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A MATRIX HANDBOOK FOR STATISTICIANS

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This book has had a long gestation period; I began writing notes for it in 1984 as a partial distraction when my first wife was fighting a terminal illness. Although I continued to collect material on and off over the years, I turned my attention to writing in other fields instead. However, in my recent “retirement”, I finally decided to bring the book to birth as I believe even more strongly now of the need for such a book. Vectors and matrices are used extensively throughout statistics, as evidenced by appendices in many books (including some of my own), in published research papers, and in the extensive bibliography of Puntanen et al. [1998]. In fact, C. R. Rao [1973a] devoted his first chapter to the topic in his pioneering book, which many of my generation have found to be a very useful source. In recent years, a number of helpful books relating matrices to statistics have appeared on the scene that generally assume no knowledge of matrices and build up the subject gradually. My aim was not to write such a how-to-do-it book, but simply to provide an extensive list of results that people could look up – very much like a dictionary or encyclopedia. I therefore assume that the reader already has a basic working knowledge of vectors and matrices. Although the book title suggests a statistical orientation, I hope that the book’s wide scope will make it useful to people in other disciplines as well.

In writing this book, I faced a number of challenges. The first was what to include. It was a bit like writing a dictionary. When do you stop adding material; I guess when other things in life become more important! The temptation was to begin including almost every conceivable matrix result I could find on the grounds that one day they might all be useful in statistical research! After all, the history of science tells us that mathematical theory usually precedes applications. However,
this is not practical and my selection is therefore somewhat personal and reflects my
own general knowledge, or lack of it! Also, my selection is tempered by my ability
to access certain books and journals, so overall there is a fair dose of randomness in
the selection process. To help me keep my feet on the ground and keep my focus on
statistics, I have listed, where possible, some references to statistical applications
of the theory. Clearly, readers will spot some gaps and I apologize in advance for
leaving out any of your favorite results or topics. Please let me know about them
(e-mail: seber@stat.auckland.ac.nz). A helpful source of matrix definitions is the

My second challenge was what to do about proofs. When I first started this
project, I began deriving and collecting proofs but soon realized that the proofs
would make the book too big, given that I wanted the book to be reasonably com-
prehensive. I therefore decided to give only references to proofs at the end of each
section or subsection. Most of the time I have been able to refer to book sources,
with the occasional journal article referenced, and I have tried to give more than
one reference for a result when I could. Although there are many excellent matrix
books that I could have used for proofs, I often found in consulting a book that a
particular result that I wanted was missing or perhaps assigned to the exercises,
which often didn’t have outline solutions. To avoid casting my net too widely, I
have therefore tended to quote from books that are more encyclopedic in nature.
Occasionally, there are lesser known results that are simply quoted without proof in
the source that I have used, and I then use the words “Quoted by ...”; the reader will
need to consult that source for further references to proofs. Some of my references
are to exercises, and I have endeavored to choose sources that have at least outline
solutions (e.g., Rao and Bhimasankaram [2000] and Seber [1984]) or perhaps some
hints (e.g., Horn and Johnson [1985, 1991]); several books have solutions manuals
(e.g., Harville [2001] and Meyer [2000b]). Sometimes I haven’t been able to locate
the proof of a fairly of straightforward result, and I have found it quicker to give
an outline proof that I hope is sufficient for the reader.

In relation to proofs, there is one other matter I needed to deal with. Initially,
I wanted to give the original references to important results, but found this too
difficult for several reasons. Firstly, there is the sheer volume of results, combined
with my limited access to older documents. Secondly, there is often controversy
about the original authors. However, I have included some names of original au-
thors where they seem to be well established. We also need to bear in mind Stigler’s
maxim, simply stated, that “no scientific discovery is named after its original dis-
coverer.” (Stigler [1999: 277]). It should be noted that there are also statistical
proofs of some matrix results (cf. Rao [2000]).

The third challenge I faced was choosing the order of the topics. Because this
book is not meant to be a teach-yourself matrix book, I did not have to follow a
“logical” order determined by the proofs. Instead, I was able to collect like results
together for an easier look-up. In fact, many topics overlap, so that a logical order
is not completely possible. A disadvantage of such an approach is that concepts are
sometimes mentioned before they are defined. I don’t believe this will cause any
difficulties because the cross-referencing and the index will, hopefully, be sufficiently
detailed for definitions to be readily located.

My fourth challenge was deciding what level of generality I should use. Some
authors use a general field for elements of matrices, while others work in a framework
of complex matrices, because most results for real matrices follow as a special case.
Most books with the word "statistics" in the title deal with real matrices only. Although the complex approach would seem the most logical, I am aware that I am writing mainly for the research statistician, many of whom are not involved with complex matrices. I have therefore used a mixed approach with the choice depending on the topic and the proofs available in the literature. Sometimes I append the words "real case" or "complex case" to a reference to inform the reader about the nature of the proof referenced. Frequently, proofs relating to real matrices can be readily extended with little change to those for the complex case.

In a book of this size, it has not been possible to check the correctness of all the results quoted. However, where a result appears in more than one reference, one would have confidence in its accuracy. My aim has been to try and faithfully reproduce the results. As we know with data, there is always a percentage that is either wrong or incorrectly transcribed. This book won't be any different. If you do find a typo, I would be grateful if you could e-mail me so that I can compile a list of errata for distribution.

With regard to contents, after some notation in Chapter 1, Chapter 2 focuses on vector spaces and their properties, especially on orthogonal complements and column spaces of matrices. Inner products, orthogonal projections, metrics, and convexity then take up most of the balance of the chapter. Results relating to the rank of a matrix take up all of Chapter 3, while Chapter 4 deals with important matrix functions such as inverse, transpose, trace, determinant, and norm. As complex matrices are sometimes left out of books, I have devoted Chapter 5 to some properties of complex matrices and then considered Hermitian matrices and some of their close relatives.

Chapter 6 is devoted to eigenvalues and eigenvectors, singular values, and (briefly) antieigenvalues. Because of the increasing usefulness of generalized inverses, Chapter 7 deals with various types of generalized inverses and their properties. Chapter 8 is a bit of a potpourri: it is a collection of various kinds of special matrices, except for those specifically highlighted in later chapters such as non-negative matrices in Chapter 9 and positive and non-negative definite matrices in Chapter 10. Some special products and operators are considered in Chapter 11, including (a) the Kronecker, Hadamard, and Rao–Khatri products and (b) operators such as the vec, vech, and vec-permutation (commutation) operators. One could fill several books with inequalities so that in Chapter 12 I have included just a selection of results that might have some connection with statistics. The solution of linear equations is the topic of Chapter 13, while Chapters 14 and 15 deal with partitioned matrices and matrices with a pattern.

A wide variety of factorizations and decompositions of matrices are given in Chapter 16, and in Chapter 17 and 18 we have the related topics of differentiation and Jacobians. Following limits and sequences of matrices in Chapter 19, the next three chapters involve random variables - random vectors (Chapter 20), random matrices (Chapter 21), and probability inequalities (Chapter 22). A less familiar topic, namely majorization, is considered in Chapter 23, followed by aspects of optimization in the last chapter, Chapter 24.

I want to express my thanks to a number of people who have provided me with preprints, reprints, reference material and answered my queries. These include Harold Henderson, Nye John, Simo Puntanen, Jim Schott, George Styan, Gary Tee, Goëtz Trenkler, and Yongge Tian. I am sorry if I have forgotten anyone because of the length of time since I began this project. My thanks also go to
several anonymous referees who provided helpful input on an earlier draft of the book, and to the Wiley team for their encouragement and support. Finally, special thanks go to my wife Jean for her patient support throughout this project.

GEORGE A. F. SEBER

Auckland, New Zealand
September 2007
1.1 GENERAL DEFINITIONS

Vectors and matrices are denoted by boldface letters $a$ and $A$, respectively, and scalars are denoted by italics. Thus $a = (a_i)$ is a vector with $i$th element $a_i$ and $A = (a_{ij})$ is a matrix with $i,j$th elements $a_{ij}$. I maintain this notation even with random variables, because using uppercase for random variables and lowercase for their values can cause confusion with vectors and matrices. In Chapters 20 and 21, which focus on random variables, we endeavor to help the reader by using the latter half of the alphabet $u, v, \ldots, z$ for random variables and the rest of the alphabet for constants.

Let $A$ be an $n_1 \times n_2$ matrix. Then any $m_1 \times m_2$ matrix $B$ formed by deleting any $n_1 - m_1$ rows and $n_2 - m_2$ columns of $A$ is called a submatrix of $A$. It can also be regarded as the intersection of $m_1$ rows and $m_2$ columns of $A$. I shall define $A$ to be a submatrix of itself, and when this is not the case I refer to a submatrix that is not $A$ as a proper submatrix of $A$. When $m_1 = m_2 = m$, the square matrix $B$ is called a principal submatrix and it is said to be of order $m$. Its determinant, $\det(B)$, is called an $m$th-order minor of $A$. When $B$ consists of the intersection of the same numbered rows and columns (e.g., the first, second, and fourth), the minor is called a principal minor. If $B$ consists of the intersection of the first $m$ rows and the first $m$ columns of $A$, then it is called a leading principal submatrix and its determinant is called a leading principal $m$-th order minor.
Many matrix results hold when the elements of the matrices belong to a general field $\mathcal{F}$ of scalars. For most practitioners, this means that the elements can be real or complex, so we shall use $\mathcal{F}$ to denote either the real numbers $\mathbb{R}$ or the complex numbers $\mathbb{C}$. The expression $\mathcal{F}^n$ will denote the $n$-dimensional counterpart.

If $A$ is complex, it can be expressed in the form $A = B + iC$, where $B$ and $C$ are real matrices, and its complex conjugate is $\overline{A} = B - iC$. We call $A' = (a_{ji})$ the transpose of $A$ and define the conjugate transpose of $A$ to be $A^* = \overline{A}'$. In practice, we can often transfer results from real to complex matrices, and vice versa, by simply interchanging $'$ and $^*$.

When adding or multiplying matrices together, we will assume that the sizes of the matrices are such that these operations can be carried out. We make this assumption by saying that the matrices are conformable. If there is any ambiguity we shall denote an $m \times n$ matrix $A$ by $A_{m \times n}$. A matrix partitioned into blocks is called a block matrix.

If $x$ and $y$ are random variables, then the symbols $E(y)$, $\text{var}(y)$, $\text{cov}(x, y)$, and $E(z | y)$ represent expectation, variance, covariance, and conditional expectation, respectively.

Before we give a list of all the symbols used we mention some univariate statistical distributions.

### 1.2 SOME CONTINUOUS UNIVARIATE DISTRIBUTIONS

We assume that the reader is familiar with the normal, chi-square, $t$, $F$, gamma, and beta univariate distributions. Multivariate vector versions of the normal and $t$ distributions are given in Sections 20.5.1 and 20.8.1, respectively, and matrix versions of the gamma and beta are found in Section 21.9. As some noncentral distributions are referred to in the statistical chapters, we define two univariate distributions below.

1.1. (Noncentral Chi-square Distribution) The random variable $x$ with probability density function

$$f(x) = \frac{1}{2^{\nu/2}} e^{-x^2/2} x^{(\nu/2)-1} \sum_{i=1}^{\infty} e^{-\delta/2} \left( \frac{\delta}{4} \right)^i \frac{1}{i!} \Gamma\left(\frac{1}{2} \nu + i\right) x^i$$

is called the noncentral chi-square distribution with $\nu$ degrees of freedom and non-centrality parameter $\delta$, and we write $x \sim \chi^2_{\nu}(\delta)$.

(a) When $\delta = 0$, the above density reduces to the (central) chi-square distribution, which is denoted by $\chi^2_{\nu}$.

(b) The noncentral chi-square can be defined as the distribution of the sum of the squares of independent univariate normal variables $y_i$ ($i = 1, 2, \ldots, n$) with variances 1 and respective means $\mu_i$. Thus if $y \sim N_d(\mu, I_d)$, the multivariate normal distribution, then $x = y'y \sim \chi^2_d(\delta)$, where $\delta = \mu'y\mu$ (Anderson [2003: 81–82]).

(c) $E(x) = \nu + \delta$.

Since $\delta > 0$, some authors set $\delta = \tau^2$, say. Others use $\delta/2$, which, because of (c), is not so memorable.
1.2. (Noncentral F-Distribution) If $x \sim \chi^2_m(\delta)$, $y \sim \chi^2_n$, and $x$ and $y$ are statistically independent, then $F = (x/m)/(y/n)$ is said to have a noncentral F-distribution with $m$ and $n$ degrees of freedom, and noncentrality parameter $\delta$. We write $F \sim F_{m,n}(\delta)$. For a derivation of this distribution see Anderson [2003: 185]. When $\delta = 0$, we use the usual notation $F_{m,n}$ for the F-distribution.

1.3 GLOSSARY OF NOTATION

Scalars

- $\mathcal{F}$: field of scalars
- $\mathbb{R}$: real numbers
- $\mathbb{C}$: complex numbers
- $F := \mathbb{R}$ or $\mathbb{C}$
- $z = x + iy$: a complex number
- $\bar{z} = x - iy$: complex conjugate of $z$
- $|z| = (x^2 + y^2)^{1/2}$: modulus of $z$

Vector Spaces

- $\mathbb{R}^n$: $n$-dimensional coordinate space
- $\mathbb{R}^n$: $\mathbb{F}^n$ with $\mathbb{F} = \mathbb{R}$
- $\mathbb{C}^n$: $\mathbb{F}^n$ with $\mathbb{F} = \mathbb{C}$
- $C(A)$: column space of $A$, the space spanned by the columns of $A$
- $C(A^\top)$: row space of $A$
- $N(A)$: $\{x : Ax = 0\}$, null space (kernel) of $A$
- $S(A)$: span of the set $A$, the vector space of all linear combinations of vectors in $A$
- $\dim \mathcal{V}$: dimension of the vector space $\mathcal{V}$
- $\mathcal{V}^\perp$: the orthogonal complement of $\mathcal{V}$
- $x \in \mathcal{V}$: $x$ is an element of $\mathcal{V}$
- $\mathcal{V} \subseteq \mathcal{W}$: $\mathcal{V}$ is a subset of $\mathcal{W}$
- $\mathcal{V} \subset \mathcal{W}$: $\mathcal{V}$ is a proper subset of $\mathcal{W}$ (i.e., $\mathcal{V} \neq \mathcal{W}$)
- $\mathcal{V} \cap \mathcal{W}$: intersection, $\{x : x \in \mathcal{V} \text{ and } x \in \mathcal{W}\}$
- $\mathcal{V} \cup \mathcal{W}$: union, $\{x : x \in \mathcal{V} \text{ and/or } x \in \mathcal{W}\}$
- $\mathcal{V} + \mathcal{W}$: sum, $\{x + y : x \in \mathcal{V}, y \in \mathcal{W}\}$
- $\mathcal{V} \oplus \mathcal{W}$: direct sum, $\{x + y : x \in \mathcal{V}, y \in \mathcal{W}; \mathcal{V} \cap \mathcal{W} = 0\}$
- $\langle , \rangle$: an inner product defined on a vector space
- $x \perp y$: $x$ is perpendicular to $y$ (i.e., $\langle x, y \rangle = 0$)
Complex Matrix

\[ A = B + iC \]  
complex matrix, with \( B \) and \( C \) real

\[ \overline{A} = (\overline{a_{ij}}) = B - iC \]  
complex conjugate of \( A \)

\[ A^* = \overline{A}' = (\overline{a_{ji}}) \]  
conjugate transpose of \( A \)

\[ A = A^* \]  
\( A \) is a Hermitian matrix

\[ A = -A^* \]  
\( A \) is a skew-Hermitian matrix

\[ AA^* = A^*A \]  
\( A \) is a normal matrix

Special Symbols

\[ \sup \]  
supremum

\[ \inf \]  
infernum

\[ \max \]  
maximum

\[ \min \]  
minimum

\[ \to \]  
tends to

\[ \Rightarrow \]  
implies

\[ \propto \]  
proportional to

\[ 1_n \]  
the \( n \times 1 \) vector with unit elements

\[ I_n \]  
the \( n \times n \) identity matrix

\[ 0 \]  
a vector or matrix of zeros

\[ \text{diag}(d) \]  
\( n \times n \) matrix with diagonal elements \( d' = (d_1, \ldots, d_n) \), and zeros elsewhere

\[ \text{diag}(d_1, d_2, \ldots, d_n) \]  
same as above

\[ \text{diag} A \]  
diagonal matrix; same diagonal elements as \( A \)

\[ A \geq 0 \]  
the elements of \( A \) are all non-negative

\[ A > 0 \]  
the elements of \( A \) are all positive

\[ A \succeq 0, \text{n.n.d} \]  
\( A \) is non-negative definite \((x'Ax \geq 0)\)

\[ A \succeq B, B \preceq A \]  
\( A - B \succeq 0 \)

\[ A \succ 0, \text{p.d.} \]  
\( A \) is positive definite \((x'Ax > 0 \text{ for } x \neq 0)\)

\[ A \succ B, B \prec A \]  
\( A - B > 0 \)

\[ x \ll y \]  
\( x \) is (strongly) majorized by \( y \)

\[ x \ll_w y \]  
\( x \) is weakly submajorized by \( y \)

\[ x \ll^w y \]  
\( x \) is weakly supermajorized by \( y \)

\[ A' = (a_{ji}) \]  
the transpose of \( A \)

\[ A^{-1} \]  
inverse of \( A \) when \( A \) is nonsingular

\[ A^- \]  
weak inverse of \( A \) satisfying \( AA^-A = A \)

\[ A^+ \]  
Moore-Penrose inverse of \( A \)

\[ \text{trace} A \]  
sum of the diagonal elements of a square matrix \( A \)

\[ \text{det} A \]  
determinant of a square matrix \( A \)

\[ \text{rank} A \]  
rank of \( A \)

\[ \text{per} A \]  
permanent of a square matrix \( A \)

\[ \text{mod}(A) \]  
modulus of \( A = (a_{ij}) \), given by \(|a_{ij}|\)

\[ \text{Pf}(A) \]  
pfaffian of \( A \)

\[ \rho(A) \]  
spectral radius of a square matrix \( A \)

\[ \kappa_v(A) \]  
condition number of an \( m \times n \) matrix, \( v = 1, 2, \infty \)
\langle x, y \rangle \quad \text{inner product of } x \text{ and } y

\| x \| \quad \text{a norm of vector } x \quad (= \langle x, x \rangle^{1/2})

\| x \|_2 \quad \text{length of } x \quad (= (x^*x)^{1/2})

\| x \|_p \quad L_p \text{ vector norm of } x \quad (= \sum_{i=1}^n |x_i|^p)^{1/p})

\| x \|_{\infty} \quad L_\infty \text{ vector norm of } x \quad (= \max_i |x_i|)

\| A \|_p \quad \text{a generalized matrix norm of } m \times n \text{ matrix } A

\quad (= \sum_{i=1}^m \sum_{j=1}^n |a_{ij}|^p)^{1/p}, \quad p \geq 1)

\| A \|_F \quad \text{Frobenius norm of matrix } A \quad (= (\sum_i \sum_j |a_{ij}|^2)^{1/2})

\| A \|_{\nu, \text{in}} \quad \text{generalized matrix norm for } m \times n \text{ matrix } A \text{ induced by a vector norm } \| \cdot \|_\nu

\| A \|_{\nu, \text{in}} \quad \text{unitarily invariant norm of } m \times n \text{ matrix } A

\| A \|_{\nu, \text{in}} \quad \text{orthogonally invariant norm of } m \times n \text{ matrix } A

\| A \| \quad \text{matrix norm of square matrix } A

\| A \| \quad \text{matrix norm for a square matrix } A \text{ induced by a vector norm } \| \cdot \|_\nu

A_{m \times n} \quad m \times n \text{ matrix}

(A, B) \quad \text{matrix partitioned by two matrices } A \text{ and } B

(a_1, \ldots, a_n) \quad \text{matrix partitioned by column vectors } a_1, \ldots, a_n

A \otimes B \quad \text{Kronecker product of } A \text{ and } B

A \circ B \quad \text{Hadamard (Schur) product of } A \text{ and } B

A \odot B \quad \text{Rao–Khatri product of } A \text{ and } B

\text{vec } A_{m \times n} \quad m n \times 1 \text{ vector formed by writing the columns of } A \text{ one below the other}

\text{vec } A_{m \times m} \quad \frac{1}{2} m(m + 1) \times 1 \text{ vector formed by writing the columns of the lower triangle of } A \text{ (including the diagonal elements) one below the other}

I_{(m, n)} \text{ or } K_{nm} \quad \text{vec-permutation (commutation) matrix}

G_n \text{ or } D_n \quad \text{duplication matrix}

P_n \text{ or } N_n \quad \text{symmetrizer matrix}

\lambda (A) \quad \text{eigenvalue of a square matrix } A

\sigma (B) \quad \text{singular value of any matrix } B
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VECTORS, VECTOR SPACES, AND CONVEXITY

Vector spaces and subspaces play an important role in statistics, the key ones being orthogonal complements as well as the column and row spaces of matrices. Projections onto vector subspaces occur in topics like least squares, where orthogonality is defined in terms of an inner product. Convex sets and functions arise in the development of inequalities and optimization. Other topics such as metric spaces and coordinate geometry are also included in this chapter. A helpful reference for vector spaces and their properties is Kollo and von Rosen [2005: section 1.2].

2.1 VECTOR SPACES

2.1.1 Definitions

**Definition 2.1.** If $S$ and $T$ are subsets of some space $V$, then $S \cap T$ is called the intersection of $S$ and $T$ and is the set of all vectors in $V$ common to both $S$ and $T$. The sum of $S$ and $T$, written $S + T$, is the set of all vectors in $V$ that are a sum of a vector in $S$ and a vector in $T$. Thus

$$W = S + T = \{w : w = s + t, s \in S \text{ and } t \in T\}.$$  

(In most applications $S$ and $T$ are vector subspaces, defined below.)

**Definition 2.2.** A vector space $U$ over a field $F$ is a set of elements $\{u\}$ called vectors and a set $F$ of elements called scalars with four binary operations ($+\,, \cdot\,, \ast$, and $\circ$) that satisfy the following axioms.
(1) $\mathcal{F}$ is a field with regard to the operations $+$ and $\cdot$.

(2) For all $u$ and $v$ in $\mathcal{U}$ we have the following:

(i) $u \ast v \in \mathcal{U}$.

(ii) $u \ast v = v \ast u$.

(iii) $(u \ast v) \ast w = u \ast (v \ast w)$ for all $w \in \mathcal{U}$.

(iv) There is a vector $0 \in \mathcal{U}$, called the zero vector, such that $u \ast 0 = u$ for all $u \in \mathcal{U}$.

(v) For each $u \in \mathcal{U}$ there exists a vector $-u \in \mathcal{U}$ such that $u \ast (-u) = 0$.

(3) For all $\alpha$ and $\beta$ in $\mathcal{F}$ and all $u$ and $v$ in $\mathcal{U}$ we have:

(i) $\alpha \circ u \in V$.

(ii) There exists an element in $\mathcal{F}$ called the unit element such that $1 \circ u = u$.

(iii) $(\alpha + \beta) \circ u = (\alpha \circ u) \ast (\beta \circ u)$.

(iv) $\alpha \circ (u \ast v) = (\alpha \circ u) \ast (\alpha \circ v)$.

(v) $(\alpha \cdot \beta) \circ u = \alpha \circ (\beta \circ u)$.

We note from (2) that $\mathcal{U}$ is an abelian group under "$\ast$". Also, we can replace "$\ast$" by "$+$" and remove "$.$" and "$\circ$" without any ambiguity. Thus (iv) and (v) of (3) above can be written as $\alpha(u + v) = \alpha u + \alpha v$ and $(\alpha \beta)u = \alpha(\beta u)$, which we shall do in what follows.

Normally $\mathcal{F} = \mathbb{F}$, where $\mathbb{F}$ denotes either $\mathbb{R}$ or $\mathbb{C}$. However, one field that has been useful in the construction of experimental designs such as orthogonal Latin squares, for example, is a finite field consisting of a finite number of elements. A finite field is known as a Galois field. The number of elements in any Galois field is $p^m$, where $p$ is a prime number and $m$ is a positive integer. For a brief discussion see Rao and Rao [1998: 6–10].

If $\mathcal{F}$ is a finite field, then a vector space $\mathcal{U}$ over $\mathcal{F}$ can be used to obtain a finite projective geometry with a finite set of elements or "points" $S$ and a collection of subsets of $S$ or "lines." By identifying a block with a "line" and a treatment with a "point," one can use the projective geometry to construct balanced incomplete block designs—as, for example, described by Rao and Rao [1998: 48–49].

For general, less abstract, references on this topic see Friedberg et al. [2003], Lay [2003], and Rao and Bhimasankaram [2000].

**Definition 2.3.** A subset $V$ of a vector space $\mathcal{U}$ that is also a vector space is called a subspace of $\mathcal{U}$.

**2.1.** $V$ is a vector subspace if and only if $\alpha u + \beta v \in V$ for all $u$ and $v$ in $V$ and all $\alpha$ and $\beta$ in $\mathcal{F}$. Setting $\alpha = \beta = 0$, we see that $0$, the zero vector in $\mathcal{U}$, must belong to every vector subspace.

**2.2.** The set $V$ of all $m \times n$ matrices over $\mathcal{F}$, along with the usual operations of addition and scalar multiplication, is a vector space. If $m = n$, the subset $\mathcal{A}$ of all symmetric matrices is a vector subspace of $V$.

**Proofs.** Section 2.1.1.


2.2. Harville [1997: chapters 3 and 4].
2.1.2 Quadratic Subspaces

Quadratic subspaces arise in certain inferential problems such as the estimation of variance components (Rao and Rao [1998: chapter 13]). They also arise in testing multivariate linear hypotheses when the variance–covariance matrix has a certain structure or pattern (Rogers and Young [1978: 204] and Seeley [1971]). Klein [2004] considers their use in the design of mixture experiments.

**Definition 2.4.** Suppose \( B \) is a subspace of \( A \), where \( A \) is the set of all \( n \times n \) real symmetric matrices. If \( B \in B \) implies that \( B^2 \in B \), then \( B \) is called a *quadratic subspace* of \( A \).

2.3. If \( A_1 \) and \( A_2 \) are real symmetric idempotent matrices (i.e., \( A_i^2 = A_i \)) with \( A_1 A_2 = 0 \), and \( A \) is the set of all real symmetric \( n \times n \) matrices, then

\[
B = \{ \alpha_1 A_1 + \alpha_2 A_2 : \alpha_1 \text{ and } \alpha_2 \text{ real} \},
\]

is a quadratic subspace of \( A \).

2.4. If \( B \) is a quadratic subspace of \( A \), then the following hold.

(a) If \( A \in B \), then the Moore–Penrose inverse \( A^+ \in B \).

(b) If \( A \in B \), then \( AA^+ \in B \).

(c) There exists a basis of \( B \) consisting of idempotent matrices.

2.5. The following statements are equivalent.

(1) \( B \) is a quadratic subspace of \( A \).

(2) If \( A, B \in B \), then \( (A + B)^2 \in B \).

(3) If \( A, B \in B \), then \( AB + BA \in B \).

(4) If \( A \in B \), then \( A^k \in B \) for \( k = 1, 2, \ldots \).

2.6. Let \( B \) be a quadratic subspace of \( A \). Then:

(a) If \( A, B \in B \), then \( ABA \in B \).

(b) Let \( A \in B \) be fixed and let \( C = \{ ABA : B \in B \} \). Then \( C \) is a quadratic subspace of \( B \).

(c) If \( A, B, C \in B \), then \( ABC + CBA \in B \).

**Proofs.** Section 2.1.2.

2.3. This follows from the definition and noting that \( A_2 A_1 = 0 \).

2.1.3 Sums and Intersections of Subspaces

**Definition 2.5.** Let $V$ and $W$ be vector subspaces of a vector space $U$. As with sets, we define $V + W$ to be the sum of the two vector subspaces. If $V \cap W = \emptyset$ (some authors use $\{0\}$), we say that $V$ and $W$ are disjoint vector subspaces (Harville [1997] uses the term "essentially disjoint"). Note that this differs from the notion of disjoint sets, namely $V \cap W = 0$, which we will not need. When $V$ and $W$ are disjoint, we refer to the sum as a direct sum and write $V \oplus W$. Also $V \cap W$ is called the intersection of $V$ and $W$.

The ordered pair $(\cap, \subseteq)$ forms a lattice of subspaces so that lattice theory can be used to determine properties relating to the sum and intersection of subspaces. Kollo and von Rosen [2006: section 1.2] give detailed lists of such properties, and some of these are given below.

2.7. Let $A$, $B$, and $C$ be vector subspaces of $U$.

(a) $A \cap B$ and $A + B$ are vector subspaces. However, $A \cup B$ need not be a vector space. Here $A \cap B$ is the smallest subspace containing $A$ and $B$, and $A + B$ is the largest. Also $A + B$ is the smallest subspace containing $A \cup B$. By smallest subspace we mean one with the smallest dimension.

(b) If $U = A \oplus B$, then every $u \in U$ can be expressed uniquely in the form $u = a + b$, where $a \in A$ and $b \in B$.

(c) $A \cap (A + B) = A + (A \cap B) = A$.

(d) (Distributive)

(i) $A \cap (B + C) \supseteq (A \cap B) + (A \cap C)$.

(ii) $A + (B \cap C) \subseteq (A + B) \cap (A + C)$.

(e) In the following results we can interchange $+$ and $\cap$.

(i) $[A \cap (B + C)] + B = [(A + B) \cap C] + B$.

(ii) $A \cap [B + (A \cap C)] = (A \cap B) + (A \cap C)$.

(iii) $A \cap (B + C) = A \cap [B \cap (A + C)] + C$.

(iv) $(A \cap B) + (A \cap C) + (B \cap C) = [A + (B \cap C)] \cap [B + (A \cap C)]$.

(v) $A \cap B = [(A \cap B) + (A \cap C)] \cap [(A \cap B) + (B \cap C)]$.

**Proofs.** Section 2.1.3.

2.7a. Schott [2005: 68].

2.7b. Assume $u = a_1 + b_1$ so that $a - a_1 = -(b - b_1)$, with the two vectors being in disjoint subspaces; hence $a = a_1$ and $b = b_1$.

2.7c-e. Kollo and von Rosen [2006: section 1.2].

2.7d. Harville [2001: 163, exercise 4].
2.1.4 Span and Basis

**Definition 2.6.** We can always construct a vector space $\mathcal{U}$ from $\mathcal{F}$, called an $n$-tuple space, by defining $\mathbf{u} = (u_1, u_2, \ldots, u_n)'$, where each $u_i \in \mathcal{F}$.

In practice, $\mathcal{F}$ is usually $\mathbb{F}$ and $\mathcal{U}$ is $\mathbb{F}^n$. This will generally be the case in this book, unless indicated otherwise. However, one useful exception is the vector space consisting of all $m \times n$ matrices with elements in $\mathcal{F}$.

**Definition 2.7.** Given a subset $A$ of a vector space $\mathcal{V}$, we define the span of $A$, denoted by $S(A)$, to be the set of all vectors obtained by taking all linear combinations of vectors in $A$. We say that $A$ is a generating set of $S(A)$.

2.8. Let $A$ and $B$ be subsets of a vector space. Then:

(a) $S(A)$ is a vector space (even though $A$ may not be).

(b) $A \subseteq S(A)$. Also $S(A)$ is the smallest subspace of $\mathcal{V}$ containing $A$ in the sense that every subspace of $\mathcal{V}$ containing $A$ also contains $S(A)$.

(c) $A$ is a vector space if and only if $A = S(A)$.

(d) $S[S(A)] = S(A)$.

(e) If $A \subseteq B$, then $S(A) \subseteq S(B)$.

(f) $S(A) \cup S(B) \subseteq S(A \cup B)$.

(g) $S(A \cap B) \subseteq S(A) \cap S(B)$.

**Definition 2.8.** A set of vectors $v_i$ ($i = 1, 2, \ldots, r$) in a vector space are linearly independent if $\sum_{i=1}^{r} a_i v_i = \mathbf{0}$ implies that $a_1 = a_2 = \cdots = a_r = 0$. A set of vectors that are not linearly independent are said to be linearly dependent. For further properties of linearly independent sets see Rao and Bhimasankaram [2000: chapter 1].

The term “vector” here and in the following definitions is quite general and simply refers to an element of a vector space. For example, it could be an $m \times n$ matrix in the vector space of all such matrices; Harville [1997: chapters 3 and 4] takes this approach.

**Definition 2.9.** A set of vectors $v_i$ ($i = 1, 2, \ldots, r$) span a vector space $\mathcal{V}$ if the elements of $\mathcal{V}$ consist of all linear combinations of the vectors (i.e., if $\mathbf{v} \in \mathcal{V}$, then $\mathbf{v} = a_1 v_1 + \cdots + a_r v_r$). The set of vectors is called a generating set of $\mathcal{V}$. If the vectors are also linearly independent, then the $v_i$ form a basis for $\mathcal{V}$.

2.9. Every vector space has a basis. (This follows from Zorn’s lemma, which can be used to prove the existence of a maximal linearly independent set of vectors, i.e., a basis.)

**Definition 2.10.** All bases contain the same number of vectors so that this number is defined to be the dimension of $\mathcal{V}$.

2.10. Let $\mathcal{V}$ be a subspace of $\mathcal{U}$. Then:

(a) Every linearly independent set of vectors in $\mathcal{V}$ can be extended to a basis of $\mathcal{U}$.
(b) Every generating set of \( V \) contains a basis of \( V \).

2.11. If \( V \) and \( W \) are vector subspaces of \( U \), then:

(a) If \( V \subseteq W \) and \( \dim V = \dim W \), then \( V = W \).

(b) If \( V \subseteq W \) and \( W \subseteq V \), then \( V = W \). This is the usual method for proving the equality of two vector subspaces.

(c) \( \dim(V + W) = \dim(V) + \dim(W) - \dim(V \cap W) \).

2.12. If the columns of \( A = (a_1, \ldots, a_r) \) and the columns of \( B = (b_1, \ldots, b_r) \) both form a basis for a vector subspace of \( \mathbb{F}^n \), then \( A = BR \), where \( R = (r_{ij}) \) is \( r \times r \) and nonsingular.

**Proofs.** Section 2.1.4.


2.9. Halmos [1958].


2.11a–b. Proofs are straightforward.


2.12. Firstly, \( a_j = \sum_i b_ir_{ij} \) so that \( A = BR \). Now assume \( \text{rank} R < r \); then \( \text{rank} A \leq \min\{ \text{rank} B, \text{rank} R \} < r \) by (3.12), which is a contradiction.

2.1.5 **Isomorphism**

**Definition 2.11.** Let \( V_1 \) and \( V_2 \) be two vector spaces over the same field \( \mathcal{F} \). Then a map (function) \( \phi \) from \( V_1 \) to \( V_2 \) is said to be an **isomorphism** if the following hold.

1. \( \phi \) is a bijection (i.e., \( \phi \) is one-to-one and onto).
2. \( \phi(u + v) = \phi(u) + \phi(v) \) for all \( u, v \in V_1 \).
3. \( \phi(\alpha u) = \alpha \phi(u) \) for all \( \alpha \in \mathcal{F} \) and \( u \in V_1 \).

\( V_1 \) is said to be **isomorphic** to \( V_2 \) if there is an isomorphism from \( V_1 \) to \( V_2 \).

2.13. Two vector spaces over a field \( \mathcal{F} \) are isomorphic if and only if they have the same dimension.

**Proofs.** Section 2.1.5.

2.2 INNER PRODUCTS

2.2.1 Definition and Properties

The concept of an inner product is an important one in statistics as it leads to ideas of length, angle, and distance between two points.

**Definition 2.12.** Let \( V \) be a vector space over \( \mathbb{F} \) (i.e., \( \mathbb{R} \) or \( \mathbb{C} \)), and let \( x, y, \) and \( z \) be any vectors in \( V \). An inner product \( \langle \cdot, \cdot \rangle \) defined on \( V \) is a function \( \langle x, y \rangle \) of two vectors \( x, y \in V \) satisfying the following conditions:

1. \( \langle x, y \rangle = \overline{\langle y, x \rangle} \), the complex conjugate of \( \langle y, x \rangle \).
2. \( \langle x, x \rangle \geq 0 \); \( \langle x, x \rangle = 0 \) implies that \( x = 0 \).
3. \( \langle \alpha x, y \rangle = \alpha \langle x, y \rangle \), where \( \alpha \) is a scalar in \( \mathbb{F} \).
4. \( \langle x + y, z \rangle = \langle x, z \rangle + \langle y, z \rangle \).

When \( V \) is over \( \mathbb{R} \), (1) becomes \( \langle x, y \rangle = \langle y, x \rangle \), a symmetry condition. Inner products can also be defined on infinite-dimensional spaces such as a Hilbert space. A vector space together with an inner product is called an inner product space. A complex inner product space is also called a unitary space, and a real inner product space is called a Euclidean space.

The norm or length of \( x \), denoted by \( ||x|| \), is defined to be the positive square root of \( \langle x, x \rangle \). We say that \( x \) has unit length if \( ||x|| = 1 \). More general norms, which are not associated with an inner product, are discussed in Section 4.6.

We can define the angle \( \theta \) between \( x \) and \( y \) by

\[
\cos \theta = \frac{\langle x, y \rangle}{||x|| ||y||}.
\]

The distance between \( x \) and \( y \) is defined to be \( d(x, y) = ||x - y|| \) and has the properties of a metric (Section 2.4). Usually, \( V = \mathbb{R}^n \) and \( \langle x, y \rangle = x'y \) in defining angle and distance.

Suppose (2) above is replaced by the weaker condition

\( (2') \langle x, x \rangle \geq 0 \). (It is now possible that \( \langle x, x \rangle = 0 \), but \( x \neq 0 \).)

We then have what is called a semi-inner product (quasi-inner product) and a corresponding seminorm. We write \( \langle x, y \rangle_s \) for a semi-inner product.

2.14. For any inner product the following hold:

\( \langle x, \alpha y + \beta z \rangle = \alpha \langle x, y \rangle + \beta \langle x, z \rangle \).

\( \langle x, 0 \rangle = \langle 0, x \rangle = 0 \).

\( \langle \alpha x, \beta y \rangle = \alpha \langle x, y \rangle = \alpha \beta \langle x, y \rangle \).

2.15. The following hold for any norm associated with an inner product.

\( ||x + y|| \leq ||x|| + ||y|| \) (triangle inequality).

\( ||x - y|| + ||y|| \geq ||x|| \).
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(c) \(\|x + y\|^2 + \|x - y\|^2 = 2\|x\|^2 + 2\|y\|^2\) (parallelogram law).

(d) \(\|x + y\|^2 = \|x\|^2 + \|y\|^2\) if \(\langle x, y \rangle = 0\) (Pythagoras theorem).

(e) \(\langle x, y \rangle + \langle y, x \rangle \leq 2\|x\| \cdot \|y\|\).

2.16. (Semi-Inner Product) The following hold for any semi-inner product \(\langle \cdot, \cdot \rangle_s\) on a vector space \(V\).

(a) \(\langle 0, 0 \rangle_s = 0\)

(b) \(\|x + y\|_s \leq \|x\|_s + \|y\|_s\).

(c) \(\mathcal{N} = \{x \in V : \|x\|_s = 0\}\) is a subspace of \(V\).

2.17. (Schwarz Inequality) Given an inner product space, we have for all \(x\) and \(y\)

\[\langle x, y \rangle^2 \leq \langle x, x \rangle \langle y, y \rangle,\]

or

\[|\langle x, y \rangle| \leq \|x\| \cdot \|y\|,\]

with equality if either \(x\) or \(y\) is zero or \(x = ky\) for some scalar \(k\). We can obtain various inequalities from the above by changing the inner product space (cf. Section 12.1).

2.18. Given an inner product space and unit vectors \(u, v,\) and \(w\), then

\[\sqrt{1 - |\langle u, v \rangle|^2} \leq \sqrt{1 - |\langle u, w \rangle|^2} + \sqrt{1 - |\langle w, v \rangle|^2}.\]

Equality holds if and only if \(w\) is a multiple of \(u\) or of \(v\).

2.19. Some inner products are as follows.

(a) If \(V = \mathbb{R}^n\), then common inner products are:

(1) \(\langle x, y \rangle = y^*x = \sum_{i=1}^n x_i y_i\) (= \(x'y\)). If \(x = y\), we denote the norm by \(\|x\|_2\), the so-called Euclidean norm.

The minimal angle between two vector subspaces \(V\) and \(W\) in \(\mathbb{R}^n\) is given by

\[\cos \theta_{\text{min}} = \max_{x \in V, y \in W} \frac{(x'y)^2}{\|x\|_2 \cdot \|y\|_2}.\]

For some properties see Meyer [2000a: section 5.15].

(2) \(\langle x, y \rangle = y'Ax\) (= \(x'Ay\)), where \(A\) is a positive definite matrix.

(b) If \(V = \mathbb{C}^n\), then we can use \(\langle x, y \rangle = y^*x = \sum_{i=1}^n x_i y_i\).

(c) Every inner product defined on \(\mathbb{C}^n\) can be expressed in the form \(\langle x, y \rangle = y^*Ax = \sum_i \sum_j a_{ij} x_i y_j\), where \(A = (a_{ij})\) is a Hermitian positive definite matrix. This follows by setting \(\langle e_i, e_j \rangle = a_{ij}\) for all \(i, j\), where \(e_i\) is the \(i\)th column of \(I_n\). If we have a semi-inner product, then \(A\) is Hermitian non-negative definite. (This result is proved in Drygas [1970: 29], where symmetric means Hermitian.)
2.20. Let \( \mathcal{V} \) be the set of all \( m \times n \) real matrices, and in scalar multiplication all scalars belong to \( \mathbb{R} \). Then:

(a) \( \mathcal{V} \) is vector space.

(b) If we define \( \langle A, B \rangle = \text{trace}(A'B) \), then \( \langle , \rangle \) is an inner product.

(c) The corresponding norm is \( \langle A, A \rangle^{1/2} = (\sum_{i=1}^{m} \sum_{j=1}^{n} a_{ij}^2)^{1/2} \). This is the so-called Frobenius norm \( \|A\|_F \) (cf. Definition 4.16 below (4.7)).

Proofs. Section 2.2.1.


2.15. We begin with the Schwarz inequality \( |\langle x, y \rangle| = |\langle y, x \rangle| \leq \|x\| \cdot \|y\| \) of (2.17). Then, since \( \langle x, y \rangle + \langle y, x \rangle \) is real,

\[
\langle x, y \rangle + \langle y, x \rangle \leq |\langle x, y \rangle + \langle y, x \rangle| \leq |\langle x, y \rangle| + |\langle y, x \rangle| \leq 2\|x\| \cdot \|y\|,
\]

which proves (e). We obtain (a) by writing \( \|x + y\|^2 = \langle x + y, x + y \rangle \) and using (e); the rest are straightforward. See also Rao and Rao [1998: 54].


2.17. There are a variety of proofs (e.g., Schott [2005: 36] and Ben-Israel and Greville [2003: 7]). The inequality also holds for quasi-inner (semi-inner) products (Harville [1997: 255]).


2.2.2 Functionals

Definition 2.13. A function \( f \) defined on a vector space \( \mathcal{V} \) over a field \( \mathbb{F} \) and taking values in \( \mathbb{F} \) is said to be a linear functional if

\[
f(\alpha_1 x_1 + \alpha_2 x_2) = \alpha_1 f(x_1) + \alpha_2 f(x_2)
\]

for every \( x_1, x_2 \in \mathcal{V} \) and every \( \alpha_1, \alpha_2 \in \mathbb{F} \). For a discussion of linear functionals and the related concept of a dual space see Rao and Rao [1998: section 1.7].

2.21. (Riesz) Let \( \mathcal{V} \) be an an inner product space with inner product \( \langle , \rangle \), and let \( f \) be a linear functional on \( \mathcal{V} \).

(a) There exists a unique vector \( z \in \mathcal{V} \) such that

\[
f(x) = \langle x, z \rangle \text{ for every } x \in \mathcal{V}.
\]

(b) Here \( z \) is given by \( z = \overline{f(u)} u \), where \( u \) is any vector of unit length in \( \mathcal{V}^\perp \).

Proofs. Section 2.2.2.

2.2.3 Orthogonality

**Definition 2.14.** Let \( \mathcal{U} \) be a vector space over \( F \) with an inner product \( \langle \cdot, \cdot \rangle \), so that we have an inner product space. We say that \( x \) is *perpendicular* to \( y \), and we write \( x \perp y \), if \( \langle x, y \rangle = 0 \).

2.22. A set of vectors that are mutually orthogonal—that is, are pairwise orthogonal for every pair—are linearly independent.

**Definition 2.15.** A basis whose vectors are mutually orthogonal with unit length is called an *orthonormal basis*. An orthonormal basis of an inner product space always exists and it can be constructed from any basis by the Gram–Schmidt orthogonalization process of (2.30).

2.23. Let \( \mathcal{V} \) and \( \mathcal{W} \) be vector subspaces of a vector space \( \mathcal{U} \) such that \( \mathcal{V} \subseteq \mathcal{W} \). Any orthonormal basis for \( \mathcal{V} \) can be enlarged to form an orthonormal basis for \( \mathcal{W} \).

**Definition 2.16.** Let \( \mathcal{U} \) be a vector space over \( F \) with an inner product \( \langle \cdot, \cdot \rangle \), and let \( \mathcal{V} \) be a subset or subspace of \( \mathcal{U} \). Then the *orthogonal complement* of \( \mathcal{V} \) with respect to \( \mathcal{U} \) is defined to be

\[
\mathcal{V}^\perp = \{ x : \langle x, y \rangle = 0 \text{ for all } y \in \mathcal{V} \}.
\]

If \( \mathcal{V} \) and \( \mathcal{W} \) are two vector subspaces, we say that \( \mathcal{V} \perp \mathcal{W} \) if \( \langle x, y \rangle = 0 \) for all \( x \in \mathcal{V} \) and \( y \in \mathcal{W} \).

2.24. Suppose \( \text{dim } \mathcal{U} = n \) and \( \alpha_1, \alpha_2, \ldots, \alpha_n \) is an orthonormal basis of \( \mathcal{U} \). If \( \alpha_1, \ldots, \alpha_r \) \((r < n)\) is an orthonormal basis for a vector subspace \( \mathcal{V} \) of \( \mathcal{U} \), then \( \alpha_{r+1}, \ldots, \alpha_n \) is an orthonormal basis for \( \mathcal{V}^\perp \).

2.25. If \( S \) and \( T \) are subsets or subspaces of \( \mathcal{U} \), then we have the following results:

(a) \( S^\perp \) is a vector space.

(b) \( S \subseteq (S^\perp)^\perp \) with equality if and only if \( S \) is a vector space.

(c) If \( S \) and \( T \) both contain \( 0 \), then \( (S + T)^\perp = S^\perp \cap T^\perp \).

2.26. If \( \mathcal{V} \) is a vector subspace of \( \mathcal{U} \), a vector space over \( F \), then:

(a) \( \mathcal{V}^\perp \) is a vector subspace of \( \mathcal{U} \), by (2.25a) above.

(b) \( (\mathcal{V}^\perp)^\perp = \mathcal{V} \).

(c) \( \mathcal{V} \oplus \mathcal{V}^\perp = \mathcal{U} \). In fact every \( u \in \mathcal{U} \) can be expressed uniquely in the form \( u = x + y \), where \( x \in \mathcal{V} \) and \( y \in \mathcal{V}^\perp \).

(d) \( \text{dim}(\mathcal{V}) + \text{dim}(\mathcal{V}^\perp) = \text{dim}(\mathcal{U}) \).

2.27. If \( \mathcal{V} \) and \( \mathcal{W} \) are vector subspaces of \( \mathcal{U} \), then:

(a) \( \mathcal{V} \subseteq \mathcal{W} \) if and only if \( \mathcal{V} \perp \mathcal{W}^\perp \).

(b) \( \mathcal{V} \subseteq \mathcal{W} \) if and only if \( \mathcal{W}^\perp \subseteq \mathcal{V}^\perp \).

(c) \( (\mathcal{V} \cap \mathcal{W})^\perp = \mathcal{V}^\perp + \mathcal{W}^\perp \) and \( (\mathcal{V} + \mathcal{W})^\perp = \mathcal{V}^\perp \cap \mathcal{W}^\perp \).
For more general results see Kollo and von Rosen [2005: section 1.2].

**Definition 2.17.** Let $\mathcal{V}$ and $\mathcal{W}$ be vector subspaces of $\mathcal{U}$, a vector space over $\mathbb{F}$, and suppose that $\mathcal{V} \subseteq \mathcal{W}$. Then the set of all vectors in $\mathcal{W}$ that are perpendicular to $\mathcal{V}$ form a vector space called the orthogonal complement of $\mathcal{V}$ with respect to $\mathcal{W}$, and is denoted by $\mathcal{V} \perp \cap \mathcal{W}$. Thus

$$
\mathcal{V} \perp \cap \mathcal{W} = \{ w : w \in \mathcal{W}, \langle w, v \rangle = 0 \text{ for every } v \in \mathcal{V} \}.
$$

2.28. Let $\mathcal{V} \subseteq \mathcal{W}$. Then

(a) (i) $\dim(\mathcal{V} \perp \cap \mathcal{W}) = \dim(\mathcal{W}) - \dim(\mathcal{V})$.
(ii) $\mathcal{W} = \mathcal{V} \oplus (\mathcal{V} \perp \cap \mathcal{W})$.

(b) From (a)(ii) we have $\mathcal{U} = \mathcal{W} \oplus \mathcal{V} \perp = \mathcal{V} \oplus (\mathcal{V} \perp \cap \mathcal{W}) \oplus \mathcal{V} \perp$.

The above can be regarded as an orthogonal decomposition of $\mathcal{U}$ into three orthogonal subspaces. Using this, vectors can be added to any orthonormal basis of $\mathcal{V}$ to form an orthonormal basis of $\mathcal{W}$, which can then be extended to form an orthonormal basis of $\mathcal{U}$.

2.29. Let $\mathcal{A}$, $\mathcal{B}$, and $\mathcal{C}$ be vector subspaces of $\mathcal{U}$. If $\mathcal{B} \perp \mathcal{C}$ and $\mathcal{A} \perp \mathcal{C}$, then $\mathcal{A} \cap (\mathcal{B} \oplus \mathcal{C}) = \mathcal{A} \cap \mathcal{B}$.

2.30. (Classical Gram–Schmidt Algorithm) Given a basis $x_1, x_2, \ldots, x_n$ of an inner product space, there exists an orthonormal basis $q_1, q_2, \ldots, q_n$ given by $q_1 = x_1/\|x_1\|$, $q_j = w_j/\|w_j\|$ $(j = 2, \ldots, n)$, where

$$
w_j = x_j - \langle x_j, q_1 \rangle q_1 - \langle x_j, q_2 \rangle q_2 - \cdots - \langle x_j, q_{j-1} \rangle q_{j-1}.
$$

This expression gives the algorithm for computing the basis. If we require an orthogonal basis only without the square roots involved with the normalizing, we can use $w_1 = x_1$ and, for $j = 2, 3, \ldots, n$,

$$
w_j = x_j - \frac{\langle x_j, w_1 \rangle w_1}{\langle w_1, w_1 \rangle} - \cdots - \frac{\langle x_j, w_{j-1} \rangle w_{j-1}}{\langle w_{j-1}, w_{j-1} \rangle}.
$$

Also the vectors can be replaced by matrices using a suitable inner product such as $\langle A, B \rangle = \text{trace}(A'B)$.

2.31. Since, from (2.9), every vector space has a basis, it follows from the above algorithm that every inner product space has an orthonormal basis.

2.32. Let $\{ \alpha_1, \alpha_2, \ldots, \alpha_n \}$ be an orthonormal basis of $\mathcal{V}$, and let $x, y \in \mathcal{V}$ be any vectors. Then, for an inner product space:

(a) $x = \langle x, \alpha_1 \rangle \alpha_1 + \langle x, \alpha_2 \rangle \alpha_2 + \cdots + \langle x, \alpha_n \rangle \alpha_n$.

(b) (Parseval’s identity) $\langle x, y \rangle = \sum_{i=1}^n \langle x, \alpha_i \rangle \langle \alpha_i, y \rangle$.

Conversely, if this equation holds for any $x$ and $y$, then $\alpha_1, \ldots, \alpha_n$ is an orthonormal basis for $\mathcal{V}$.

(c) Setting $x = y$ in (b) we have

$$
\|x\|^2 = |\langle x, \alpha_1 \rangle|^2 + |\langle x, \alpha_2 \rangle|^2 + \cdots + |\langle x, \alpha_n \rangle|^2.
$$
(d) (Bessel’s inequality) \( \sum_{i=1}^{k} \langle x, \alpha_i \rangle \leq \|x\|^2 \) for each \( k \leq n \).

Equality occurs if and only if \( x \) belongs to the space spanned by the \( \alpha_i \).

**Proofs.** Section 2.2.3.


2.25a. If \( x_1, x_2 \in S \perp \), then \( \langle x_1, y \rangle = 0 \) for all \( y \in S \) and \( \langle \alpha_1 x_1 + \alpha_2 x_2, y \rangle = \alpha_1 \langle x_1, y \rangle + \alpha_2 \langle x_2, y \rangle = 0 \), i.e., \( \alpha_1 x_1 + \alpha_2 x_2 \in S \perp \).

2.25b. If \( x \in S \), then \( \langle x, y \rangle = 0 \) for all \( y \in S \perp \) and \( x \in (S \perp) \perp \). By (a), \( (S \perp) \perp \) is a vector space even if \( S \) is not; then use (2.26b).

2.25c. If \( x \) belongs to the left-hand side (LHS), then \( \langle x, s + t \rangle = \langle x, s \rangle + \langle x, t \rangle = 0 \) for all \( s \in S \) and all \( t \in T \). Setting \( s = 0 \), then \( \langle x, t \rangle = 0 \); similarly, \( \langle x, s \rangle = 0 \) and \( LHS \subseteq RHS \). The argument reverses.


2.27a–b. Harville [1997: 172].


2.28a(i). Follows from (2.26d) with \( U = W \).

2.28a(ii). If \( x \in RHS \), then \( x = y + z \) where \( y \in V \subseteq W \) and \( z \in W \) so that \( x \in W \) and \( RHS \subseteq LHS \). Then use (i) to show \( \dim(RHS) = \dim(LHS) \).

2.29. Kollo and von Rosen [2005: 29].


2.32d. Rao [1973a: 10].

### 2.2.4 Column and Null Spaces

**Definition 2.18.** If \( A \) is a matrix (real or complex), then the space spanned by the columns of \( A \) is called the column space of \( A \), and is denoted by \( C(A) \). (Some authors, including myself in the past, call this the range space of \( A \) and write \( R(A) \).) The corresponding row space of \( A \) is \( C(A') \), which some authors write as \( R(A) \); hence my choice of notation to avoid this confusion. The null space or kernel, \( N(A) \) of \( A \), is defined as follows:

\[
N(A) = \{ x : Ax = 0 \}.
\]

The following results are all expressed in terms of complex matrices, but they clearly hold for real matrices as well.

2.33. From the definition of a vector subspace we find that \( C(A) \) and \( N(A) \) are both vector subspaces.
2.34. Let $A$ and $B$ both have $n$ columns. If any one of the following conditions holds, then all three hold:

1. $C(A') \subseteq C(B').$
2. $N(B) \subseteq N(A).$
3. $A(I_n - B^{-}B) = 0.$

If (3) holds for a particular weak inverse $B^{-}$, then (3) holds for any weak inverse $B^{-}$.

2.35. Let $A$ be any complex matrix.

(a) $N(A^*A) = N(A).$
(b) $C(AA^*) = C(A).$
(c) Two more results follow from (a) and (b) by interchanging $A$ and $A^*$.

In most applications $A$ is real so that $A^* = A'$.

2.36. $N(A) \subseteq C(I - A)$ and $N(I - A) \subseteq C(A)$.

2.37. If $x \perp y$ when $\langle x, y \rangle = x^*y = 0$, and $A$ is an $m \times n$ complex matrix, then $N(A) = \{C(A^*)\}^\perp$. We therefore have an orthogonal decomposition

$$N(A) \oplus C(A^*) = \mathbb{F}^n \text{ and } \dim N(A) + \dim C(A^*) = n.$$ 

We get a further result by interchanging the roles of $A$ and $A^*$. Note that $\dim[C(A^*)] = \text{rank } A^* = \text{rank } A$, by (3.3c).

2.38. If $A$ is $m \times n$ and $B$ is $m \times p$, then $C(B) \subseteq C(A)$ if and only if there exists an $n \times p$ matrix $R$ such that $AR = B$. Furthermore, if $p = n$, $C(A) = C(B)$ if and only if there exists such a nonsingular $R$. Similar results are available for row spaces by simply taking transposes. Thus if $C$ is $q \times n$, then $C(C') \subseteq C(A')$ if and only if there exists a $q \times m$ matrix $S$ such that $SA = C$.

2.39. The following hold for conformable matrices:

(a) If $C(A) \subseteq C(B)$, then $C(A'B) = C(A').$
(b) $C(B_1) \subseteq C(B_2)$ implies that $C(A'B_1) \subseteq C(A'B_2)$.
(c) $C(B_1) = C(B_2)$ implies that $C(A'B_1) = C(A'B_2)$.
(d) If $C(A + BE) \subseteq C(B)$ for some conformable $E$, then $C(A) \subseteq C(B)$.
(e) If $C(A) \subseteq C(B)$, then $C(A + BE) \subseteq C(B)$ for any conformable $E$.

Proofs. Section 2.2.4.

2.34. Scott and Styan [1985: 210].
2.35. Meyer [2000a: 212–213].
2.36. Note that $Bx = 0$ if and only if $x = (I - B)x$. Set $B = A$ and $B = I - A$. 


2.39. Quoted by Kollo and von Rosen [2005: 49]. For (a) we first have $\mathcal{C}(A'B) \subseteq \mathcal{C}(A')$. Then, from (2.35), $A'x = A'Ay = A'BRy \in \mathcal{C}(A'B)$, by (2.38), i.e., $\mathcal{C}(A') \subseteq \mathcal{C}(A'B)$. The rest are straightforward.

### 2.3 PROJECTIONS

**Definition 2.19.** A square matrix $P$ such that $P^2 = P$ is said to be **idempotent**.

In this section we focus on the geometrical properties of such matrices, which are used extensively in statistics. Algebraic properties are considered in Section 8.6.

#### 2.3.1 General Projections

**Definition 2.20.** Let the vector space $\mathcal{U}$ be the direct sum of two vector spaces $V_1$ and $V_2$ so that $\mathcal{U} = V_1 \oplus V_2$ (i.e., $V_1 \cap V_2 = 0$). Then every vector $v \in \mathcal{V}$ has a unique decomposition $v = v_1 + v_2$, where $v_i \in V_i$ $(i = 1, 2)$. The transformation $v \to v_1$ is called the projection of $v$ on $V_1$ along $V_2$. Here uniqueness follows by assuming another decomposition $v = w_1 + w_2$ so that $v_1 - w_1 = -(v_2 - w_2)$, which implies $v_i = w_i$ for $i = 1, 2$, otherwise $V_1 \cap V_2 \neq 0$. Usually $\mathcal{U} = \mathbb{F}^n$, and the following hold if $\mathbb{F}$ is $\mathbb{R}$ or $\mathbb{C}$.

2.40. The above projection on $V_1$ along $V_2$ can be represented by an $n \times n$ matrix $P$ called a **projector** or **projection matrix** so that $Pv = v_1$. Also $P$ is unique and idempotent.

2.41. Using the above notation, $v = P \cdot v + (I_n - P) \cdot v = v_1 + v_2$, so that $v_2 = (I_n - P) \cdot v$ is the projection of $v$ on $V_2$ along $V_1$. Here $P$ and $I_n - P$ are unique and idempotent, and $$P(I_n - P) = 0.$$  

2.42. Using the above notation, we can identify $V_1$ and $V_2$ as follows:

(a) $\mathcal{C}(P) = \mathcal{V}_1$.

(b) $\mathcal{C}(I_n - P) = \mathcal{V}_2$.

(c) If $P$ is idempotent, then from (8.61) we obtain $$\mathcal{C}(P) \oplus \mathcal{N}(P) = \mathcal{V}_1 \oplus \mathcal{V}_2.$$  

2.43. Using the notation of (2.42), suppose that $\mathcal{V}_1 = \mathcal{C}(A)$, where $A$ is $n \times n$ of rank $r$. Let $A = R_{n \times r}C_{r \times n}$ be a full-rank factorization of $A$ (cf. 3.5). Then $$P = R(CR)^{-1}C$$ is the projection onto $\mathcal{V}_1$ along $\mathcal{V}_2$. 

Proofs. Section 2.3.1.

2.40. Assume two projectors $P_i$ ($i = 1, 2$), then $(P_1 - P_2)v = v_1 - v_2 = 0$ for all $v$ so that $P_1 = P_2$. Now $v_1 = v_1 + 0$ is the unique decomposition of $v_1$ so that $P^2v = P(Pv) = Pv_1 = v_1 - Pv$ for all $v$ so that $P^2 = P$.


2.42a. $\mathcal{C}(P) \subseteq \mathcal{V}_1$ as $P$ projects onto $\mathcal{V}_1$. Conversely, if $v_1 \in \mathcal{V}_1$, then $Pv_1 = v_1$, and $\mathcal{V}_1 \subseteq \mathcal{C}(P)$; (b) is similar.

2.43. Meyer [2000a: 634].

2.3.2 Orthogonal Projections

Definition 2.21. Suppose $\mathcal{U}$ has an inner product $\langle \cdot , \cdot \rangle$, and let $\mathcal{V}$ be a vector subspace with orthogonal complement $\mathcal{V}^\perp$, namely

$$\mathcal{V}^\perp = \{ x : \langle x, y \rangle = 0, \text{ for every } y \in \mathcal{V} \}.$$  

Then $\mathcal{U} = \mathcal{V} \oplus \mathcal{V}^\perp$ so that every $v \in \mathcal{U}$ can be expressed uniquely in the form $v = v_1 + v_2$, where $v_1 \in \mathcal{V}$ and $v_2 \in \mathcal{V}^\perp$. The vectors $v_1$ and $v_2$ are called the orthogonal projections of $v$ onto $\mathcal{V}$ and $\mathcal{V}^\perp$, respectively (we shall omit the words "along $\mathcal{V}^\perp$" and "along $\mathcal{V}$", respectively). Orthogonal projections will, of course, share the same properties as general projections. If $\mathcal{V} = \mathcal{C}(A)$, we shall denote the orthogonal projection $P_\mathcal{V}$ onto $\mathcal{V}$ by $P_A$. In what follows we assume that $\mathcal{U} = \mathbb{F}^n$.

2.44. Using the above notation, $v_1 = P_\mathcal{V}v$ and $v_2 = (I_n - P_\mathcal{V})v$, where $P_\mathcal{V}$ and $I_n - P_\mathcal{V}$ are unique idempotent matrices. The matrix $P_\mathcal{V}$ is said to be the orthogonal projector or orthogonal projection matrix of $\mathbb{F}^n$ onto $\mathcal{V}$, while $P_{\mathcal{V}}^\perp = I_n - P_\mathcal{V}$ is the orthogonal projector of $\mathbb{F}^n$ onto $\mathcal{V}^\perp$. As we shall see below, the definition of orthogonality depends on the definition of $\langle x, y \rangle$.

2.45. If $\mathbb{F}^n = \mathbb{R}^n$ and $\langle x, y \rangle = x'y$, then from the orthogonality we have

$$P_\mathcal{V}(I - P_\mathcal{V}) = 0,$$

and $P_\mathcal{V}$ is symmetric as well as being idempotent.

2.46. Let $\mathbb{F}^n = \mathbb{C}^n$ and define $\langle x, y \rangle = y^*Ax$, where $A$ is a Hermitian positive definite matrix. Note that $x \bot y$ if $y^*Ax = 0$ (cf. 2.19c).

(a) Let $P_\mathcal{V}$ be the orthogonal projection matrix that projects onto $\mathcal{V}$. Then $P_\mathcal{V}^2 = P_\mathcal{V}$ and $AP_\mathcal{V}$ is Hermitian, that is,

$$AP_\mathcal{V} = P_\mathcal{V}^*A.$$  

(Note that $P_\mathcal{V}$ is generally not Hermitian. However, if $A = I_n$, then $P_\mathcal{V}$ is Hermitian.)

(b) $\mathcal{C}(P_\mathcal{V}) = \mathcal{V}$ and $\mathcal{C}(I_n - P_\mathcal{V}) = \mathcal{V}^\perp$ (from 2.42). Also

$$P_\mathcal{V}^*A(I_n - P_\mathcal{V}) = AP_\mathcal{V}(I_n - P_\mathcal{V}) = 0.$$
(c) Let $\mathcal{V} = \mathcal{C}(X)$. Then
\[
P_\mathcal{V} = X(X^*AX)^{-}X^*A,
\]
which is unique for any weak inverse $(X^*AX)^{-}$ and therefore invariant. Also $P_{\mathcal{V}^\perp} = I_n - P_\mathcal{V}$.

(d) If $\mathcal{V} = \mathcal{C}(X)$, then $P_\mathcal{V}X = X$.

2.47. Of particular interest is a special case of (2.46) above, namely $\langle x, y \rangle = x'V^{-}y$, where $V$ is positive definite and $x, y \in \mathbb{R}^n$. Because of its statistical importance in a variety of nonlinear models including nonlinear regression (e.g., generalized or weighted least squares) and multinomial models, $\langle x, y \rangle$ has been called the weighted inner product space (Wei [1997]). We now list some special cases of the previous general theory. Let $X$ be $n \times p$ of rank $p$ and $\mathcal{V} = \mathcal{C}(X)$. Then:

(a) $P_\mathcal{V} = X(X'V^{-}X)^{-}X'V^{-}1$, which implies $P_\mathcal{V}^2 = P_\mathcal{V}$ and $P_\mathcal{V}'V^{-1} = V^{-1}P_\mathcal{V}$. Here $(X'V^{-}X)^{-}$ is any weak inverse of $X'V^{-}X$. Further properties of $P_\mathcal{V}$ (with $V^{-}$ replaced by $V$) are given by Harville [2001: 106-112].

(b) If the columns of $Q$ and $N$ are respectively orthonormal bases of $\mathcal{V}$ and $\mathcal{V}^\perp$, then $P_\mathcal{V} = QQ'V^{-1}$ and $P_{\mathcal{V}^\perp} = NN'V^{-1}$, where $P_\mathcal{V} + P_{\mathcal{V}^\perp} = I_n$.

(c) From (b), $Q'V^{-1}N = 0$.

We can set $V = I$ is the above to get the unweighted case.

2.48. Let $V$ be an $n \times n$ positive definite matrix, $G$ an $n \times g$ matrix of rank $g$ ($g \leq n$), and $F$ an $n \times f$ matrix ($f = n - g$) of rank $f$ such that $G'F = 0$. Then
\[
VF(F'VF)^{-1}F' + G(G'V^{-1}G)^{-1}G'V^{-1} = I_n.
\]

2.49. Let $\mathbb{F}^n = \mathbb{C}^n$, $\mathbf{v} \in \mathbb{C}^n$, and define $\langle x, y \rangle = x^*y$, i.e., $A = I_n$ in (2.46). Then:

(a) $P_\mathcal{V}$ is an orthogonal projection matrix on some vector space if and only if $P_\mathcal{V}$ is idempotent and Hermitian.

(b) From (2.42) we have $\mathcal{V} = \mathcal{C}(P_\mathcal{V})$.

(c) Let $T = (t_1, t_2, \ldots, t_p)$, where the columns $t_i$ of $T$ form an orthonormal basis for $\mathcal{V}$. Then $P_\mathcal{V} = TT^*$, and the projection of $\mathbf{v}$ onto $\mathcal{V}$ is $v_1 = TT^*\mathbf{v} = \sum_{i=1}^pt_i^*\mathbf{v}t_i$.

(d) If $\mathcal{V} = \mathcal{C}(X)$, then $P_\mathcal{V} = X(X^*X)^{-}X^* = XX^+$, where $(X^*X)^{-}$ is a weak inverse of $X^*X$ and $X^+$ is the Moore–Penrose inverse of $X$. When the columns of $X$ are linearly independent, $P_\mathcal{V} = X(X^*X)^{-1}X^*$.

(e) Let $\mathcal{V} = \mathcal{N}(A)$, the null space of $A$. Then, since $\mathcal{V}^\perp = \mathcal{C}(A^*)$ (by 2.37), $P_\mathcal{V} = I_n - A^*(AA^*)^{-}A$.

(f) If $\mathbb{F}^n = \mathbb{R}^n$, then the previous results hold by replacing $*$ by $'$ and replacing Hermitian by real symmetric. For example, if $\mathcal{V} = \mathcal{C}(A)$, then $P_\mathcal{V} = A(A'A)^{-}A'$. Furthermore, $x'P_\mathcal{V}x = xP_\mathcal{V}'P_\mathcal{V}x = y'y \geq 0$, so that $P_\mathcal{V}$ is non-negative definite. This result is used frequently in this book.
2.50. Let $A$ be an $n \times m$ real matrix and $B$ an $n \times p$ real matrix. Assuming that $(x, y) = x'y$, let $P_D$ denote the orthogonal projection onto $C(D)$ for any matrix $D$.

(a) $C(A) \cap C(B) = C[A(I_m - P_V)]$, where $V = C[A'(I - P_B)]$.

(b) $C(A, B) = C(A) \oplus C[(I - P_A)B]$.

(c) From (b) we have $P_{(A,B)} = P_A + (I - P_A)B$.

(d) $C(A) \subseteq C(B)$ if and only if $P_B - P_A$ is non-negative definite, and $C(A) \subseteq C(B)$ if and only if $P_B - P_A$ is positive definite.

The above results are particularly useful in partitioned linear models.

2.51. (Some Subspace Properties) Let $\omega$, $\Omega$, and $V$ be vector subspaces in $\mathbb{R}^n$ with $\omega \subseteq \Omega$, and let $P_\omega$ and $P_\Omega$ be the respective orthogonal projectors onto $\omega$ and $\Omega$ with respect to the inner product $(x, y) = x'y$ defined on $\mathbb{R}^n$. Thus $P_\omega$ and $P_\Omega$ are symmetric and idempotent. The following results hold (see also (2.53c)).

(a) $P_\Omega P_\omega = P_\omega P_\Omega = P_\omega$.

(b) $P_{\omega^\perp \cap \Omega} = P_\Omega - P_\omega$.

(c) $AP_\Omega A'$ is nonsingular if and only if the rows of $A$ are linearly independent and $C(A') \cap \Omega^\perp = 0$.

(d) If $\omega = \Omega \cap N(A)$, where $N(A)$ is the null space of $A$, then:

(i) $\omega^\perp \cap \Omega = C(P_\Omega A')$.

(ii) $P_{\omega^\perp \cap \Omega} = P_\Omega A'(AP_\Omega A')^{-1}AP_\Omega$, where $(AP_\Omega A')^{-1}$ is any weak inverse of $AP_\Omega A'$.

(e) Let $\Omega = C(X) = C(X_1, X_2)$, where the columns of $n \times p$ $X$ are linearly independent, and let $\omega = C(X_1)$, where $\dim(\omega) = r$.

(i) We have from (c), with $V = \omega^\perp$ and $P_\omega = X_1(X_1'X_1)^{-1}X_1' (= P_1$, say), that $X_2'(I_n - P_1)X_2$ is nonsingular.

(ii) $\omega = \Omega \cap N[X_2'(I_n - P_1)]$.

(iii) It follows from (b) and (d)(ii)) that

$$P_\Omega - P_\omega = (I_n - P_1)X_2[X_2'(I_n - P_1)X_2]^{-1}X_2'(I_n - P_1).$$

By interchanging the subscripts 1 and 2, a further result can be obtained.

Note that (a)–(d) are used in testing a linear hypothesis for a linear regression model (e.g., Seber [1977: sections 3.9.3 and 4.5] and Seber and Lee [2003: theorems 4.1 and 4.3]); (e) is related to subset regression (see Seber and Wild [1989: Appendix D] for a summary).

2.52. If $\Omega$ and $\omega_i$ ($i = 1, 2, \ldots, k$) are vector subspaces of $\mathbb{R}^n$ satisfying $\omega_i \subset \Omega$, with inner product $(x, y) = x'y$, then the following results are equivalent:

(1) $P_{\omega_1 \cap \omega_2 \cap \cdots \cap \omega_i} - P_{\omega_1 \cap \omega_2 \cap \cdots \cap \omega_{i-1}} = P_\Omega - P_{\omega_i}$ for $i = 1, 2, \ldots, k$. 
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(2) \( \omega_i^+ \cap \Omega \perp \omega_j^+ \cap \Omega \) for all \( i, j = 1, 2, \ldots, k; \quad i \neq j. \)

(3) \( \omega_i^+ \cap \Omega \subset \omega_j \) for all \( i, j = 1, 2, \ldots, k; \quad i \neq j. \)

The above results are useful in testing a sequence of nested hypotheses in an analysis of variance, when there are equal numbers of observations per cell (balanced designs) leading to an underlying orthogonal structure (cf. Darroch and Silvey [1963], Seber [1980: section 6.2], and Seber and Lee [2003: 203]).

2.53. Let \( \omega_1 \) and \( \omega_2 \) be vector subspaces of \( \mathbb{R}^n \) with inner product \( \langle x, y \rangle = x'y. \)

(a) \( P = P_{\omega_1} + P_{\omega_2} \) is an orthogonal projector if and only if \( \omega_1 \perp \omega_2, \) in which case \( P_{\omega_1} + P_{\omega_2} = P_\omega, \) where \( \omega = \omega_1 \oplus \omega_2. \)

(b) If \( \omega_1 = C(A) \) and \( \omega_2 = C(B) \) in (a), then \( \omega_1 \oplus \omega_2 = C(A, B). \)

(c) The following statements are equivalent:

(1) \( P_{\omega_1} - P_{\omega_2} \) is an orthogonal projection matrix.

(2) \( \|P_{\omega_1}x\|_2 \geq \|P_{\omega_2}x\|_2 \) for all \( x \in \mathbb{R}^n. \)

(3) \( P_{\omega_1}P_{\omega_2} = P_{\omega_2}. \)

(4) \( P_{\omega_2}P_{\omega_1} = P_{\omega_1}. \)

(5) \( \omega_2 \subset \omega_1. \)

(d) \( P_{\omega_1 \cap \omega_2} = 2P_{\omega_1}(P_{\omega_1} + P_{\omega_2})^+P_{\omega_2} = 2P_{\omega_2}(P_{\omega_1} + P_{\omega_2})^+P_{\omega_1}. \) Here \( B^+ \) denotes the Moore–Penrose inverse of \( B. \)

The above results hold for \( \mathbb{C}^n \) if \( \langle x, y \rangle = y'x \) and \( ' \) is replaced by \( * \).

**Definition 2.22.** (Centering) Let \( a = (a_i) \) be an \( n \times 1 \) real vector, and let \( \bar{a} = \sum_{i=1}^{n} a_i/n. \) We say that the \( a \) is centered when we transform \( a_i \) to \( b_i = a_i - \bar{a}. \)

If we have the \( n \times p \) matrix \( A = (a_1, a_2, \ldots, a_n)' = (a^{(1)}, a^{(2)}, \ldots, a^{(p)}) \) and \( \bar{a} = n^{-1} \sum_{i=1}^{n} a_i, \) then we say that \( A \) is row centered if we transform it to the matrix \( B = (a_1 - \bar{a}, a_2 - \bar{a}, \ldots, a_n - \bar{a})'. \)

If \( \bar{a}^{(col)} = \sum_{j=1}^{p} a^{(j)}/p, \) then we say that \( A \) is column centered if we form the matrix \( C = (a^{(1)} - \bar{a}^{(col)}, a^{(2)} - \bar{a}^{(col)}, \ldots, a^{(p)} - \bar{a}^{(col)}). \)

We say that \( A \) is double-centered if we apply both row and column centering.

2.54. Using the above notation, we have the following results:

(a) We can write \( \bar{a} = 1_n'a/n \) so that \( (\bar{a}) = n^{-1}1_n'1_n'a = P_{1_n}a, \) where \( P_{1_n} = n^{-1}1_n'1_n \) represents the orthogonal projection of \( \mathbb{R}^n \) onto \( 1_n. \) Furthermore, \( b = a - (\bar{a}) = (I_n - P_{1_n})a, \) where \( I_n - P_{1_n} \) represents an orthogonal projection perpendicular to \( 1_n; \) this projection matrix is called a centering matrix.

(b) \( \bar{a} = A1_n'/n \) and \( B = A - 1_n \bar{a}' = (I_n - P_{1_n})A. \)

(c) \( \bar{a}^{(col)} = A1_p/p \) and \( C = A(I_p - P_{1_p}). \)

(d) When \( A \) is double centered we obtain \( D = (I_n - P_{1_n})A(I_p - P_{1_p}), \) where \( d_{ij} = a_{ij} - \bar{a}_i - \bar{a}_j - \bar{a}, \quad \bar{a}_i = \sum_j a_{ij}/p, \quad \bar{a}_j = \sum_i a_{ij}/n, \) and \( \bar{a} = \sum_i \sum_j a_{ij}/(np). \)
Centering is used extensively in statistics, for example linear regression (Seber and Lee [2003: section 3.11.1 and section 11.7 for computing algorithms]) and principal component analysis, and double centering is used in classical metric scaling, in principal component analysis (Jolliffe [1992: section 14.2.3]), and in the singular-spectrum analysis (SAS) of times series, where it is applied to trajectory matrices (Golyandina et al. [2001: section 4.4, 272]).

**Proofs.** Section 2.3.2.

2.46. Rao [1973a: 47].

2.47. Wei [1997: 185–187].

2.48. Seber [1984: 536].

2.49. Seber and Lee [2003: Appendices B1 and B2, real case].

2.50a. Quoted by Rao and Mitra [1971: 118, exercise 7a].

2.50b–d. Sengupta and Jammalamadaka [2003: 39, 47]; (c) uses (2.44).


2.51d(ii). If $x \in C(X_1) = \omega$, then $P_1 x = x$, $X_2(I_n - P_1)x = 0$, and $x \in \mathcal{N}(X_2(I_n - P_1))$. Conversely, if $x = X_1\alpha_1 + X_2\alpha_2 \in \Omega$ and $0 = X_2(I_n - P_1)x = X_2(I_n - P_1)X_2\alpha_2$ (since $P_1X_1 = X_1$), then $\alpha_2 = 0$ (by (i)) and $x \in C(X_1)$.

2.52. Seber [1980: section 6.2].

2.53a. $P$ is clearly symmetric and idempotent if and only $P_{\omega_1}P_{\omega_2} = -P_{\omega_2}P_{\omega_1}$. Multiplying on the left by $P_{\omega_2}$ shows that $P_{\omega_1}P_{\omega_2}$ is symmetric and therefore $P_{\omega_1}P_{\omega_2} = 0$. Furthermore, since $P_{\omega_i}$ is idempotent, we have from (2.35)

$$C(P_{\omega_1} + P_{\omega_2}) = C\left(\begin{pmatrix} P_{\omega_1} & P_{\omega_2} \\ P_{\omega_2} & P_{\omega_1} \end{pmatrix}\right) = C(P_{\omega_1}, P_{\omega_2}) = \omega_1 \oplus \omega_2.$$

2.53b. $A'B = 0$ implies that $PAPB = 0$.

2.53c. Quoted, less generally, by Isotalo et al. [2005a: 61]. The proofs are straightforward. For (2), note that for a symmetric idempotent matrix, $x'Ax = x'A'Ax = ||Ax||^2_2$.


### 2.4 METRIC SPACES

**Definition 2.23.** Let $S$ be a subset of $\mathbb{R}^n$. By a **metric** for $S$ we mean a real-valued function $d(\cdot, \cdot)$ on $S \times S$ such that:

(a) $d(x, y) \geq 0$ for all $x, y \in S$ with equality if and only if $x = y$ ($d$ is positive definite).
(b) \( d(x, y) = d(y, x) \) for all \( x, y \in S \) \((d \) is symmetric).

(c) \( d(x, y) \leq d(x, z) + d(y, z) \) for all \( x, y, z \in S \) \((\) triangle inequality). If we replace (c) by the stronger condition

\[
(c') \quad d(x, y) \leq \max[d(x, z), d(y, z)],
\]
d is called an ultrametric. Note that \((c')\) implies (c).

Definition 2.24. A metric space is a pair \((S, d)\) consisting of a set \(S\) and a metric \(d\) for \(S\).

2.55. If \(d\) is a metric, then so are \(d_1, d_2,\) and \(d_3,\) where
\[
\begin{align*}
d_1(x, y) &= d(x, y)/(1 + d(x, y)), \\
d_2(x, y) &= \sqrt{d(x, y)}, \\
d_3(x, y) &= kd(x, y) \quad (k > 0).
\end{align*}
\]

2.56. If \(d\) is a metric, then \(D(x, y) = [d(x, y)]^2\) is not necessarily a metric.

2.57. (Canberra metric) If \(x\) and \(y\) have positive elements, then the function
\[
d(x, y) = \frac{1}{n} \sum_{j=1}^{n} \frac{|x_j - y_j|}{x_j + y_j}
\]
is a metric.

2.58. (Minkowski Metrics) The function \(\Delta_p\) is a metric, where
\[
\Delta_p(x, y) = \left( \sum_{i=1}^{n} |x_i - y_i|^p \right)^{1/p}, \quad p > 0.
\]
The most common ones are \(p = 1\) \((\) the city block metric\) and \(p = 2\) \((\) the Euclidean metric\). Various scaled versions of \(\Delta_1\) have also been used.

2.59. \(\Delta_{\infty}(x, y) = \sup_{1 \leq i \leq n} |x_i - y_i|,\) for all \(x\) and \(y,\) is a metric.

Definition 2.25. The Mahalanobis distance is defined to be
\[
d(x, y) = \{ (x - y)' A (x - y) \}^{1/2},
\]
where \(A\) is positive definite. Here \(d\) is a metric. The Mahalanobis angle \(\theta\) between \(x\) and \(y\) subtended at the origin is defined by
\[
\cos \theta = \frac{x' Ay}{(x' Ax)^{1/2} (y' Ay)^{1/2}}.
\]

Definition 2.26. A sequence of points \(\{x_i\}\) in \(S\) for a metric space \((S, d)\) is called a Cauchy sequence if, for every \(\epsilon > 0,\) there exists a positive integer \(N\) such the \(d(x_i, x_j) < \epsilon\) for all \(i, j > N.\)

A sequence \(\{x_i\}\) converges to a point \(x\) if, for every \(\epsilon > 0,\) there exists a positive integer \(N\) such that \(d(x, x_i) < \epsilon\) for all \(i > N.\)
A metric space is said to be complete if every Cauchy sequence converges to a point in $S$.

**Definition 2.27.** Let $f$ be a mapping of a metric space $(S, d)$ into itself. We call $f$ a contraction if there exists a constant $c$ with $0 < c \leq 1$ such that

$$d(f(x), f(y)) \leq cd(x, y), \quad \text{for all } x, y \in S.$$ 

If $0 < c < 1$, we say that $f$ is a strict contraction. If $f(x) = x$, then $x$ is referred to as a fixed point of $f$.

2.60. (Contraction Mapping Theorem) Let $f$ be a strict contraction of a complete metric space into itself. Then $f$ has one and only one fixed point and, for any point $y \in S$, the sequence

$$y, f(y), f^2(y), f^3(y), \ldots,$$

where $f^n(y) = f(f^{n-1}(y))$, converges to the fixed point.

2.61. Let $(S, d)$ be a metric space with $S = \mathbb{C}^n$ and $d(x, y) = \|x - y\|_2$. A matrix $A$ is a contraction, that is

$$\|Ax - Ay\|_2 \leq c\|x - y\|_2 \quad \text{for } 0 < c \leq 1,$$

if and only if $\sigma_{\text{max}}(A) \leq 1$, where $\sigma_{\text{max}}(A)$ is the maximum singular value of $A$. Further necessary and sufficient conditions for a matrix to be a contraction are given by Zhang [1999: section 5.4].

**Proofs.** Section 2.4.

2.55–2.57. Seber [1984: : 392, exercises 7.4–7.6, see the solutions].

2.58. Seber [1984: 352]. Use Minkowski's inequalities (12.17b) and $x_i - z_i = x_i - y_i + y_i - z_i$ to prove the triangle inequality.

2.59. Use the properties of sup.


## 2.5 CONVEX SETS AND FUNCTIONS

**Definition 2.28.** A subset $C$ of $\mathbb{R}^n$ is called convex if, for any two points $x_1, x_2 \in C$, the line segment joining $x_1$ and $x_2$ is contained in $C$, that is,

$$\alpha x_1 + (1 - \alpha) x_2 \in C \quad \text{for } 0 \leq \alpha \leq 1.$$

We will list some properties of convex sets below. For a more comprehensive discussion see Berkovitz [2002], Kelly and Weiss [1979], Lay [1982], and Rockafellar [1970].

2.62. If $C_1$ and $C_2$ are convex sets in $\mathbb{R}^n$, then:

(a) $C_1 \cap C_2$ is convex.
(b) $C_1 + C_2$ is convex.

(c) $C_1 \cup C_2$ need not be convex.

These results clearly hold for any finite number of convex sets. The result (a) also holds for a countably infinite number of convex sets.

2.63. Given any set $A \in \mathbb{R}^n$, the set $C_A$ of points generated by taking the convex combination of every finite set of points $x_i$ in $A$, namely

$$\alpha_1 x_1 + \alpha_2 x_2 + \cdots + \alpha_k x_k \quad (\text{each } \alpha_i \geq 0 \text{ and } \sum_i \alpha_i = 1)$$

is a convex set containing $A$. The set $C_A$ is the smallest convex set containing $A$ and is called the convex hull of $A$. It is also the intersection of all convex sets containing $A$.

**Definition 2.29.** Given $A$ a set in $\mathbb{R}^n$, we define $x$ to be an inner (interior) point of $A$ if there is an open sphere with center $x$ that is a subset of $A$; that is, there exists $\delta > 0$ such that

$$S_\delta = \{y : y \in \mathbb{R}^n, (y - x)'(y - x) < \delta\} \subseteq A.$$

A boundary point $x$ of $A$ (not necessarily belonging to $A$) is such that every open sphere with center $x$ contains points both in $A$ and in $A^c$, the complement of $A$ with respect to $\mathbb{R}^n$.

A point $x$ is a limit (accumulation) point if, for every $\delta > 0$, $S_\delta$ contains at least one point of $S$ distinct from $x$.

The closure of set $A$ is obtained by adding to it all its boundary points not already in it, and is denoted by $\overline{A}$. It can also be obtained by adding to $S$ all its limit points.

The set $A$ is closed if $A = \overline{A}$, while the set is open if $A^c$, the complement of $A$, is closed. For any set $A$, $\overline{A}$ is the smallest closed set containing $A$.

An exterior point of $A$ is a point in $\overline{A}^c$. A point $x \in A$ is an extreme point of $A$ if there are no distinct points $x_1$ and $x_2$ in $A$ such that $x = \alpha x_1 + (1 - \alpha)x_2$ for some $\alpha$ ($0 < \alpha < 1$)

A set $A$ is bounded if it is contained in an open sphere $S_\delta$ for some $\delta > 0$.

A set which is closed and bounded is said to be compact. For some properties of open and closed sets see Magnus and Neudecker [1999: 66–69].

The above results generalize to more general spaces using a more general distance metric other than $\|x - y\|_2$.

2.64. Let $C$ be a convex set.

(a) The closure $\overline{C}$ is convex.

(b) $C$ and $\overline{C}$ have the same inner, boundary, and exterior points.

(c) Let $x$ be an inner point and $y$ a boundary point of $C$. Then the points $\alpha x + (1 - \alpha)y$ are inner points of $C$ for $0 < \alpha \leq 1$ and exterior points of $C$ for $\alpha > 1$

(d) If $T$ is an open subset of $\mathbb{R}^n$ and $T \subseteq \overline{C}$, then $T \subseteq C$. 
2.65. (Separation theorems)

(a) Let \( C \) be a closed convex subset and suppose \( 0 \notin C \). Then there exists a vector \( a \) such that \( a'x > 0 \) for all \( x \in C \).

(b) Let \( C \) be a convex set and \( y \) an exterior point. Then there exists a unit vector \( u \) (i.e., \( \|u\|_2 = 1 \)) such that

\[
\inf_{x \in C} u'x > u'y.
\]

(c) Let \( C \) be a convex set and \( y \) a point not in \( C \), or a boundary point if in \( C \). Then there exists a supporting plane through \( y \); that is, there exists a nonzero vector \( a \neq 0 \) such that \( a'x \geq a'y \) for all \( x \in C \), or equivalently \( \inf_{x \in C} a'x = a'y \), if \( y \) is a boundary point.

(d) Let \( C_1 \) and \( C_2 \) be convex sets with no inner point in common. Then there exists a hyperplane \( a'x = b \) separating the two sets; that is, there exists a vector \( a \) and a scalar \( b \) such that \( a'x \geq b \) for all \( x \in C_1 \) and \( a'y \leq b \) for all \( y \in C_2 \). This also implies that \( a'x_1 \geq a'x_2 \) for all \( x_1 \in C_1 \) and all \( x_2 \in C_2 \).

If \( C_1 \) and \( C_2 \) are also closed, we have strict separation so that there exist \( a \) and \( b \) such that \( a'x > b \) for \( x \in C_1 \) and \( a'y < b \) for \( y \in C_2 \).

(e) Let \( C \) be a convex subset, symmetric about \( 0 \), so that if \( x \in C \), then \( -x \in C \) also. Let \( f(x) \geq 0 \) be a function for which (i) \( f(x) = f(-x) \), (ii) \( C_\alpha = \{x : f(x) \geq \alpha\} \) is convex for any positive \( \alpha \), and (iii) \( \int_C f(x) \, dx < \infty \). Then

\[
\int_C f(x + cy) \, dx \geq \int_C f(x + y) \, dx,
\]

for all \( 0 \leq c \leq 1 \) and \( y \in \mathbb{R}^n \).

2.66. (Convex Hull) If \( C_A \) is the convex hull of a subset \( A \subset \mathbb{R}^n \), then every point of \( A \) can be expressed as a convex combination of at most \( n + 1 \) points in \( A \).

2.67. (Extreme Points) If \( C \) is a closed bounded convex set, it is spanned by its extreme points; that is, every point in \( C \) can be expressed as a linear combination of its extreme points. Also \( C \) has extreme points in every supporting hyperplane.

**Definition 2.30.** A real valued function \( f \) is **convex** in an interval \( I \) of \( \mathbb{R} \) if

\[
f(\alpha x + (1 - \alpha)y) \leq \alpha f(x) + (1 - \alpha)f(y), \quad \text{all } \alpha \text{ such that } 0 < \alpha < 1,
\]

for all \( x, y \in I \) \( (x \neq y) \). The function \( f \) is said to be **strictly convex** if \( \leq \) is replaced by \( < \) above.

We say that \( f \) is (strictly) **concave** if \(-f\) is (strictly) convex. A linear function is both convex and concave. A similar definition applies if \( x \) is replaced by a vector or matrix.

A vector convex function is defined along the same lines. We say that \( f \) is **convex** if

\[
f(\alpha x + (1 - \alpha)y) \leq \alpha f(x) + (1 - \alpha)f(y)
\]

for every \( \alpha \) such that \( 0 \leq \alpha \leq 1 \) and \( x, y \in \mathbb{R}^n \); \( f \) is **concave** if \(-f\) is convex. Here \( a \preceq b \) means \( a_i \leq b_i \) for all \( i \).
The following functions are convex.

(a) \(-\log x \ (x > 0)\).
(b) \(x^p, \ p > 1 \ (x > 0)\).

They can be used to establish a number of well-known inequalities (e.g., Horn and Johnson [1985: 535–536]).

The function

\[ f(A) = \log \det A \]

is a strictly concave function on the convex set of Hermitian positive definite matrices.

Every convex and every concave function is continuous on its interior. However, a convex function may have a discontinuity at a boundary point and may not be differentiable at an interior point.

Every increasing convex (respectively concave) function of a convex (respectively concave) function is convex (respectively concave). Every strictly increasing convex (respectively concave) function of a strictly convex (respectively concave) function is strictly convex (respectively concave).

(Weirstrass's Theorem) Let \( S \) be a compact subset of a real or complex vector space. If \( f : S \rightarrow \mathbb{R} \) is a continuous function, then there exist points \( x_{\min}, x_{\max} \in S \) such that

\[ f(x_{\min}) \leq f(x) \leq f(x_{\max}) \quad \text{for all } x \in S. \]

**Definition 2.31.** The numerical range (field of values) of an \( n \times n \) complex matrix \( A \) is

\[ \{ x^*Ax : \|x\| = 1, x \in \mathbb{C}^n \}. \]

(Toeplitz–Hausdorff) The numerical range of an \( n \times n \) complex matrix is a convex compact subset of \( \mathbb{C}^n \). For further properties of a field of values see Gustafson and Rao [1997] and Horn and Johnson [1991].
2.6 COORDINATE GEOMETRY

Occasionally one may need some results from coordinate geometry. Some of these are listed below for easy reference.

2.6.1 Hyperplanes and Lines

2.74. The equation of a hyperplane passing through the points \( x_1, x_2, \ldots, x_n \) in \( \mathbb{R}^n \) can be expressed in the form

\[
\det \begin{pmatrix}
1 & 1 & 1 & \cdots & 1 \\
x & x_1 & x_2 & \cdots & x_n
\end{pmatrix} = 0.
\]

2.75. Given the points \( x_1 = (a_1, b_1, c_1)' \) and \( x_2 = (a_2, b_2, c_2)' \) in \( \mathbb{R}^3 \), then the equation of the line through the points is

\[
\frac{x - a_1}{a_1 - a_2} = \frac{y - b_1}{b_1 - b_2} = \frac{z - c_1}{c_1 - c_2}.
\]

If the two points are \( A \) and \( B \), then \( a_1 - a_2 = AB \cos \theta_1 \), and so on, so that we can replace the denominators of the above line by the direction cosines \( \cos \theta_i \) of the line with respect to each axis. Then \( \cos \theta_1^2 + \cos \theta_2^2 + \cos \theta_3^2 = 1 \). This result clearly generalizes to two points in \( \mathbb{R}^n \).

2.76. Given the plane \( ax + by + cz + d = 0 \) in \( \mathbb{R}^3 \), a normal vector to the plane is given by \( (a, b, c)' \), and the perpendicular distance of the point \( x_1 = (x_1, y_1, z_1)' \) from the plane is

\[
\frac{|ax_1 + by_1 + cz_1 + d|}{\sqrt{a^2 + b^2 + c^2}}.
\]

This result clearly generalises to \( \mathbb{R}^n \). Given the plane \( a'x + d = 0 \), the distance of \( x_1 \) from the plane is \( (a'x_1 + d)/\|a\|_2 \).

2.77. Given \( 0 < \alpha < 1 \), then \( z = (1 - \alpha)x + \alpha y \) divides the line segment joining \( x \) and \( y \) in the proportion \( \alpha : (1 - \alpha) \).

Proofs. Section 2.6.1.

2.77. Abadir and Magnus [2005: 6].

2.6.2 Quadratics

2.78. If \( A \) is an \( n \times n \) symmetric indefinite matrix (i.e., has both positive and negative eigenvalues), then \( (x - a)'A(x - a) \leq c \) with \( c > 0 \) is a hyperboloid with center \( a \).

2.79. If \( A \) is an \( n \times n \) positive definite matrix, then \( (x - a)'A(x - a) \leq c \) with \( c > 0 \) is an ellipsoid with center \( a \). By shifting the origin to \( a \) and rotating the ellipsoid, the latter can be expressed in a standard form \( \sum_{i=1}^n \lambda_i z_i^2 \leq c \) with \( \lambda_i > 0 \) \((i = 1, 2, \ldots, n)\), where the \( \lambda_i \) are the eigenvalues of \( A \). Setting all the \( z_i \)'s equal to
zero except $z_j$, we see that the lengths of the semi-major axes are $b_j = \sqrt{c/\lambda_j}$ for $j = 1, 2, \ldots, n$, and the volume of the ellipsoid is

$$v = \frac{\pi^{n/2}}{\Gamma(\frac{n}{2} + 1)} \prod_{j=1}^{n} b_j = \frac{\pi^{n/2} c^{n/2}}{\Gamma(\frac{n}{2} + 1)(\det A)^{1/2}},$$

by (6.17c). Such a volume arises in finding the constant associated with various elliptical multivariate distributions such as the multivariate normal and the multivariate $t$-distributions (cf. Chapter 20).

2.80. (Quadrics) If $x \in \mathbb{R}^n$, then a general quadric is $Q = 0$, where $Q = x'Ax + 2b'x + c$ and $A$ is an $n \times n$ symmetric matrix. Let $x_1$ and $x_2$ be two points in $\mathbb{R}^n$ that we denote by $P_1$ and $P_2$, respectively. From (2.77), the coordinates of the point $P$ dividing the line $P_1P_2$ in the ratio $\mu : 1$ is given by $(1 + \mu)^{-1}(x_1 + \mu x_2)$. Let $Q_{ij} = x'_iAx_j + b'_i x_i + b'_j x_j + c$.

(a) Substituting for $P$ we find that $P$ lies on the quadric if

$$\mu^2 Q_{22} + 2\mu Q_{12} + Q_{11} = 0.$$

This is a quadratic in $\mu$ so that an arbitrary line meets a quadric in two points.

(b) (Tangent Plane) If $P_1$ lies on $Q = 0$, then $Q_{11} = 0$ and one root $\mu$ is zero. If $P_1P_2$ is a tangent, then the other root must also be zero; that is, the sum of the roots is zero and $Q_{12} = 0$. As $P_2$ varies subject to $Q_{12} = 0$, $P_2$ lies on $Q_1 = 0$, so that

$$x'_1Ax + b'(x_1 + x) + c = 0,$$

is the tangent plane at $x_1$.

(c) (Tangent Cone) Suppose $P_1$ and $P_2$ are not on $Q = 0$, but $P_1P_2$ touches the quadric so that the equation in $\mu$ has equal roots, i.e., $Q_{11}Q_{22} = Q_{12}^2$. Therefore as $P_2$ varies subject to this condition, we trace out the tangent cone from $P_1$, namely,

$$Q_{11}Q = Q_1^2.$$

(d) (Envelope) Suppose $Q = x'Ax - 1 = 0$, where $A$ is nonsingular, is a central quadric (i.e., $b = 0$). Then using (c), $a'x = 1$ touches the quadric if $a'A^{-1}a = 1$. As $a$ varies, $a'A^{-1}a = 1$ is the envelope equation.

2.6.3 Areas and Volumes

2.81. In two dimensions the area of a triangle with vertices $(x_i, y_i)'$, $i = 1, 2, 3$ is $\frac{1}{2} |\Delta|$, where

$$\Delta = \det \begin{pmatrix} 1 & x_1 & y_1 \\ 1 & x_2 & y_2 \\ 1 & x_3 & y_3 \end{pmatrix}.$$

The three points are collinear if and only if $\Delta = 0$. 
2.82. If \( V = (v_1, v_2, \ldots, v_p) \), where the \( v_i \) are vectors in \( \mathbb{R}^n \), then the square of the two-dimensional volume of the parallelootope with \( v_1, \ldots, v_p \) as principal edges is \( \det(V'V) \). A 2-dimensional parallelootope is a parallelogram; in this case we get the square of the area. When \( p = 3 \) we have the conventional parallelopiped. For statistical applications see Anderson [2003: section 7.5].

2.83. From (2.74), the four points \((x_i, y_i, z_i)', i = 1, 2, 3, 4, \) in three dimensions are coplanar if and only if

\[
\det \begin{pmatrix}
1 & 1 & 1 & 1 \\
x_1 & x_2 & x_3 & x_4 \\
y_1 & y_2 & y_3 & y_4 \\
z_1 & z_2 & z_3 & z_4
\end{pmatrix} = 0.
\]

Proofs. Section 2.6.3.

2.81. Cullen [1997: 121].

2.82. Anderson [2003: 266]. For the area of a parallelogram see Basilevsky [1983: 64].
CHAPTER 3

RANK

The concept of rank undergirds much of matrix theory. In statistics it is frequently linked to the concept of degrees of freedom. Both equalities and inequalities are considered in this chapter, and partitioned matrices play an important role.

3.1 SOME GENERAL PROPERTIES

All the matrices in this section are defined over a general field $\mathcal{F}$, unless otherwise stated.

**Definition 3.1.** The rank, denoted by $\text{rank} \ A$ ( = $r$, say), of a matrix $A$ is $\dim \mathcal{C}(A)$, the dimension of the column space of $A$. Here $r$ is also called the *column rank* of $A$. The *row rank* is $\dim \mathcal{C}(A')$. If $A$ is $m \times n$ of rank $m$ (respectively $n$), then $A$ is said to have full *row* (respectively *column*) rank. An $n \times n$ matrix $A$ is said to be *nonsingular* if $\text{rank} \ A = n$.

As noted in Section 2.2.4, an associated vector space of $\mathcal{C}(A)$ is the null space $\mathcal{N}(A)$, and its dimension is called the *nullity*.

3.1. $\text{rank} \ A' = \text{rank} \ A = r$ so that the row rank equals the column rank.

3.2. Let $A$ be an $m \times n$ matrix of rank $r$ ($r \leq \min \{m, n\}$).

(a) $A$ has $r$ linearly independent columns and $r$ linearly independent rows.

(b) There exists an $r \times r$ nonzero principal minor. When $r < \min \{m, n\}$, all principal minors of larger order than $r$ are zero.
(c) If \( B \) is \( m \times p \) and \( C(B) \subseteq C(A) \), then \( \text{rank} B \leq \text{rank} A \).

3.3. Let \( A \) be an \( m \times n \) matrix over \( \mathbb{F} \).

(a) \( \text{rank} A + \text{nullity} A = \text{number of columns of } A \).

(b) Suppose \( A \) is real, then
\[
\text{rank}(A'A) = \text{rank}(AA') = \text{rank} A.
\]

(c) Suppose \( A \) is complex, then:

(i) \( \text{rank} A = \text{rank} \bar{A} \).

(ii) Since \( \text{rank} \bar{A} = \text{rank} A' \) by (3.1), we have \( \text{rank} A = \text{rank} A^* \).

(iii) \( \text{rank} A = \text{rank}(AA^*) = \text{rank}(A^*A) \).

Thus, combining the above,
\[
\text{rank} A = \text{rank} \bar{A} = \text{rank} A^* = \text{rank}(AA^*) = \text{rank}(A^*A).
\]

(d) If \( A \) is complex, it is not necessarily true that \( \text{rank} A'A = \text{rank} A \).

3.4. We consider two special cases of rank.

(a) If \( \text{rank} A = 0 \), then \( A = 0 \). This is a simple but key result that can be used to prove the equality of two matrices.

(b) If \( \text{rank} A = 1 \), then there exist nonzero \( a \) and \( b \) such that \( A = ab' \).

3.5. (Full-Rank Factorization) Any \( m \times n \) real or complex matrix \( A \) of rank \( r \) \((r > 0)\) can be expressed in the form \( A_{m \times n} = C_{m \times r}R_{r \times n} \), where \( C \) and \( R \) have (full) rank \( r \). We call this a full-rank factorization. The columns of \( C \) may be an arbitrary basis of \( C(A) \), and then \( R \) is uniquely determined, or else the rows of \( R \) may be an arbitrary basis of \( C(A') \), and then \( C \) is uniquely determined. Note that \( C \) has a left inverse, namely \((C'C)^{-1}C'\), and \( R \) has a right inverse, \( R'(RR')^{-1} \). Two full-rank factorizations can be obtained from the singular value decomposition of \( A \) (cf. 16.34e).

3.6. If \( A \) and \( B \) are \( m \times n \) matrices, then \( \text{rank} A = \text{rank} B \) if and only if there exist a nonsingular \( m \times m \) matrix \( C \) and an \( n \times n \) nonsingular matrix \( D \) such that \( A = CBD \).

3.7. If \( C(B) = C(C) \), then \( \text{rank}(AB) = \text{rank}(AC) \) for all \( A \).

3.8. If \( V \) is Hermitian non-negative definite, then \( V = RR^* \) (by 10.10) and \( \text{rank}(AV) = \text{rank}(AR) \) for all \( A \).

Proofs. Section 3.1.


3.2. (a) and (c) follow from the definition; for (b) see Meyer [2000a: 215].

3.3a. Follows from (2.37) and (c)(ii) below. See also Seber and Lee [2003: 458].
3.3c(i). Rao and Bhimasankaram [2000: 145].
3.3c(iii). Ben-Israel and Greville [2003: 46] and Meyer [2000a: 212].
3.3d. For a counter example consider \( A = (1, i)'(1, 1) \).
3.4b. Abadir and Magnus [2005: 80].
3.5. Ben-Israel and Greville [2003: 26], Marsaglia and Styan [1974a: theorem 1], and Searle [1982: 175].
3.6. If \( \text{rank } A = \text{rank } B = r \), then by (16.33a) \( A \) and \( B \) are equivalent to the same diagonal matrix. The converse follows from (3.14a).
3.7. Follows from \( C(AB) = C(AC) \).
3.8. By (10.10), \( V = RR^* \) and from (2.35) we have \( C(V) = C(R) \). The result follows from (3.7).

### 3.2 MATRIX PRODUCTS

All the matrices in this section are real or complex.

3.9. Given conformable matrices \( A \) and \( B \), we have the following.

(a) \( \text{rank } (BA) = \text{rank } A \) if \( B \) has full row rank.

(b) \( \text{rank } (AC) = \text{rank } A \) if \( C \) has full column rank.

(c) \( \text{rank } (A'AB) = \text{rank } (AB) = \text{rank } (ABB') \).

3.10. Let \( A \) and \( B \) be \( m \times n \) and \( n \times p \) matrices, respectively. Then:

(a) \( \text{rank } (AB) = \text{rank } B - \dim \{ \mathcal{N}(A) \} \cap \mathcal{C}(B) \} \).

(b) \( \text{rank } (AB) = \text{rank } A - \dim \{ \mathcal{C}(A') \cap \mathcal{N}(B) \} \).

The above results immediately give us conditions for \( \text{rank } (AB) = \text{rank } A \) and \( \text{rank } (AB) = \text{rank } B \). Other conditions are given in (3.13c) and (3.13d) below.

3.11. Let \( A \) be a square matrix. If \( \text{rank } (A^m) = \text{rank } (A^{m+1}) \), then \( \text{rank } (A^m) = \text{rank } (A^n) \) for all \( n \geq m \).

3.12. \( \text{rank } (AB) \leq \min \{ \text{rank } A, \text{rank } B \} \).

3.13. Let \( A \) have \( n \) columns and \( B \) have \( n \) rows. Let \( A^- \) and \( B^- \) be any weak inverses of \( A \) and \( B \), respectively. Then:

\[
\text{rank} \left( \begin{array}{cc} 0 & A \\ B & I_n \end{array} \right) = \text{rank } A + \text{rank } (B, I_n - A^- A)
\]
\[
= \text{rank } \left( \begin{array}{c} A \\ I_n - BB^- \end{array} \right) + \text{rank } B
\]
\[
= \text{rank } A + \text{rank } B + \text{rank } [(I_n - BB^-)(I_n - A^- A)]
\]
\[
= n + \text{rank } (AB).
\]
We can deduce the following.

(a) \( \text{rank}(B, I_n - A^{-1}A) = \text{rank} B + \text{rank} [(I_n - BB^{-})(I_n - A^{-1}A)] \).

(b) \( \text{rank} \left( \begin{bmatrix} A & \mathbf{0} \\ I_n - BB^{-} \end{bmatrix} \right) = \text{rank} A + \text{rank} [(I_n - BB^{-})(I_n - A^{-1}A)] \).

(c) \( \text{rank}(AB) = \text{rank} A \) if and only if \( (B, I_n - A^{-1}A) \) has full row rank \( n \).

(d) \( \text{rank}(AB) = \text{rank} B \) if and only if \( (I_n \cdot A^{-1}A) \) has full column rank \( n \).

(e) (Sylvester)
\[
\text{rank}(AB) \geq \text{rank} A + \text{rank} B - n,
\]
with equality if and only if \( (I_n - BB^{-})(I_n - A^{-1}A) = 0 \). This result also follows from the Frobenius inequality (3.18b) by setting \( B = I_n \).

If \( AB = 0 \), \( \text{rank} A + \text{rank} B \leq n \).


(a) If \( P \) and \( Q \) are any conformable nonsingular matrices,
\[
\text{rank}(PAQ) = \text{rank} A.
\]

(b) If \( C \) has full column rank and \( R \) has full row rank, then
\[
\text{rank} A = \text{rank}(CA) = \text{rank}(AR).
\]

3.15. If \( A \) is \( p \times q \) of rank \( q \) and \( B \) is \( q \times r \) of rank \( r \), then \( AB \) is \( p \times r \) of rank \( r \).

3.16. If \( \text{rank}(AB) = \text{rank} A \), then \( C(AB) = C(A) \).

3.17. Suppose that the following products of matrices exist. Then:

(a) \( \text{rank}(XA) = \text{rank} A \) implies \( \text{rank}(XAF) = \text{rank}(AF) \) for every \( F \).

(b) \( \text{rank}(AY) = \text{rank} A \) implies \( \text{rank}(KAY) = \text{rank}(KA) \) for every \( K \).

3.18. Let \( A, B, \) and \( C \) be conformable matrices, and let \( (AB)^{-} \) and \( (BC)^{-} \) be any weak inverses. Then:

(a)
\[
\text{rank} \left( \begin{bmatrix} \mathbf{0} & AB \\ BC & B \end{bmatrix} \right) = \text{rank}(AB) + \text{rank}(BC) + \text{rank} L
\]
\[
= \text{rank} B + \text{rank}(ABC),
\]
where \( L = [I - BC(BC)^{-}]B[I - (AB)^{-}(AB)]. \)

(b) (Frobenius Inequality) From (a) we have
\[
\text{rank}(ABC) \geq \text{rank}(AB) + \text{rank}(BC) - \text{rank} B,
\]
with equality if and only if \( L = 0 \).
3.19. Let $V$ be a non-negative definite $n \times n$ matrix, and let $X$ be an $n \times p$ matrix. Then the following statements are equivalent.

1. $\text{rank}(X'VX) = \text{rank} X$.
2. $\text{rank}(X'V^+X) = \text{rank} X$, where $V^+$ is the Moore–Penrose inverse of $V$.
3. $C(X'VX) = C(X')$.
4. $C(X) \cap [C(V)]^\perp = \mathbf{0}$.

Also $\text{rank}(X'VX) = p$ if and only if $\text{rank} X = p$ and $C(X) \cap [C(V)]^\perp = \mathbf{0}$.

**Proofs.** Section 3.2.

3.9. Abadir and Magnus [2005: 82, 85].


3.11. Meyer [2000a: 394] and Ben-Israel and Greville [2003: 155]; see also Section 3.8.


3.14a. By (3.12), $\text{rank} A = \text{rank}(P^{-1}PA) \leq \text{rank}(PA) \leq \text{rank} A$.


3.15. Let $ABx = 0$. Then using (3.5), we can take a left inverse of $A$ and then a left inverse of $B$ to get $x = 0$ so that the columns of $AB$ are linearly independent.


### 3.3 MATRIX CANCELLATION RULES

3.20. Let $A$ be any $m \times n$ matrix over $\mathbb{F}$.

(a) If $C$ has full column rank and $R$ has full row rank, then using left and right inverses, respectively, we have that $CA = CB$ implies $A = B$ and $PR = QR$ implies $P = Q$.

(b) If $\text{rank}(XA) = \text{rank} A$, then $XAG = XAH$ implies $AG = AH$.

(c) If $\text{rank}(AY) = \text{rank} A$, then $LAY = MAY$ implies $LA = MA$. 
3.21. The following are useful for deriving some cancellation rules when the real or complex matrix $A$ can be a function of other matrices.

(a) $A^*A = 0$ implies that $A = 0$.

(b) $\text{trace}(A^*A) = 0$ implies that $A = 0$.

We can interchange $A$ and $A^*$.

3.22. For real or complex matrices we have the following results.

(a) If $PX^* = QXX^*$, then from (3.21a) above and

$$\left(PXX^* - QXX^*\right)(P^* - Q^*) \equiv (PX - QX)(PX - QX)^*,$$

we have $PX = QX$. We can also replace $X$ by $X^*$.

(b) $X^*XAYY^* = 0$ implies $XAY = 0$. Special cases follow by setting $X$ or $Y$ equal to the identity matrix.

(c) $A'AB = A'C$ if and only if $AB = AA^+C$, where $A^+$ is the Moore–Penrose inverse of $A$.

Proofs. Section 3.3


3.22b. Use (3.21b) and $\text{trace}[(XAY)(XAY)^*] = \text{trace}(X^*XAYY^*A^*) = 0$.

3.22c. Magnus and Neudecker [1999: 34].

3.4 MATRIX SUMS

3.23. Let $A$ and $B$ be any $m \times n$ matrices over $\mathcal{F}$, and let $(A, B)^-$ and $(A_B)^-$ be any weak inverses. Define

$$M = \left[I_{2m} - \begin{pmatrix} A & 0 \\ B & 0 \end{pmatrix} \begin{pmatrix} A_B & 0 \\ B & 0 \end{pmatrix}^{-1} \right] \begin{pmatrix} A & 0 \\ B & 0 \end{pmatrix} \left[I_{2n} - (A, B)^-(A, B) \right].$$

(a) From (2.11c), taking transposes and noting that rank $C = \text{rank} C'$ for any $C$, we have the following results.

$$\dim[C(A) \cap C(B)] = \text{rank} A + \text{rank} B - \text{rank}(A, B) \ (= c \ \text{say}),$$

$$\dim[C(A') \cap C(B')] = \text{rank} A + \text{rank} B - \text{rank} \begin{pmatrix} A \\ B \end{pmatrix} \ (= d \ \text{say}).$$

(b) $0 \leq \text{rank} M \leq \min\{c, d\}$. Hence $c = 0$ or $d = 0$ implies $M = 0$. 
(c) \[
\begin{bmatrix}
0 & A & B \\
A & A & 0 \\
B & 0 & B
\end{bmatrix}
\] 
\[
= \text{rank}(A, B) + \text{rank}\left(\begin{bmatrix}
A \\
B
\end{bmatrix}\right) + \text{rank} M \\
= \text{rank} A + \text{rank} B + \text{rank}(A + B).
\]

From the above we have the following:

(i) \(\text{rank}(A, B) + \text{rank}\left(\begin{bmatrix}
A \\
B
\end{bmatrix}\right) + \text{rank} M = \text{rank} A + \text{rank} B + \text{rank}(A + B)\).

(ii) \(\text{rank} A + \text{rank} B - c - d \leq \text{rank}(A + B) \leq \text{rank} A + \text{rank} B - \max\{c, d\}\). Equality on the left occurs if and only if \(M = 0\), and equality on the right occurs if and only if \(\text{rank} M = \min\{c, d\}\).

(iii) \(\text{rank}(A + B) \geq \text{rank}(A, B) + \text{rank}\left(\begin{bmatrix}
A \\
B
\end{bmatrix}\right) - \text{rank} A - \text{rank} B\), with equality if and only if \(M = 0\).

(d) The following hold for any \(A\) and \(B\) of the same size.

(i) \(\text{rank}(A + B) \leq \text{rank}(A, B) \leq \text{rank} A + \text{rank} B\).

(ii) \(\text{rank}(A + B) \leq \text{rank}\left(\begin{bmatrix}
A \\
B
\end{bmatrix}\right) \leq \text{rank} A + \text{rank} B\).

(e) From the above:

(i) \(\text{rank}(A + B) = \text{rank}(A, B)\) if and only if \(d = \text{rank} M\).

(ii) \(\text{rank}(A + B) = \text{rank}\left(\begin{bmatrix}
A \\
B
\end{bmatrix}\right)\) if and only if \(c = \text{rank} M\).

(iii) \(\text{rank}(A, B) = \text{rank} A + \text{rank} B\) if and only if \(c = 0\). When \(c = 0\), \(M = 0\) and \(\text{rank} M = 0 = c\) so that \(\text{rank}(A + B) = \text{rank}\left(\begin{bmatrix}
A \\
B
\end{bmatrix}\right)\).

(iv) \(\text{rank}\left(\begin{bmatrix}
A \\
B
\end{bmatrix}\right) = \text{rank} A + \text{rank} B\) if and only if \(d = 0\). When \(d = 0\), \(M = 0\) and \(\text{rank} M = 0 = d\) so that \(\text{rank}(A + B) = \text{rank}(A, B)\).

(v) \(\text{rank}(A + B) = \text{rank} A + \text{rank} B\) if and only if \(c = d = 0\).

3.24. If \(A\) and \(B\) are \(n \times n\) matrices over \(F\), then, since \(AB - I_n = (A - I_n)B + B - I_n\), we have from (3.23e(iii)) and (3.12) that \(\text{rank}(AB - I_n) \leq \text{rank}(A - I_n) + \text{rank}(B - I_n)\).

**Definition 3.2.** Suppose that \(A = \sum_{i=1}^{k} A_i\), where each matrix is \(m \times n\). We say that we have rank additivity if \(\text{rank} A = \sum_{i=1}^{k} \text{rank} A_i\).

3.25. Let \(A\) and \(B\) be nonnull \(m \times n\) matrices over \(F\) with respective ranks \(r\) and \(s\). If any one of the following conditions hold, then they all hold.

(1) \(\text{rank}(A + B) = \text{rank} A + \text{rank} B\) (i.e., rank additivity).
(2) There exist nonsingular matrices $\mathbf{F}$ and $\mathbf{G}$ such that

$$
\mathbf{A} = \mathbf{F} \begin{pmatrix}
\mathbf{I}_r & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & 0
\end{pmatrix} \mathbf{G} \quad \text{and} \quad \mathbf{B} = \mathbf{F} \begin{pmatrix}
0 & 0 & 0 \\
0 & \mathbf{I}_s & 0 \\
0 & 0 & 0
\end{pmatrix} \mathbf{G}.
$$

The above matrices are partitioned in the same way, and the bordering zero matrices are of appropriate size; some of the latter matrices are absent if $\mathbf{A} + \mathbf{B}$ has full rank.

(3) $\dim[\mathcal{C}(\mathbf{A}) \cap \mathcal{C}(\mathbf{B})] = \dim[\mathcal{C}(\mathbf{A}') \cap \mathcal{C}(\mathbf{B}')] = 0$; that is, $c = d = 0$ in (3.23a).

(4) $\text{rank}(\mathbf{A}, \mathbf{B}) = \text{rank} \left( \begin{pmatrix} \mathbf{A} \\ \mathbf{B} \end{pmatrix} \right) = \text{rank} \mathbf{A} + \text{rank} \mathbf{B}$.

(5) $\begin{pmatrix} \mathbf{A} \\ \mathbf{B} \end{pmatrix} (\mathbf{A} + \mathbf{B})^{-}(\mathbf{A}, \mathbf{B}) = \begin{pmatrix} \mathbf{A} & 0 \\ 0 & \mathbf{B} \end{pmatrix}$.

(6) $\text{rank} \mathbf{A} = \text{rank}[[\mathbf{A}(\mathbf{I}_n - \mathbf{B}^{-}\mathbf{B})]] = \text{rank}[[\mathbf{I}_m - \mathbf{BB}^{-}]\mathbf{A}]$.

(7) $\text{rank} \mathbf{B} = \text{rank}[[\mathbf{B}(\mathbf{I}_n - \mathbf{A}^{-}\mathbf{A})]] = \text{rank}[[\mathbf{I}_m - \mathbf{AA}^{-}]\mathbf{B}]$.

(8) $\text{rank} \mathbf{A} = \text{rank}[[\mathbf{A}(\mathbf{I}_n - \mathbf{B}^{-}\mathbf{B})]]$ and $\text{rank} \mathbf{B} = \text{rank}[[\mathbf{I}_m - \mathbf{AA}^{-}]\mathbf{B}]$.

(9) $\text{rank} \mathbf{A} = \text{rank}[[\mathbf{I}_m - \mathbf{BB}^{-}]\mathbf{A}]$ and $\text{rank} \mathbf{B} = \text{rank}[[\mathbf{B}(\mathbf{I}_n - \mathbf{A}^{-}\mathbf{A})]]$.

Here $\mathbf{A}^{-}, \mathbf{B}^{-}$, and $(\mathbf{A} + \mathbf{B})^{-}$ are any choices of weak inverses. If any one of (5) to (9) hold for a particular pair of weak inverses, then they hold for any pair.

3.26. Suppose that $\mathbf{A} = \sum_{i=1}^{k} \mathbf{A}_i$, where matrices are all $m \times n$ over $\mathcal{F}$. We now give a number of results about rank additivity. As idempotent matrices play a role in this theory, the reader should also refer to Section 8.6.1.

(a) The following three conditions are equivalent.

(1) We have rank additivity.

(2) $\text{rank}(\mathbf{A}_1, \mathbf{A}_2, \ldots, \mathbf{A}_k) = \text{rank} \begin{pmatrix}
\mathbf{A}_1 \\
\mathbf{A}_2 \\
\vdots \\
\mathbf{A}_k
\end{pmatrix} = \sum_{i=1}^{k} \text{rank} \mathbf{A}_i$.

(3) $\mathbf{A}_i \mathbf{A}^{-} \mathbf{A}_i = \mathbf{A}_i$ and $\mathbf{A}_i \mathbf{A}^{-} \mathbf{A}_j = \mathbf{0}$ for all $i, j$ ($i \neq j$) where $\mathbf{A}^{-}$ is any choice of a weak inverse of $\mathbf{A}$.

If (3) holds for a particular weak inverse, then all three conditions hold for any weak inverse.

(b) Suppose $\mathbf{A}$ is idempotent (i.e., $\mathbf{A}^2 = \mathbf{A}$). Then the following three conditions are equivalent.

(1) We have rank additivity.

(2) $\text{rank}(\mathbf{A}_1, \mathbf{A}_2, \ldots, \mathbf{A}_k) = \text{rank} \begin{pmatrix}
\mathbf{A}_1 \\
\mathbf{A}_2 \\
\vdots \\
\mathbf{A}_k
\end{pmatrix} = \sum_{i=1}^{k} \text{rank} \mathbf{A}_i$. 


(3) \(A_i^2 = A_i\) and \(A_iA_j = 0\) for all \(i, j (i \neq j)\).

(c) If \(r_i = \text{rank } A_i\) \((i = 1, 2, \ldots, k)\), we have rank additivity if and only if there are nonsingular matrices \(F\) and \(G\) such that

\[
\begin{pmatrix}
I_{r_1} & 0 & \ldots & 0 & 0 \\
0 & 0 & \ldots & 0 & 0 \\
0 & 0 & \ldots & 0 & 0 \\
0 & 0 & \ldots & 0 & 0 \\
0 & 0 & \ldots & 0 & 0 \\
\end{pmatrix} = F \begin{pmatrix} A_1 \\ \vdots \\ A_k \end{pmatrix} G,
\]

Furthermore, if the \(A_i\) are real (respectively complex), there exist orthogonal (respectively unitary) \(P\) and \(Q\) and diagonal \(D\) such that \(F = PD\) and \(G = Q\), that is there exists a simultaneous singular value decomposition.

3.27. Let \(A = \sum_{i=1}^{k} A_i\), where the matrices are real (or complex with \('\) replaced by \(\ast\)).

(a) We assume that the matrices are not necessarily square.

(i) If \(A_i' A_j = 0\) and \(A_i A_j' = 0\) for all \(i, j (i \neq j)\), then the rank is additive.

(ii) If the rank is additive, then \(A_i A_j' = 0\) for all \(i, j (i \neq j)\) if and only if \(A_j A_j' = A A_j' (j = 1, \ldots, k)\).

(b) We assume that the matrices are square.

(i) If \(\text{rank}(A_i^2) = \text{rank } A_i\) and \(A_i A_j = 0\) for all \(i, j (i \neq j)\), then the rank is additive.

(ii) If the rank is additive, then \(A_i A_j = 0\) for all \(i, j (i \neq j)\) if and only if \(A_j A_j = A A_j (j = 1, \ldots, k)\).

(c) If the \(A_i\) are all real symmetric or Hermitian non-negative definite matrices and

\[
(\sum_{i=1}^{k} c_i A_i) A = (\sum_{j=1}^{k} A_j / c_j) A
\]

holds for some distinct positive scalars \(c_i\) and for some choice of weak inverse \(A^{-}\), then the rank is additive.
Conversely, if the rank is additive, then the above equation holds for every choice of distinct positive $c_1, \ldots, c_k$ and for every choice of a weak inverse.

**Proofs.** Section 3.4.


3.25. Marsaglia and Styan [1974a: theorem 11]; see also Harville [1997: 445] for (3) and Harville [2001: 29, exercise 29] for (4) and (6)–(9).


3.26b. Marsaglia and Styan [1974a: corollary 13.1]. Note that $AAA = A$ so that we can set $A^- = A$ in (a).


3.27b. Marsaglia and Styan [1974a: theorem 15].

3.26c. Marsaglia and Styan [1974a: theorem 16].

### 3.5 MATRIX DIFFERENCES

3.28. $\text{rank}(A - B) \geq |\text{rank } A - \text{rank } B|$. 

3.29. Let $A$ and $B$ be $m \times n$ matrices over $\mathcal{F}$. Then results on the rank of $A + B$ immediately lead to the results on the rank of $A - B$ by simply substituting $-B$ for $B$. We can also use the fact that $\text{rank}(A - B) = \text{rank } A - \text{rank } B$ if and only if $\text{rank}(A - B) + \text{rank } B = \text{rank } A$.

(a) Let

$$N = \begin{bmatrix} I_{2m} - \begin{pmatrix} A & 0 \\ B & -B \end{pmatrix} \end{bmatrix} \begin{pmatrix} A & 0 \\ 0 & -B \end{pmatrix} \begin{bmatrix} I_{2n} - (A, B)^-(A, B) \end{bmatrix}.$$ 

Then

$$\text{rank}(A - B) = \text{rank}(A, B) + \text{rank} \begin{pmatrix} A \\ B \end{pmatrix} + \text{rank } N - \text{rank } A - \text{rank } B.$$

(b) $\text{rank}(A - B) = \text{rank } A - \text{rank } B$ if and only if $N = 0$ and $\text{rank}(A, B) = \text{rank } A = \text{rank} \begin{pmatrix} A \\ B \end{pmatrix}$. Furthermore, if just the latter equation is true, then

$$\text{rank } N = \text{rank}(BA^-B - B).$$

3.30. Let $A$ and $B$ be $m \times n$ matrices over $\mathcal{F}$. If one of the following five conditions is true, then all five are true.

1. $\text{rank}(A - B) = \text{rank } A - \text{rank } B$. 

(2) $\mathcal{C}(B) \subset \mathcal{C}(A), \mathcal{C}(B') \subset \mathcal{C}(A')$ and $BA^-B = B$.

(3) $\operatorname{rank}(A, B) = \operatorname{rank} A = \operatorname{rank} \left( \frac{A}{B} \right)$ and $BA^-B = B$.

(4) $AA^-B = BA^-A = BA^-B = B$.

(5) $\operatorname{rank}(A - B) = \operatorname{rank}[(A(I_n - B^-B))] = \operatorname{rank}[(I_m - BB^-)A]$, where $A^-$ and $B^-$ are any choices of weak inverses. If any one of (2) to (5) holds for any particular set of weak inverses, then all the conditions hold for every weak inverse.

3.31. Let $A$ and $B$ be $m \times n$ matrices over $\mathcal{F}$ with ranks $r$ and $s$, respectively. Then:

(a) $\operatorname{rank}(A - B) = \operatorname{rank} A - \operatorname{rank} B$ if and only if there exist nonsingular matrices $F$ and $G$ such that

$$
A = F \begin{pmatrix}
I_s & 0 & 0 \\
0 & I_{r-s} & 0 \\
0 & 0 & 0
\end{pmatrix} G \quad \text{and} \quad B = F \begin{pmatrix}
I_s & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & 0
\end{pmatrix} G,
$$

where the matrices are similarly partitioned and the bordering zero matrices are of appropriate size; some are absent if $A$ or $B$ has full rank.

(b) If $A$ and $B$ are real (complex) matrices, there exist orthogonal (unitary) matrices $P$ and $Q$ such that

$$
A = P \begin{pmatrix}
D_1 & 0 & 0 \\
0 & D_2 & 0 \\
0 & 0 & 0
\end{pmatrix} Q \quad \text{and} \quad B = P \begin{pmatrix}
0 & 0 & 0 \\
0 & D_2 & 0 \\
0 & 0 & 0
\end{pmatrix} Q,
$$

where $D_1$ and $D_2$ are nonsingular diagonal matrices.

3.32. If $A$ and $B$ are nonsingular $n \times n$ matrices, then from the identity $A - B = -B(A^{-1} - B^{-1})A$ and (3.14a),

$$
\operatorname{rank}(A^{-1} - B^{-1}) = \operatorname{rank}(A - B) = \operatorname{rank}(B - A).
$$

Furthermore, $A^{-1} - B^{-1}$ is nonsingular if and only if $B - A$ is nonsingular.

3.33. (Wedderburn–Guttman) Let $A$ be an $m \times n$ matrix of rank $r$, and let $M$ and $N$ be $m \times s$ and $n \times s$ matrices, respectively, such that $M'AN$ is nonsingular. Then

$$
\operatorname{rank}[A - N(M'AN)^{-1}M'A] = r - s,
$$

with

$$
\operatorname{rank}[AN(M'AN)^{-1}M'A] = \operatorname{rank}[M'AN] = s.
$$

This theorem has been used in psychometrics.

3.34. (Idempotent Matrices) Let $P$ and $Q$ be $n \times n$ idempotent matrices. Then

$$
\operatorname{rank}(P - Q) = \operatorname{rank} \left( \frac{P}{Q} \right) + \operatorname{rank}(P, Q) - \operatorname{rank} P - \operatorname{rank} Q
$$

$$
= \operatorname{rank}(P - PQ) + \operatorname{rank}(PQ - Q)
$$

$$
= \operatorname{rank}(P - QP) + \operatorname{rank}(QP - Q).$$
Proofs. Section 3.5.

3.28. Abadir and Magnus [2005: 81].


3.31. Marsaglia and Styan [1974a: theorem 18].

3.32. Harville [1997: 420].

3.33. Takane and Yanai [2005]. They also discuss the case when $M'AN$ is rectangular.

3.34. Tian and Styan [2001]. They also give an extensive list of similar results including those for $P + Q$.

### 3.6 PARTITIONED AND PATTERNED MATRICES

Some partitioned matrices have already been mentioned above in passing so there will be a slight overlap with the following, which focuses exclusively on partitioned matrices.

3.35. (Column Partitions) Let $A$ be an $m \times n$ matrix and $B$ be an $m \times q$ matrix, both over $\mathbb{F}$.

(a) $C(A) \cap C[(I_m - AA^-)B] = 0$, where $A^-$ is any weak inverse of $A$.

(b) $\text{rank}(A, B) = \text{rank}(A, (I_m - AA^-)B)$.

(c) $\text{rank}(A, B) = \text{rank}A + \text{rank}[(I - AA^-)B] = \text{rank}B + \text{rank}[(I - BB^-)A]$.

The second result is obtained by interchanging $A$ and $B$.

Note that $AA^- = P_A$ is idempotent, thus representing an (oblique) projection onto $C(A)$ (by 7.2c); also $P_AA = A$.

3.36. (Row Partitions) Let $A$ be an $m \times n$ matrix and $C$ be an $q \times n$ matrix, both over $\mathbb{F}$.

(a) $A$ and $C(I_n - A^- A)$ have disjoint row spaces (i.e., only have the zero vector in common).

(b) $\text{rank} \begin{pmatrix} A \\ C \end{pmatrix} = \text{rank} \begin{pmatrix} A \\ C(I_n - A^- A) \end{pmatrix}$.
(c)\[
\text{rank}\begin{pmatrix} A \\ C \end{pmatrix} = \text{rank} A + \text{rank}[C(I - A^{-}A)] \\
= \text{rank} C + \text{rank}[A(I - C^{-}C)].
\]

Note that \((A^{-}A)' = P_{A^{'}}\), where \(P_{A^{'}}\) is the (oblique) projection onto \(C(A')\) (by 7.2c).

3.37. For conformable matrices \(A\), \(B\), and \(C\) over \(\mathcal{F}\) and for any choice of weak inverse \(A^{-}\), we have the following:

(a) \(\text{rank}(AB, [I - AA^{-}]C) = \text{rank}(AB) + \text{rank}([I - AA^{-}]C).\)

(b) \(\text{rank}\begin{pmatrix} BA \\ C[I - A^{-}A] \end{pmatrix} = \text{rank}(BA) + \text{rank}(C[I - A^{-}A]).\)

3.38. If all four matrices are conformable, we have

\[\text{rank}\begin{pmatrix} A & B \\ C & D \end{pmatrix} = \text{rank}\begin{pmatrix} B & A \\ D & C \end{pmatrix} = \text{rank}\begin{pmatrix} C & D \\ A & B \end{pmatrix} = \text{rank}\begin{pmatrix} D & C \\ B & A \end{pmatrix}.\]

3.39. The following hold for any conformable \(A\), \(B\), and \(C\) over \(\mathcal{F}\).

(a) For all weak inverses \(A^{-}\) and \(B^{-}\),

\[
\text{rank}\begin{pmatrix} 0 & A \\ B & C \end{pmatrix} = \text{rank} A + \text{rank}[B, C(I - A^{-}A)]
\]

\[= \text{rank} B + \text{rank}\begin{pmatrix} A \\ (I - BB^{-})C \end{pmatrix}
\]

\[\leq \text{rank} A + \text{rank} B + \text{rank} C,
\]

with equality if and only if \(C(B) \cap C(C) = 0\) and \(C(A') \cap C(C') = 0\). If \(B\) or \(C\) (or both) is nonsingular, then the rank of the left-hand side is \(\text{rank} A + \text{rank} B\).

(b) \(\text{rank}\begin{pmatrix} 0 & A \\ B & C \end{pmatrix} = \text{rank} C + \text{rank}[A(I - C^{-}C)] + \text{rank}[(I - CC^{-})B]
\]

\[+ \text{rank} D,
\]

for \(D = (I - UU^{-})AC^{-}B(I - V^{-}V)\), with \(U = A(I - C^{-}C)\) and \(V = (I - CC^{-})B\). The weak inverses may be any (possibly different) choices except that the \(C^{-}\) in the middle of \(D\) must be the same as that chosen in either \(U\) or \(V\).

3.40. (Generalized Schur Complement) Let \(E, F, G,\) and \(H\) be conformable matrices over \(\mathcal{F}\), and let \(A\) be given by

\[A = \begin{pmatrix} E & F \\ G & H \end{pmatrix}.
\]
(a) We have the following results.

(i) $$\text{rank } \mathbf{A} = \text{rank } \mathbf{E} + \text{rank } \begin{pmatrix} 0 & (\mathbf{I} - \mathbf{E}^{-\dagger}) \mathbf{F} \\ \mathbf{G} (\mathbf{I} - \mathbf{E}^{-\dagger}) & \mathbf{H} - \mathbf{G} \mathbf{E}^{-\dagger} \mathbf{F} \end{pmatrix}$$

holds for any three generalized inverses $$\mathbf{E}^{-\dagger}$$. Here $$\mathbf{S} = \mathbf{H} - \mathbf{G} \mathbf{E}^{-\dagger} \mathbf{F}$$ is the generalized Schur complement of $$\mathbf{A}$$ with respect to $$\mathbf{E}$$ and is written as $$(\mathbf{A}/\mathbf{E})$$ (cf. Section 14.1).

(ii) If $$\mathbf{G} = \mathbf{0}$$, then $$\text{rank } \mathbf{A} \geq \text{rank } \mathbf{E} + \text{rank } \mathbf{H}$$. The same is true if we have $$\mathbf{F} = \mathbf{0}$$ instead.

(iii) Let $$\tilde{\mathbf{E}}$$ be a particular weak inverse of $$\mathbf{E}$$. Then

$$\text{rank } \mathbf{A} = \text{rank } \mathbf{E} + \text{rank } (\mathbf{H} - \mathbf{G} \tilde{\mathbf{E}}^- \mathbf{F})$$

if and only if

$$\begin{align*}
\mathbf{U} &= -(\mathbf{I} - \mathbf{E} \mathbf{E}^{-\dagger}) \mathbf{F} \mathbf{S}^- \mathbf{G} (\mathbf{I} - \mathbf{E}^{-\dagger}) = \mathbf{0}, \\
\mathbf{V} &= (\mathbf{I} - \mathbf{E} \mathbf{E}^{-\dagger}) \mathbf{F} (\mathbf{I} - \mathbf{S}^- \mathbf{S}) = \mathbf{0}, \\
\mathbf{W} &= (\mathbf{I} - \mathbf{S} \mathbf{S}^-) \mathbf{G} (\mathbf{I} - \mathbf{E}^{-\dagger}) = \mathbf{0},
\end{align*}$$

where $$\mathbf{A}^-$$ and $$\mathbf{S}^-$$ are any choices of weak inverses. Since, by (7.20), $$(\mathbf{I} - \mathbf{E} \mathbf{E}^{-\dagger}) \mathbf{E} = \mathbf{0}$$ and $$(\mathbf{I} - \mathbf{E}^{-\dagger}) \mathbf{E}' = \mathbf{0}$$, the above three conditions are satisfied when $$\mathcal{C}(\mathbf{F}) \subseteq \mathcal{C}(\mathbf{E})$$ and $$\mathcal{C}(\mathbf{G}') \subseteq \mathcal{C}(\mathbf{E}')$$ (Schott [2005: 265]). This is the case, for example, when $$\mathbf{A}$$ is non-negative definite and $$\mathbf{E}$$ and $$\mathbf{H}$$ are both square, that is, $$\mathbf{G} = \mathbf{F}'$$ (cf. 14.8c). The above result follows from (iv) below. Other conditions for the above to hold that relate to ranks are given by Tian [2002: 204].

From (3.38) we can interchange $$\mathbf{E}$$ and $$\mathbf{H}$$, and $$\mathbf{F}$$ and $$\mathbf{G}$$, in the above results, as we have done in (v) and (vi) below.

(iv) Using the above notation,

$$\text{rank } \mathbf{A} = \text{rank } \mathbf{E} + \text{rank } \mathbf{S} + \text{rank } \mathbf{V} + \text{rank } \mathbf{W} + \text{rank } \mathbf{Z},$$

where $$\mathbf{Z} = (\mathbf{I} - \mathbf{V} \mathbf{V}^-) \mathbf{U} (\mathbf{I} - \mathbf{W}^- \mathbf{W})$$ and any weak inverses can be used.

(v) If $$\mathbf{E}$$ is square and nonsingular, then the three conditions of (iii) are satisfied and

$$\text{rank } \mathbf{A} = \text{rank } \mathbf{E} + \text{rank } (\mathbf{H} - \mathbf{G} \mathbf{E}^{-1} \mathbf{F}).$$

(vi) If $$\mathbf{H}$$ is square and nonsingular, then

$$\text{rank } \mathbf{A} = \text{rank } \mathbf{H} + \text{rank } (\mathbf{E} - \mathbf{F} \mathbf{H}^{-1} \mathbf{G}).$$

(vii) With appropriate matrix substitutions we have from (v) and (vi)

$$\text{rank } \begin{pmatrix} \mathbf{I}_m & \mathbf{B} \\ \mathbf{B}' & \mathbf{I}_n \end{pmatrix} = n + \text{rank } (\mathbf{I}_m - \mathbf{B} \mathbf{B}') = m + \text{rank } (\mathbf{I}_n - \mathbf{B}' \mathbf{B}).$$
(b) \( \text{rank } A = \text{rank } E + \text{rank } X + \text{rank } Y + \text{rank } T \), where

\[
\begin{align*}
X &= (I - EE^{-})F, \\
Y &= G(I - E^{-}E), \\
\end{align*}
\]

Any choices of weak inverses can be used.

**3.41.** If \( A \) is \( m \times n \) and \( B \) is \( n \times m \), then

\[ \text{rank}(I_m - AB) = \text{rank}(I_n - BA) + m - n. \]

**Proofs.** Section 3.6.


3.36. Marsaglia and Styan [1974a: theorem 5].


3.38. Interchange rows then columns.


3.40a. Marsaglia and Styan [1974a: theorem 19 and corollary 19.1] with their restrictions in (i) and (iv) removed by Ouellette [1981: 228–229]; (ii) is proved by Abadir and Magnus [2005: 121–122]; (v) and (vi) are proved by Schott [2005: 265–266] and Abadir and Magnus [2005: 123].


3.41. Abadir and Magnus [2005: 124]. See also Groß [1999].

### 3.7 MAXIMAL AND MINIMAL RANKS

This topic presents some very powerful tools for handling matrix problems, as shown in a series of papers by Yongge Tian. For example, one can find the maximum and minimum ranks of an expression and then find conditions when these two are equal; this will give us the rank, subject to the conditions. One way of proving that two matrix expressions are equal is to prove that the rank of their difference is zero.

For some history of this topic see Tian [2000], and for some detailed results see Tian [2002].

**3.42.** For conformable matrices,

\[
\min_{X_1, X_2} \text{rank}(A - BX_1 - CX_2) = \text{rank} \begin{pmatrix} A & B \\ C & 0 \end{pmatrix} - \text{rank } B - \text{rank } C,
\]

where the minimization is with respect to all conformable \( X_1 \) and \( X_2 \).
3.43. For conformable matrices, define \( p(X_1, X_2) = A - B_1X_1C_1 - B_2X_2C_2 \). Then:

(a)

\[
\min_{X_1, X_2} \text{rank}[p(X_1, X_2)] = \text{rank} \begin{pmatrix} A \\ C_1 \\ C_2 \end{pmatrix} + \text{rank}(A, B_1, B_2) + \max \left\{ \text{rank} \begin{pmatrix} A & B_1 \\ C_2 & 0 \end{pmatrix} - \text{rank} \begin{pmatrix} A & B_1 \\ C_2 & 0 \end{pmatrix}, \text{rank} \begin{pmatrix} A & B_2 \\ C_1 & 0 \end{pmatrix} - \text{rank} \begin{pmatrix} A & B_2 \\ C_1 & 0 \end{pmatrix} \right\}.
\]

(b)

\[
\max_{X_1, X_2} p(X_1, X_2) = \min \left\{ \text{rank}(A, B_1, B_2), \text{rank} \begin{pmatrix} A \\ C_1 \\ C_2 \end{pmatrix}, \text{rank} \begin{pmatrix} A & B_1 \\ C_2 & 0 \end{pmatrix} - \text{rank} \begin{pmatrix} A & 0 \\ C & D \end{pmatrix} - \text{rank} \begin{pmatrix} A & 0 \\ 0 & B \\ C & D \end{pmatrix} \right\}.
\]

3.44. (Generalized Schur Complement) Let

\[ M = \begin{pmatrix} A & B \\ C & D \end{pmatrix}, \]

then we recall from (3.40) that the generalized Schur complement of \( A \) in \( M \) \((M/A)\) is \( S_A = D - CA^{-}B \), where \( A^{-} \) is any weak inverse \( A \) (We have changed the notation for \( M \) to fit in with the proofs for the following results.) Then

\[
\max_{A^{-}} \text{rank}(S_A) = \min \left\{ \text{rank}(C, D), \text{rank} \begin{pmatrix} B \\ D \end{pmatrix}, \text{rank} M - \text{rank} A \right\}
\]

and

\[
\min_{A^{-}} \text{rank}(S_A) = \text{rank} A + \text{rank}(C, D) + \text{rank} \begin{pmatrix} B \\ D \end{pmatrix} + \text{rank} M - \text{rank} \begin{pmatrix} A & 0 \\ 0 & B \\ C & D \end{pmatrix} - \text{rank} \begin{pmatrix} A & 0 \\ 0 & B \\ C & D \end{pmatrix}.
\]

Proofs. Section 3.7.

3.42. Tian [2000].
3.43. Tian [2002]. He shows there is some simplification when \( C(B_1) \subseteq C(B_2) \) and \( C(C_2') \subseteq C(C_1') \). By equating (a) and (b), he obtains necessary and sufficient conditions for \( \text{rank}[p(X_1, X_2)] \) to be invariant with respect to \( X_1 \) and \( X_2 \). He then finds similar conditions for \( C[p(X_1, X_2)] \) to be invariant.

3.44. Tian [2002: 201]. He uses the fact that \( A^{-} \) is a solution of \( AXA = A \). He also gives necessary and sufficient conditions for the rank and column space of \( S_A \) to be invariant with respect to the choice of \( A^{-} \). Some rank and other properties of \( CA^{-}B, A^{-}B, CA^{-}, \) and \( A - AB^{-}A \) are given by Tian [2002: 206–207].

### 3.8 MATRIX INDEX

**Definition 3.3.** If \( A \) is an \( n \times n \), there exists a positive integer \( k \) (1 \( \leq k \leq n \)) such that \( \text{rank}(A^k) = \text{rank}(A^{k+1}) \). The smallest \( k \) for which this is true is called the **index** of \( A \). If \( A \) is nonsingular, \( k = 0 \), where \( A^0 = I_n \). The basis for the definition comes from the following results and (3.11).

3.45. If \( A \) is an \( n \times n \) complex matrix, then:

(a) \( N(A^0) \subseteq N(A) \subseteq N(A^2) \subseteq \cdots \subseteq N(A^k) \subseteq N(A^{k+1}) \subseteq \cdots \).

(b) \( C(A^0) \supseteq C(A) \supseteq C(A^2) \supseteq \cdots \supseteq C(A^k) \supseteq C(A^{k+1}) \supseteq \cdots \).

There is equality at some point, in fact at the same value of \( k \) in both cases. What this means is that the index \( k \) is the smallest integer at which \( C(A^k) \) stops shrinking and \( N(A^k) \) stops growing.

3.46. Let \( A \) have index \( k \).

(a) All matrices \( \{A^l : l \geq k\} \) have the same rank, the same column space, and the same null space.

(b) Their transposes \( \{(A^l)^t : l \geq k\} \) have the same rank, the same column space, and the same null space.

(c) Their conjugate transposes \( \{(A^l)^* : l \geq k\} \) have the same rank, the same column space, and the same null space.

(d) For no \( l \) less than \( k \) do \( A^l \) and a higher power of \( A \) (or their transposes or conjugate transposes) have the same range or the same null space.

(e) For \( l \geq k \)

\[
C(A^l) \cap N(A^l) = 0 \quad \text{and} \quad C(A^l) \oplus N(A^l) = \mathbb{C}^n.
\]

**Proofs.** Section 3.8

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Chapter 4

Chapter 4

Matrix Functions: Inverse, Transpose, Trace, Determinant, and Norm

The topics considered in this chapter might be regarded as the “bread and butter” or, changing the metaphor, the working tools for someone using linear algebra in their research. I have not included rank, generalized inverse, and eigenvalues, as I have a separate chapter for each of these topics.

4.1 Inverse

Definition 4.1. An \( m \times n \) matrix \( A \) is said to have a right inverse if there exists an \( n \times m \) matrix \( B \) such that \( AB = I_m \). It is said to have a left inverse if there exists an \( n \times m \) matrix \( C \) such that \( CA = I_n \). These inverses are generally not unique.

Definition 4.2. If \( A \) is \( n \times n \) and \( \text{rank} \, A = n \), then \( A \) is said to be nonsingular and has an inverse denoted by \( A^{-1} \) that satisfies \( AA^{-1} = A^{-1}A = I_n \). An equivalent definition is that \( A \) is nonsingular if and only if \( \det A \neq 0 \). A square matrix that is not nonsingular (i.e., \( \det A = 0 \)) is said to be singular. Inverses, both algebraic and numerical, can be computed using Matlab (Leon [2007: chapter 71], Maple (Jeffrey and Corless [2007: chapter 72]), and Mathematica (Ruskeepää [2007: chapter 73]).

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4.2. If \( A \) is \( n \times n \) and \( AB = I_n \), then \( B = A^{-1} \).

4.3. If \( A \) and \( B \) are nonsingular matrices of the same size, then \( (AB)^{-1} = B^{-1}A^{-1} \).

4.4. If \( A \) is nonsingular and \( c \neq 0 \), then \( (cA)^{-1} = c^{-1}A^{-1} \).

4.5. If \( A \) is nonsingular, then \( A^{-1} \) is a continuous function of the elements of \( A \).

Proofs. Section 4.1.


4.5. Schott [2005: 199].

4.2 TRANSPOSE

Definition 4.3. If \( A = (a_{ij}) \) is real or complex, we define \( A^* = (\bar{a}_{ji}) \) to be the conjugate transpose of \( A \). When \( A \) is real, \( A^* = A' \).

4.6. (Basic Results)

(a) \((AB)^* = B^*A^* \).

(b) \((\alpha A)^* = \bar{\alpha}A^* \).

(c) If \( A \) is a nonsingular matrix, then \((A^{-1})^* = (A^*)^{-1} \).

4.7. Suppose \( A \) and \( B \) are real matrices, where \( A \) is \( p \times m \) and \( B \) is \( p \times n \), with \( m \leq n \). Then \( AA' = BB' \) if and only if there exists an \( m \times n \) matrix \( H \) with \( HH' = I_m \) such that \( AH = B \).

Proofs. Section 4.2.


4.3 TRACE

Definition 4.4. If \( A = (a_{ij}) \) is an \( n \times n \) matrix, then the sum of the diagonal elements is called the trace of \( A \) and is denoted by \( \text{trace} A \). Thus

\[
\text{trace} A = \sum_{i=1}^{n} a_{ii} = \text{trace} A'.
\]

4.8. Let \( A \) be \( m \times n \), and let \( A^- \) be any weak inverse of \( A \). Then, from (7.2d),

\[
\text{trace}(A^-A) = \text{trace}(AA^-) = \text{rank} A.
\]
4.9. If $A$ is real and symmetric, then

$$\text{rank } A \geq \frac{(\text{trace } A)^2}{\text{trace}(A^2)}.$$ 

For related results see (6.21).

4.10. If $A$ is an $n \times n$ real matrix with real eigenvalues and exactly $t$ of them are nonzero, then

$$(\text{trace } A)^2 \leq t \text{trace}(A^2).$$

4.11. Let $A$ be an $n \times n$ real matrix.

(a) If $A$ has real eigenvalues, then $(\text{trace } A)^2 \leq \text{rank}(A) \text{trace}(A^2)$.

(b) If $A$ is symmetric, $(\text{trace } A)^2 = \text{rank}(A) \text{trace}(A^2)$ if and only if there is a non-negative integer $k$ such that $A^2 = kA$.

(c) If $A$ is symmetric, then $A^2 = A$ if and only if $\text{rank } A = \text{trace } A = \text{trace}(A^2)$.

(d) $\text{trace}(A'A) \geq \text{trace}(A^2)$, with equality if and only if $A$ is symmetric.

4.12. If $A$ is an $n \times n$ real or complex matrix, then $A$ can be written as $A = XY - YX$ for some $n \times n$ matrices $X$ and $Y$ if and only if $\text{trace } A = 0$.

4.13. Let $A$ be $m \times n$ and $B$ be $n \times m$, both real or complex matrices.

(a) We have

$$\text{trace}(AB) = \text{trace}(BA) = \text{trace}(A'B') = \text{trace}(B'A')$$

$$= \sum_{i=1}^{m} \sum_{j=1}^{n} a_{ij}b_{ji} = \sum_{i=1}^{m} \sum_{j=1}^{n} a_{ij}b'_{ij}.$$ 

(b) If $m = n$ and either $A$ or $B$ is symmetric, then

$$\text{trace}(AB) = \sum_{i=1}^{n} \sum_{j=1}^{n} a_{ij}b_{ij}.$$ 

This result is particularly useful in statistics.

4.14. Suppose $A$ is $m \times n$, $B$ is $n \times p$, and $C$ is $p \times n$. Then

$$\text{trace}(ABC) = \text{trace}(BCA) = \text{trace}(CAB).$$

4.15. Let $C$ be an $m \times n$ real or complex matrix. Then

$$\text{trace}(C^*C) = \text{trace}(CC^*) = \sum_{i=1}^{m} \sum_{j=1}^{n} |c_{ij}|^2.$$ 

Hence $\text{trace}(C^*C) = 0$ implies that $C = 0$.

4.16. Suppose the $m \times n$ matrix $E_{ij}$ has 1 in the $i, j$th position and zeros elsewhere. If $A$ is $n \times m$, we have $\text{trace}(E_{ij}A) = a_{ji} = a'_{ij}$. 
4.17. If \( R \) is \( n \times n \) and nonsingular, \( \text{trace}(R^{-1}AR) = \text{trace}(ARR^{-1}) = \text{trace}(A) \).

4.18. If \( A \) and \( B \) are real symmetric matrices, then \( \text{trace}[(AB)^2] \leq \text{trace}(A^2B^2) \).

4.19. If \( A \) is \( n \times n \), \( B \) is \( m \times m \), and \( A \otimes B \) is the Kronecker product, then (cf. 11.11(ii))

\[
\text{trace}(A \otimes B) = \text{trace}(A) \text{trace}(B).
\]

4.20. If \( A \) is \( n \times n \) and \( x \) is \( n \times 1 \), then \( x'Ax = \text{trace}(x'Ax) = \text{trace}(Ax'x) \).

4.21. If \( A \) is \( m \times n \), then \( \text{trace}(AX) = 0 \) for every \( n \times m \) \( X \) if and only if \( A = 0 \).

4.22. If \( A \) is \( n \times n \), then \( \text{trace}(AX) = 0 \) for all Hermitian \( X \) if and only if \( A = 0 \).

4.23. If \( A \) is an \( n \times n \) Hermitian matrix and \( \text{trace}A \geq \Re\text{trace}(AU) \) for all unitary matrices \( U \), then \( A \) is non-negative definite. Here \( \Re \) is the “real part.”

4.24. Let \( A \) be an \( n \times n \) matrix with singular value decomposition \( A = P\Sigma Q^* \), where \( P \) and \( Q \) are \( n \times n \) unitary matrices, \( \Sigma = \text{diag}(\sigma_1(A), \ldots, \sigma_n(A)) \), and the \( \sigma_i(A) \) are the ordered singular values of \( A \). Let \( U_n \) be the collection of all \( n \times n \) unitary matrices. Then

\[
\max_{U \in U_n} \Re\text{trace}(AU) = \sum_{i=1}^{n} \sigma_i(A),
\]

and the maximum is attained at \( U_0 = QP^* \) (which need not be unique).

4.25. Let \( A \) be \( m \times n \) and \( B \) be \( n \times m \) matrices, and define \( U_n \) as in (4.24) above. Then

\[
\max_{U \in U_n, V \in U_m} \Re\text{trace}(AUBV) = \sum_{i=1}^{p} \sigma_i(A)\sigma_i(B),
\]

where \( p = \min\{m, n\} \) and \( \sigma(\cdot) \) is a singular value.

4.26. Let \( A \) and \( B \) be \( n \times n \) non-negative definite matrices. Then:

(a) \( \text{trace}A \geq 0 \) with equality if and only if \( A = 0 \).

(b) \( \text{trace}(AB) \geq 0 \) with equality if and only if \( AB = 0 \).

4.27. Let \( A \) and \( B \) be \( n \times n \) positive definite matrices. Then:

(a) \( \text{trace}A > 0 \).

(b) \( \text{trace}(AB) > 0 \).

Proofs. Section 4.3.

4.8. \( AA^\ast \) is a projection onto \( \mathcal{C}(A) \) and is therefore idempotent so that its rank equals its trace.


4.11d. Follows from \( \text{trace}[(A - A'')(A - A')] = 2[\text{trace}(A'A) - \text{trace}(A^2)] \geq 0 \).
   We can interchange the subscripts \(i\) and \(j\).
4.14. Use (4.13a) with \(AB\) and \(C\), and so on.
4.15. \(\text{trace}(C^*C) = \sum_i \sum_j c_{ij}^*c_{ji} = \sum_i \sum_j c_{ji}c_{ji}\).
4.16. Use (4.13a).
4.21. Use (4.16) for all \(E_{ij}\).
4.27a. Each \(a_{ii} > 0\) from (10.33b).
4.27b. We have \(\text{trace}(AB) = \text{trace}(A^{1/2}BA^{1/2})\), where (cf. 10.32) \(A^{1/2}\) is
   the positive definite square root of \(A\), and \(A^{1/2}BA^{1/2}\) is positive definite.
   Now apply (a) to \(\text{trace}(A^{1/2}BA^{1/2})\).

4.4 DETERMINANTS

Determinants arise in many places in this book. In this section I concentrate on
some basic properties, but the reader should also refer to Chapter 14 on partitioned
matrices and Chapter 15 on patterned matrices. Determinants of special matrices
are given in Chapter 8, and the differentiation of determinants is given in Chapters
17 and 18.

4.4.1 Introduction

**Definition 4.5.** The determinant of a square matrix \(A = (a_{ij})\), denoted by
\(\text{det}(A)\), is defined as

(1) \[ \text{det}(A) = \sum \varepsilon_{j_1,j_2,\ldots,j_n} a_{1j_1}a_{2j_2}\cdots a_{nj_n}, \]
   where \(\varepsilon_{j_1,j_2,\ldots,j_n}\) is +1 or −1 according as \(\{j_1,j_2,\ldots,j_n\}\) is an even or odd number
   of permutations of the integers \(\{1,2,\ldots,n\}\), with the summation extending
   over all \(n\) such possible permutations. Thus \(\varepsilon_{j_1,j_2,\ldots,j_n} = (-1)^{j_1+j_2+\cdots+j_n}\).

(2) Another way of expressing \(\text{det}(A)\) is
   \[ \text{det}(A) = \sum_{\pi} \text{sgn}(\pi) \prod_{i=1}^{n} a_{i\pi(i)}. \]
Here \( \pi \) is a permutation of the ordered set \( \{1, 2, \ldots, n\} \) and \( \pi(i) \) is the \( i \)th member of the permutation \( \pi \). The summation extends over all permutations, and the function \( \text{sgn}(\pi) \) is +1 or -1 depending on whether the permutation is even or odd.

4.28. (Basic Properties) Let \( A \) be an \( n \times n \) matrix.

(a) \( \det(A) = \det(A') \).

(b) If two rows (columns) of \( A \) are equal, then \( \det(A) = 0 \).

(c) If every element of a row (column) of \( A \) is zero, then \( \det(A) = 0 \).

(d) If \( B \) is obtained from \( A \) by multiplying one row (column) of \( A \) by the scalar \( k \), then \( \det(B) = k \det(A) \). In particular, \( \det(cA) = c^n \det(A) \).

(e) If \( B \) is obtained from \( A \) by interchanging any two rows (columns), then \( \det(B) = -\det(A) \).

(f) Adding to one row (column) of a square matrix any multiple of another row (column) does not affect the value of the determinant.

(g) \( \det(A) \) is a continuous function of the elements of \( A \).

Note that the transformations (d)–(f) can be represented by matrices (cf. Section 16.2.1).

4.29. (Row-Block Operations) Some of the properties of the previous result carry over to block multiplication. Let \( A \) be \( m \times m \) and \( B \) be \( n \times n \) matrices.

(a) If \( E \) is \( m \times m \), then

\[
\det \begin{pmatrix} EA & EB \\ C & D \end{pmatrix} = \det(E) \cdot \det \begin{pmatrix} A & B \\ C & D \end{pmatrix}.
\]

(b) If \( E \) is \( n \times m \), then

\[
\det \begin{pmatrix} A & B \\ C + EA & D + EB \end{pmatrix} = \det \begin{pmatrix} A & B \\ C & D \end{pmatrix}.
\]

4.30. An \( n \times n \) matrix may be written as \( A = XYX^{-1}Y^{-1} \) for some nonsingular \( n \times n \) matrices \( X \) and \( Y \) if and only if \( \det(A) = 1 \).

4.31. If \( A \) and \( B \) are \( n \times n \) matrices, then:

(a) \( \det(AB) = \det(A) \det(B) \).

(b) \( \det(AA') = \det(AA') = (\det A)^2 \).

(c) If \( A \) is nonsingular, then setting \( B = A^{-1} \) gives us \( \det(A^{-1}) = (\det A)^{-1} \).

(d) \( \det \begin{pmatrix} A & B \\ B & A \end{pmatrix} = \det(A + B) \det(A - B) \).
4.32. (Craig-Sakamoto) If A and B are \(n \times n\) real symmetric matrices, and \(c\) and \(d\) are positive scalars, then
\[
\det(I_n - sA - tB) = \det(I_n - sA) \cdot \det(I_n - tB)
\]
for all \(|s| < c\) and \(|t| < d\) if and only if \(AB = 0\).

4.33. Let \(A\) be an \(m \times n\) matrix and \(B\) be an \(n \times m\) matrix. Taking determinants of both sides of the following equivalence
\[
\begin{pmatrix}
I_m - AB & A \\
0 & I_n
\end{pmatrix}
\begin{pmatrix}
I_m & 0 \\
B & I_n
\end{pmatrix}
= \begin{pmatrix}
I_m & 0 \\
B & I_n - BA
\end{pmatrix}
\begin{pmatrix}
I_m & A \\
0 & I_n
\end{pmatrix},
\]
using (14.18) and the fact that the determinant of a triangular matrix is the product of its diagonal elements, we get
\[
\det(I_m - AB) = \det(I_n - BA).
\]
If \(n = 1\),
\[
\det(I_m - aa') = 1 - a'a.
\]

Proofs. Section 4.4.1.


4.28g. Schott [2005: 198].


4.32. Abadir and Magnus [2005: 181] and Harville [1997: 568–569; see also the theory there on polynomials].

4.4.2 Adjoint Matrix

Definition 4.6. Let \(A\) be an \(n \times n\) matrix. If a submatrix \(A_{ij}\) is formed by deleting the \(i\)th row and the \(j\)th column of \(A\), then \(\det(A_{ij})\) is called the minor of \(a_{ij}\) and the signed minor \(a_{ij} = (-1)^{i+j} \det(A_{ij})\) is called the cofactor of \(a_{ij}\). The matrix \(\text{adj}(A) = (\alpha_{ji})\) is called the adjoint (adjugate) of \(A\).

4.34. If \(A\) is \(n \times n\), then
\[
\sum_{j=1}^{n} a_{ij} \alpha_{kj} = \begin{cases} 
\det(A), & \text{if } i = k, \\
0, & \text{otherwise.}
\end{cases}
\]

4.35. If \(A\) is \(n \times n\), then \(A(\text{adj}A) = (\text{adj}A)A = \det(A)I_n\).
4.36. \( \text{adj(adjA)} = (\det A)^{n-2} A. \)

4.37. If \( A \) is nonsingular, it follows from (4.35) above that \( \text{adj}(A) = (\det A)^{-1} A \) and \( \det(\text{adjA}) = \{\det(A)\}^{n-1} \).

4.38. The following hold.

(a) \( \text{adj}(aA) = a^{n-1} \text{adjA}. \)

(b) \( \text{adj}(A') = (\text{adjA})'. \)

(c) If \( A \) is nonsingular, then \( \text{adj}(A^{-1}) = (\text{adjA})^{-1}. \)

4.39. Let \( A \) be \( n \times n. \)

(a) Let \( \text{rank} A = n - 1, \) then

\[
\text{adjA} = (-1)^{k+1} d(A) \frac{xy'}{y'(A^{k-1})^+ x},
\]

where \( k \) denotes the algebraic multiplicity of the zero eigenvalue of \( A \) (1 \( \leq k \leq n) \), \( d(A) \) is the product of the \( n - k \) non-zero eigenvalues of \( A \), \((\cdot)^+\) denotes the Moore–Penrose inverse, and \( x \) and \( y \) are \( n \times 1 \) vectors satisfying \( Ax = 0 \) and \( y'A = 0'. \) If \( k = n, \) we put \( d(A) = 1. \)

(b) If 0 is a simple eigenvalue of \( A \) (i.e., \( k = 1 \) in (a)), then \( \text{rank} A = n - 1 \) and

\[
\text{adjA} = d(A) \frac{xy'}{y'x}.
\]

Here \( d(A) \) is the product of the \( n - 1 \) nonzero eigenvalues and \( x \) and \( y \) are defined in (a).

(c) If \( \text{rank} A \leq n - 2, \) then \( \text{adjA} = 0. \)

If \( \text{rank} A = n - 1, \) then \( \text{rank}(\text{adjA}) = 1. \)

4.40. If \( A \) and \( B \) are both \( n \times n, \) then \( \text{adj}(AB) = \text{adjA} \cdot \text{adjB}. \)

Proofs. Section 4.4.2.


4.38. Rao and Bhimasankaram [2000: 245, see solution to exercise 8].


4.4.3 Compound Matrix

**Definition 4.7.** Given the \( m \times n \) matrix \( A = (a_{ij}) \), a compound matrix of \( A \) is the array of all minors of a given size \( k \), say, \( (k \leq \min\{m,n\}) \). The \( M = \binom{m}{k} \) by \( N = \binom{n}{k} \) matrix is denoted by \( A_{[k]} = (b_{\alpha\beta}) \), where we write symbolically \( \alpha = (i_1, i_2, \ldots, i_k) \) and \( \beta = (j_1, j_2, \ldots, j_k) \). Here \( b_{\alpha\beta} \) is the determinant of the submatrix obtained by selecting the intersection of the \( k \) rows \( i_1, i_2, \ldots, i_k \) and the \( k \) columns \( j_1, j_2, \ldots, j_k \). The \( MN \) elements of \( A_{[k]} \) are arranged in lexicographic order (for a numerical example see Horn and Johnson [1985: 19-20]). Compound matrices are useful for expressing a number of expansions of determinants like Sylvester's identity, the Cauchy–Binet formula and the Laplace expansion given in the next section (cf. Rao and Rao [1998: 146–154]).

4.4.1 (Basic Properties)

(a) Let \( A_{m \times p} \) and \( B_{p \times n} \) be real or complex matrices, then:

(\( i \)) \( (AB)_{[k]} = A_{[k]}B_{[k]}, \quad k \leq \min\{m, n, p\} \).

(\( ii \)) \( (cA)_{[k]} = c^kA_{[k]} \).

(b) If \( A \) is an \( m \times n \) real or complex matrix, then \( (A_{[k]})' = (A')_{[k]} \).

(c) If \( A \) is a complex matrix, then \( (A_{[k]})* = (A^*)_{[k]} \).

(d) If \( A \) is a nonsingular real or complex matrix, then \( (A_{[k]})^{-1} = (A^{-1})_{[k]} \).

**Proofs.** Section 4.4.3


4.4.4 Expansion of a Determinant

4.42. (Expanding by Row \( i \) or Column \( j \)) Referring to (4.34), we have

\[
\det(A) = \sum_{j=1}^{n} a_{ij} \alpha_{ij} \quad (\text{row } i)
\]

\[
= \sum_{i=1}^{n} a_{ij} \alpha_{ij} \quad (\text{column } j).
\]

4.43. (Expanding by the Diagonal) Consider the \( n \times n \) matrix

\[
B = A + \text{diag}(x_1, x_2, \ldots, x_n).
\]

Then \( \det(B) \) consists of the sum of all possible products of the \( x_i \) taken \( r \) at a time for \( r = n, n-1, \ldots, 2, 1, 0 \), each product being multiplied by its complementary principal minor of order \( n-r \) in \( A \). By complementary minor in \( A \) we mean the
principal minor having diagonal elements other than those associated in \( B \) with the \( x \)'s of the particular products concerned. For example,

\[
\begin{vmatrix}
  a_{11} + x_1 & a_{12} & a_{13} \\
  a_{21} & a_{22} + x_2 & a_{23} \\
  a_{31} & a_{32} & a_{33} + x_3 \\
\end{vmatrix}
\]

\[= x_1 x_2 x_3 + x_1 x_2 a_{33} + x_2 x_3 a_{11} + x_3 x_1 a_{22} + x_1 \det\left(\begin{array}{cc}
  a_{22} & a_{23} \\
  a_{32} & a_{33} \\
\end{array}\right) + x_2 \det\left(\begin{array}{cc}
  a_{11} & a_{13} \\
  a_{31} & a_{33} \\
\end{array}\right) + x_3 \det\left(\begin{array}{cc}
  a_{11} & a_{12} \\
  a_{21} & a_{22} \\
\end{array}\right) + \det(\mathbf{A}).
\]

When \( x_1 = x_2 = \cdots = x_n = x \), we have \( \det(\mathbf{B}) = \sum_{i=0}^{n} x^{n-i} s_i(\mathbf{A}) \), where \( s_i(\mathbf{A}) \) is the sum of all the principal minors of order \( i \) of \( \mathbf{A} \). We define \( s_0(\mathbf{A}) \equiv 1 \) and note that \( s_n = \det(\mathbf{A}) \).

We can obtain an expansion of \( \det(\mathbf{A}) \) by its diagonal elements by setting \( a_{ii} = 0 \) and \( x_i = a_{ii} \) for \( i = 1, 2, \ldots, n \). Such an expansion is particularly useful when many of the principal minors are zero. We note that

\[
\det(\mathbf{A} - \lambda \mathbf{I}_n) = \sum_{i=0}^{n} (-\lambda)^{n-i} s_i(\mathbf{A}),
\]

which leads to the characteristic equation \( \det(\lambda \mathbf{I}_n - \mathbf{A}) = (-1)^n \det(\mathbf{A} - \lambda \mathbf{I}_n) \).

4.44. (Expanding by \( m \) Rows—Laplace Expansion) The Laplace expansion of \( \det(\mathbf{A}) \), where \( \mathbf{A} \) is \( n \times n \), can be obtained as follows. Firstly, consider any \( m \) \( (m \geq 1) \) rows of \( \mathbf{A} \). They contain \( R = \binom{n}{m} \) minors of order \( m \). Secondly, multiply each of these minors, \( \det(\mathbf{A}_r) \) say \( (r = 1, 2, \ldots, R) \), by the determinant of the complement of \( \mathbf{A}_r \), \( \det(\mathbf{B}_{n-r}) \) say, and by a sign factor. Here the complementary minor of \( \mathbf{A}_r \) is the \((n - m)\)th-order minor derived from \( \mathbf{A} \) by deleting the \( m \) rows and columns containing \( \mathbf{A}_r \). The sign factor is \((-1)^a_r\), where \( a_r \) is the sum of the subscripts of the diagonal elements of \( \mathbf{A}_r \). Then \( \det(\mathbf{A}) \) is the sum of such products, namely

\[
\det(\mathbf{A}) = \sum_{r=1}^{R} (-1)^{a_r} \det(\mathbf{A}_r) \det(\mathbf{B}_{n-r}).
\]

For example, expanding by rows 2 and 3 we have

\[
\begin{vmatrix}
  a_{11} & a_{12} & a_{13} & a_{14} \\
  a_{21} & a_{22} & a_{23} & a_{24} \\
  a_{31} & a_{32} & a_{33} & a_{34} \\
  a_{41} & a_{42} & a_{43} & a_{44} \\
\end{vmatrix}
\]

\[= \det\left(\begin{array}{cc}
  a_{21} & a_{22} \\
  a_{31} & a_{32} \\
\end{array}\right) \cdot \det\left(\begin{array}{cc}
  a_{13} & a_{14} \\
  a_{43} & a_{44} \\
\end{array}\right) (-1)^{2+1+3+2} + \det\left(\begin{array}{cc}
  a_{21} & a_{23} \\
  a_{31} & a_{33} \\
\end{array}\right) \cdot \det\left(\begin{array}{cc}
  a_{12} & a_{14} \\
  a_{42} & a_{44} \\
\end{array}\right) (-1)^{2+1+3+3} + \cdots + \]

\[+ \det\left(\begin{array}{cc}
  a_{23} & a_{24} \\
  a_{33} & a_{34} \\
\end{array}\right) \cdot \det\left(\begin{array}{cc}
  a_{11} & a_{12} \\
  a_{41} & a_{42} \\
\end{array}\right) (-1)^{2+3+3+4}.
\]
Further extensions of the Laplace expansion method are available, many of which are named after their originators—for example, Cauchy, Binet–Cauchy (Harville [1997: 200–202] and Rao and Rao [1997: 149]), and Jacobi.

A number of other expansions are available. For example, if we are interested in relating minors of submatrices, we can use Sylvester's Determinantal Identity (Rao and Rao [1998: 151–153]). If \( C = A_{n \times p} B_{p \times n} \), we can expand \( \det C \) in terms of the sum of products of a minor of \( A \) times a minor of \( B \) using the Cauchy–Binet formula (Rao and Bhimasankaram [2000: 238] and Rao and Rao [1997: 140]).

4.45. Given the skew-symmetric matrix

\[
A = \begin{pmatrix}
0 & a & b & c \\
-a & 0 & d & e \\
-b & -d & 0 & f \\
-c & -e & -f & 0
\end{pmatrix},
\]

then \( \det(A) = (af - be + cd)^2 \).

4.46. 

\[
\det \begin{pmatrix}
a_{11}^2 & 2a_{11}a_{12} & a_{12}^2 \\
a_{11}a_{21} & a_{11}a_{22} + a_{12}a_{21} & a_{12}a_{22} \\
a_{21}^2 & 2a_{21}a_{22} & a_{22}^2
\end{pmatrix} = 4 \left\{ \det \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} \right\}^2.
\]

The above matrix occurs in genetics.

Proofs. Section 4.4.4.

4.43. Searle [1982: 106].


4.46. Quoted by Searle [1982: 114].

4.5 PERMANENTS

Definition 4.8. Let \( A \) be an \( n \times n \) real matrix. The permanent of \( A \), denoted by \( \text{per}(A) \), is defined by

\[
\text{per}(A) = \sum_{\pi} \prod_{i=1}^{n} a_{i \pi(i)},
\]

where \( \pi \) is a permutation of the ordered set \( \{1, 2, \ldots, n\} \) and \( \pi(i) \) is the \( i \)th member of the permutation \( \pi \); the summation extends over all permutations \( \pi \). This definition may be compared with the definition of a determinant. There \( \prod_{i=1}^{n} a_{i \pi(i)} \) is multiplied by either +1 or −1 depending on whether \( \pi \) is an even or odd permutation. Note that \( \text{per}(A) \) can also be defined for an \( m \times n \) matrix. For general references to permanents see Wanless [2007] and Minc [1978, 1987], and for an emphasis on applications in probability and statistics see Bapat [1990]. Permanents can be used to prove a number of properties shared by doubly stochastic matrices.
Let \( \mathcal{I} \) and \( \mathcal{J} \) be ordered subsets of \( \{1, 2, \ldots, n\} \), each with \( \#\mathcal{I} \) and \( \#\mathcal{J} \) elements, respectively (the cardinality of each set), and define the \( \#\mathcal{I} \times \#\mathcal{J} \) submatrix \( A_{(\mathcal{I}, \mathcal{J})} = (a_{ij})_{i \in \mathcal{I}, j \in \mathcal{J}} \). We must have \( \#\mathcal{I} = \#\mathcal{J} \) for \( \text{per}(A_{(\mathcal{I}, \mathcal{J})}) \) to make sense.

4.47. Let \( A \) be an \( n \times n \) matrix.
(a) \( \text{per}(A) = \text{per}(A^t) \).
(b) \( \text{per}(A) \) admits a Laplace expansion along any row or column. Thus, if \( A_{ij} \) denotes the submatrix of \( A \) obtained by deleting the \( i \)th row and the \( j \)th column of \( A \), then
\[
\text{per}(A) = \sum_{i=1}^{n} a_{ij} \text{det} A_{ij}.
\]

4.48. \( \text{per}(A_{(\mathcal{I}, \mathcal{J})}) \) does not depend on the order of elements in \( \mathcal{I} \) or \( \mathcal{J} \).

4.49. If \( A \) is an \( n \times n \) non-negative matrix (i.e., \( a_{ij} \geq 0 \) for all \( i, j \)) and \( \#\mathcal{I} + \#\mathcal{J} = n \), then
\[
\text{per}(A) \geq \text{per}(A(\mathcal{I}, \mathcal{J}^c)) \times \text{per}(A(\mathcal{I}^c, \mathcal{J}))
\]
where \( \mathcal{I}^c \) is the complement of \( \mathcal{I} \), and so on.

4.50. If \( A \) is an \( n \times n \) non-negative matrix, then \( \text{per}(A) = 0 \) if and only if there are subsets \( \mathcal{I} \) and \( \mathcal{J} \) such that
\[
\#\mathcal{I} + \#\mathcal{J} \geq n + 1 \quad \text{and} \quad A(\mathcal{I}, \mathcal{J}) = 0.
\]

4.51. Let \( A \) and \( B \) be \( n \times n \) complex matrices. Then
(a) \[ |\text{per}(AB)|^2 \leq \text{per}(AA^*) \text{det}(BB^*), \]
with equality if and only if one of the following occurs:
(1) A row of \( A \) or a column of \( B \) is \( 0 \),
(2) No row of \( A \) and no column of \( B \) consists of \( 0 \), and \( A^* = BD\Pi \), where \( D \) is a diagonal matrix and \( \Pi \) is a permutation matrix.

(b) \[ |\text{per}(A)|^2 \leq \text{per}(AA^*) \] and \[ |\text{per}(A)|^2 \leq \text{per}(A^*A) \].

(c) If \( A \) is Hermitian non-negative definite, then
(i) \( \text{per}(A) \leq n^{-1} \text{trace}(A^n) \).
(ii) \( \text{det} A \leq \text{per}(A) \).

Proofs. Section 4.5.

4.47b. Use (4.44) with \( r = 1 \) and ignore the signs.
4.48. Follows from the definition.
4.51. Marcus and Minc [1964: 118, 120]. For (b), set \( B = I \) then \( A = I \) in (a).
4.6 NORMS

Norms, both for vectors and matrices, are used for measuring distance in vector spaces and for providing a measure of how close one matrix is to another. They can therefore be used for finding the best approximation of a matrix in a given class of matrices by a matrix in another class (e.g., of lower rank). They can also be used for investigating limits of matrix sequences and series. Norms, therefore, have a role to play in statistics in the areas of inequalities, optimization, matrix approximation, matrix analysis, and numerical analysis.

4.6.1 Vector Norms

Definition 4.9. A vector norm on a real or complex vector space $\mathcal{V}$ is a real-valued function $\| \cdot \|$ satisfying the following three conditions.

1. $\|x\| \geq 0$ for all $x \in \mathcal{V}$, and $\|x\| = 0$ implies that $x = 0$ (positive definite property).
2. $\|\alpha x\| = |\alpha| \cdot \|x\|$ for all $\alpha \in \mathbb{F}$ and all $x \in \mathcal{V}$ (scalar multiplication).
3. $\|x + y\| \leq \|x\| + \|y\|$ (triangle inequality).

A vector norm is said to be unitarily invariant if $\|Ux\| = \|x\|$ for all $x \in \mathbb{C}^n$ and all $n \times n$ unitary matrices $U$.

If (1) above is replaced by

(1a) $\|x\| \geq 0$ for all $x \in \mathcal{V}$,

then $\| \cdot \|$ is called a vector seminorm.

4.52. The following hold for both a norm and a seminorm for any $x, y \in \mathcal{V}$.

(a) $\|-x\| = \|x\|$.
(b) $\|x\| - \|y\| \leq \|x - y\|$.
(c) $\|x - y\| \leq \|x\| + \|y\|$.

4.53. Every vector norm on $\mathbb{R}^n$ or $\mathbb{C}^n$ is uniformly continuous.

4.54. For finite-dimensional real or complex vector spaces, all vector norms are equivalent in the sense that if $\| \cdot \|_\alpha$ and $\| \cdot \|_\beta$ are two vector norms, then there exist positive constants $c_1$ and $c_2$ such that

$$c_1 \|x\|_\alpha \leq \|x\|_\beta \leq c_2 \|x\|_\alpha$$

for all $x$ (cf. (4.56) below for some examples).

Definition 4.10. If $p$ is a real number with $p \geq 1$ and $x$ is an $n \times 1$ vector, then

$$\|x\|_p = \left( \sum_{i=1}^{n} |x_i|^p \right)^{1/p}$$
is a norm on $\mathbb{R}^n$ or $\mathbb{C}^n$ called the $L_p$ norm. Letting $p \to \infty$, we find that

$$\|x\|_\infty = \max_{1 \leq i \leq n} |x_i|$$

is also a norm called the $L_\infty$ norm. The norms most commonly used are the $L_1$, $L_2$, and $L_\infty$ norms. In particular, the so-called Euclidean norm $L_2$ is used to define the length of a vector in $\mathbb{R}^n$ or $\mathbb{C}^n$. The function $\|x\|_p$ is not a norm for $0 < p < 1$.

**4.55.** The $L_p$ norm ($p \geq 1$) is a vector norm.

**4.56.** For all $x \in \mathbb{C}^n$ we have:

(a) $n^{-1/2} \|x\|_1 \leq \|x\|_2 \leq \|x\|_1$.

(b) $\|x\|_\infty \leq \|x\|_2 \leq n^{1/2} \|x\|_\infty$.

(c) $\|x\|_2 \leq \|x\|_1 \leq n^{1/2} \|x\|_2$.

(d) $\|x\|_\infty \leq \|x\|_1 \leq n \|x\|_\infty$.

**4.57.** Every inner product induces a norm; we simply put $\|x\| = \langle x, x \rangle^{1/2}$. However, there are norms not induced by an inner product as in (4.58c) below.

**4.58.** (Parallelogram Law)

(a) The norm induced by an inner product on a vector space (cf. 4.57) has the property

$$\|x + y\|^2 + \|x - y\|^2 = 2\|x\|^2 + 2\|y\|^2.$$

(b) Conversely, any norm on a real or complex vector space satisfying the above equation is induced by an inner product, namely

$$\langle x, y \rangle = \frac{1}{2}(\|x + y\|^2 - \|x\|^2 - \|y\|^2).$$

An alternative inner product that can be used is

$$\langle x, y \rangle = \frac{1}{4}(\|x + y\|^2 - \|x - y\|^2).$$

(c) If the parallelogram rule does not hold, then there is no inner product that induces the norm.

(d) Let $1 \leq p \leq \infty$. Then the $L_p$ norm satisfies (a) if and only if $p = 2$. Thus $L_1$, for example, does not satisfy (a) so it cannot be induced by an inner product.

**4.59.** The sum of two vector (semi)norms is a vector (semi)norm, and any positive multiple of a vector (semi)norm is also a vector (semi)norm.

**4.60.** Let $\| \cdot \|_\alpha$ and $\| \cdot \|_\beta$ be vector norms on a real or complex vector space $V$. The function $\| \cdot \|$ defined by

$$\|x\| = \max\{\|x\|_\alpha, \|x\|_\beta\}$$

is a vector norm.
4.61. (Continuity) If \( \{x_n\} \) and \( \{y_n\} \) are sequences of vectors in an inner product space such that \( \|x_n - x\| \to 0 \) and \( \|y_n - y\| \to 0 \) as \( n \to \infty \), then

(a) \( \|x_n\| \to \|x\| \) and \( \|y_n\| \to \|y\| \).

(b) \( \langle x_n, y_n \rangle \to \langle x, y \rangle \), if \( \|x\| < \infty \) and \( \|y\| < \infty \).

4.62. If \( \| \cdot \| \) is a vector norm on \( \mathbb{C}^n \) and \( R \) is a nonsingular \( n \times n \) matrix, then \( \| \cdot \|_R \) defined by

\[
\|x\|_R = \|Rx\|, \quad x \in \mathbb{C}^n
\]

is also a vector norm on \( \mathbb{C}^n \).

**Proofs.** Section 4.6.1.

4.52a. By (2) of Definition 4.9.

4.52b. Horn and Johnson [1985: 260].

4.52c. By (3) of Definition 4.9 with \( y \) replaced by \(-y\).


4.55. Conditions (1) and (2) of Definition 4.9 are readily verified (cf. Gentle [1998: 71]), and (3) follows from Minkowski's inequality (12.17a).

4.56. (b)–(d) are quoted by Golub and Van Loan [1996: 53], while (a) and (b) are proved by Rao and Bhimasankaram [2000: 258; see the solution to exercise 14].


4.58a. This follows by simply expanding \( \langle x + y, x + y \rangle \), and so on.


4.58c. Abadir and Magnus [2005: 64].

4.58d. Rao and Bhimasankaram [2000: 258; see the solution to exercise 9].

4.59–4.60. Horn and Johnson [1985: 268].

4.61. Abadir and Magnus [2005: 65].


### 4.6.2 Matrix Norms

**Definition 4.11.** We can interpret the word "vector" as simply an element of a vector space. In this case, an \( m \times n \) complex matrix \( A = (a_{ij}) \) is simply an element of the space of \( m \times n \) complex matrices. Alternatively, this space can also be identified with the vector space \( \mathbb{C}^{mn} \) by arranging the entries of each \( A \) as an \( mn \)-tuple in some order (e.g., \( \text{vec} A \)). When a norm applied to \( \text{vec} A \) satisfies the conditions of a vector norm, we call the norm a **generalized matrix norm**. Some examples follow.
4.63. (Generalized Matrix Norms) Let $A$ be an $m \times n$ matrix. Then the following are generalized matrix norms:

(a) $\|A\|_{\infty} = \max_{1 \leq i \leq m, 1 \leq j \leq n} |a_{ij}|$.

(b) $\|A\|_F = (\text{trace}(A^*A))^{1/2} = (\sum_{i=1}^{m} \sum_{j=1}^{n} |a_{ij}|^2)^{1/2}$, the Frobenius norm. (We use a subscript $F$ instead of $F = 2$ to avoid confusion later in dealing with matrix norms instead of generalized ones.)

(c) $\|A\|_p = (\sum_{i=1}^{m} \sum_{j=1}^{n} |a_{ij}|^p)^{1/p}$ ($p \geq 1$).

Definition 4.12. (Induced Norms) Given the vector norm $\| \cdot \|_v$, the generalized matrix norm induced by $\| \cdot \|_v$ for the $m \times n$ matrix $A$ is defined by

$$\|A\|_{v,in} = \sup_{x \neq 0} \frac{\|Ax\|_v}{\|x\|_v} = \sup_{x \neq 0} \left| A \left( \frac{x}{\|x\|_v} \right) \right| = \sup_{\|x\|_v = 1} \|Ax\|_v,$$

where $x \in \mathbb{C}^n$. As noted by Horn and Johnson [1985: 292], we can replace “sup” by “max” in the above definition. The most common vector norms are the $L_p$ norms with $p \geq 1$. Note that $\| \cdot \|_F$ is not an induced norm, and is not to be confused with $\| \cdot \|_2,in$ (cf. 4.66b).

4.64. The induced norm $\|A\|_{v,in}$ is a generalized matrix norm as condition (3) of Definition 4.9 in Section 4.6.1 holds.

4.65. If $A$ is $m \times n$ and $B$ is $n \times q$, then for an $L_p$ vector norm ($p \geq 1$)

$$\|AB\|_{p,in} \leq \|A\|_{p,in} \|B\|_{p,in}.$$

This result does not hold for every $\| \cdot \|_{v,in}$. Golub and Van Loan [1996: 55], in quoting the above result, note that it represents a relationship between three different norms defined on $\mathbb{R}^{m \times q}$, $\mathbb{R}^{m \times n}$ and $\mathbb{R}^{n \times q}$, respectively. They also call the above norm a matrix norm, which it is for square matrices (see Definition 4.13 below).

4.66. Let $A$ be $m \times n$. Then following are induced norms based on $L_p$ vector norms.

(a) $\|A\|_{1,in} = \max_{1 \leq j \leq n} \sum_{i=1}^{m} |a_{ij}|$.

(b) $\|A\|_{2,in} = [\lambda_{\max}(A^*A)]^{1/2} = \sigma_{\max}(A)$, where $\lambda_{\max}$ is the maximum eigenvalue of $A^*A$ and $\sigma_{\max}$ is the maximum singular value.

(c) $\|A\|_{\infty,in} = \max_{1 \leq i \leq m} \sum_{j=1}^{n} |a_{ij}|$.

4.67. If $A$ is $m \times n$ then:

(a) $\|A\|_{2,in} \leq \|A\|_F \leq n^{1/2} \|A\|_{2,in}$. (See also (4.82) below for square matrices.)

(b) $\max_{1 \leq i \leq m, 1 \leq j \leq n} |a_{ij}| \leq \|A\|_{2,in} \leq (mn)^{1/2} \max_{1 \leq i \leq m, 1 \leq j \leq n} |a_{ij}|$.

(c) $m^{-1/2} \|A\|_{1,in} \leq \|A\|_{2,in} \leq n^{1/2} \|A\|_{1,in}$.

(d) $n^{-1/2} \|A\|_{\infty,in} \leq \|A\|_{2,in} \leq m^{1/2} \|A\|_{\infty,in}$.
The above bounds on the norm $\|A\|_2,\infty$ are useful, because this norm is more difficult to compute than either $\|A\|_1,\infty$ or $\|A\|_\infty,\infty$.

**Definition 4.13.** Let $\mathcal{V}$ be the vector space of $n \times n$ complex matrices. If $A \in \mathcal{V}$, then the *matrix norm* of $A$, denoted by $|||A|||$, is any real-valued non-negative function of $A$ satisfying the following conditions.

1. $|||A||| \geq 0$ and $|||A||| = 0$ if and only if $A = 0$.
2. $|||cA||| = |c| \cdot |||A|||$; where $c$ is any scalar and $|c|$ is its modulus.
3. If $B \in \mathcal{V}$ then $|||A + B||| \leq |||A||| + |||B|||$.
4. If $C \in \mathcal{V}$ then $|||AC||| \leq |||A||| \cdot |||C|||$.

Note that the first three conditions are those of a generalized matrix norm (and of a vector norm), which can be applied to any $m \times n$ matrix. However, condition (4) applies to square matrices only. For a brief introduction to matrix norms see Meyer [2000a: section 5.2].

4.68. Let $||| \cdot |||$ be any matrix norm and $A$ any $n \times n$ matrix.

(a) (i) $\rho(A) \leq |||A|||$; where $\rho$ is the spectral radius.
   (ii) $\rho(A) = \lim_{k \to \infty} (|||A^k|||)^{1/k}$.

(b) (i) From $AI_n = A$ and Definition 4.13(4) we have $|||I_n||| \geq 1$.
   (ii) Repeated use of Definition 4.13(4) give us $|||A^k||| \leq (|||A|||)^k$ (k a positive integer).
   (iii) Using $AA^{-1} = I_n$ and Definition 4.13(4) gives us $|||A^{-1}||| \geq (|||A|||)^{-1}$.

(c) From $A = (A - B) + B$, Definition 4.13(3), and interchanging the roles of $A$ and $B$, we have $|||A||| - |||B||| \leq |||A - B|||$.

(d) $|a_{ij}| \leq \theta |||A|||$ for all $i$ and $j$, where $\theta = \max_{1 \leq i \leq n, 1 \leq j \leq n} |||E_{ij}|||$; and $E_{ij}$ is an $n \times n$ matrix with 1 in the $i, j$th position and zeros elsewhere.

(e) If $|||A|||_S = |||S^{-1}AS|||$ for all nonsingular $n \times n$ matrices $S$, then $|||A|||_S$ is a matrix norm.

4.69. Let $A$ be an $n \times n$ matrix.

(a) $|||A|||_p = (\sum_{i=1}^n \sum_{j=1}^n (|a_{ij}|^p)^{1/p}$ is a matrix norm for $1 \leq p \leq 2$. When $p = 2$ we use the notation $|||A|||_F$.

(b) If $n \geq 2$, $|||A||| = n\max_{1 \leq i \leq n, 1 \leq j \leq n} |a_{ij}|$ is a matrix norm, but $|||A|||_\infty$ of (4.63a) is not, though it is a generalized matrix norm.

4.70. Result (4.69b) above can be generalized. For every generalized matrix norm $|||A|||_\alpha$, where $A$ is $n \times n$, there is a finite positive constant $c_\alpha$ which depends on the norm such that $c_\alpha |||A|||_\alpha$ is a matrix norm.
4.71. An $n \times n$ matrix $A$ is nonsingular if there is a matrix norm $||| \cdot |||$ such that $|||I_n - A||| < 1$. In this case

$$A^{-1} = \sum_{k=0}^{\infty} (I_n - A)^k.$$ 

4.72. Given $\epsilon > 0$, there exists a matrix norm $||| \cdot |||$ such that

$$\rho(A) \leq |||A||| < \rho(A) + \epsilon,$$

where $\rho$ is the spectral radius (see also 4.68a).

**Definition 4.14.** The generalized matrix norm induced by the vector norm $\| \cdot \|_v$ for the square matrix $A$ is a matrix norm because it satisfies the four conditions of Definition 4.13. We call it the induced matrix norm and we denote it by $|||A|||_{v,in}$.


4.73. For $n \times n$ matrices, the induced matrix norm has the following properties.

(a) $|||I_n|||_{v, in} = 1$.

(b) $\|Ax\|_v \leq |||A|||_{v, in} \cdot \|x\|_v$.

(c) $|||\alpha A|||_{v, in} = |\alpha| \cdot |||A|||_{v, in}$.

(d) $||| - A|||_{v, in} = |||A|||_{v, in}$.

(e) $|||I_n + A|||_{v, in} \leq |||I_n|||_{v, in} + |||A|||_{v, in} = 1 + |||A|||_{v, in}$.

(f) $|||I_n - A|||_{v, in} \leq 1 + |||A|||_{v, in}$.

(g) Suppose $|||A|||_{v, in} < 1$.

(i) $B = I_n - A$ and $I_n + A$ are nonsingular.

(ii) From $B(I_n - A) = I_n$, we can take the norm of $B = I_n + BA$ using (e) and Definition 4.13(4) to get

$$\frac{1}{1 + |||A|||_{v, in}} \leq |||(I_n - A)^{-1}|||_{v, in} \leq \frac{1}{1 - |||A|||_{v, in}}.$$ 

By replacing $A$ by $-A$ and using (c) above we see that the same bounds apply for $|||(I_n + A)^{-1}|||_{v, in}$.

4.74. Let $A$ be an $n \times n$ matrix. The matrix norm induced by an $L_p$ vector norm is given by

$$|||A|||_{p, in} = \max_{\|x\|_p = 1} \|Ax\|_p, \quad p \geq 1.$$ 

Setting $p = 1, 2, \infty$, we have:

(a) $|||A|||_{1, in} = \max_{1 \leq j \leq n} \sum_{i=1}^{n} |a_{ij}|$.

(b) $|||A|||_{2, in} = [\lambda_{\max}(A^*A)]^{1/2} = \sigma_{\max}(A)$, where $\lambda_{\max}$ is the maximum eigenvalue of $A^*A$ and $\sigma_{\max}$ is the maximum singular value. We note that $\lambda_{\max}$ is
real and non-negative as $A^*A$ is Hermitian and non-negative definite. We note that $\lambda_{\text{max}} = \rho(A^*A)$, where $\rho$ is the spectral radius. When $A$ is Hermitian, $\|A\|_2^2 = [\rho(A^2)]^{1/2}$, which reduces to $\rho(A)$ when $A$ is also non-negative definite. For further properties of this induced norm see Meyer [2000a: 281-283].

This matrix norm is also called the spectral matrix norm.

(c) $\|A\|_{\infty,in} = \max_{1 \leq i \leq n} \sum_{j=1}^{n} |a_{ij}|.$

The inequalities given in (4.67) apply to the above matrix norms by setting $m = n$.

4.75. If $A$ and $B$ are non-negative definite $n \times n$ matrices, then:

(a) $\|A^s B^s\|_{2,in} \leq \|AB\|_{s,in}^2$ for $0 \leq s \leq 1$.

(b) If $\|AB\|_{2,in} \leq 1$, then $\|A^s B^s\|_{2,in} \leq 1$ for $0 \leq s \leq 1$.

(c) $\|AB\|_{2,in}^t \leq \|A^t B^t\|_{2,in}^t$ for $t \geq 1$.

4.76. Let $\| \cdot \|_{\alpha}$ and $\| \cdot \|_{\beta}$ be two given vector norms on $\mathbb{C}^n$, and let $\| \cdot \|_{\alpha,in}$ and $\| \cdot \|_{\beta,in}$ denote the respective induced matrix norms on the space $V$ of $n \times n$ matrices.

(a) Define

$$R_{\alpha,\beta} = \max_{x \neq 0} \frac{\|x\|_\alpha}{\|x\|_\beta} \quad \text{and} \quad R_{\beta,\alpha} = \max_{x \neq 0} \frac{\|x\|_\beta}{\|x\|_\alpha}.$$

Then

$$\max_{A \neq 0} \frac{\|A\|_{\alpha,in}}{\|A\|_{\beta,in}} = \max_{A \neq 0} \frac{\|A\|_{\beta,in}}{\|A\|_{\alpha,in}} = R_{\alpha,\beta} R_{\beta,\alpha}.$$

(b) $\|A\|_{\alpha,in} = \|A\|_{\beta,in}$ for all $A \in V$ if and only if there is a positive constant $c$ such that $\|x\|_\alpha = c \|x\|_\beta$ for all $x \in \mathbb{C}$.

(c) $\|A\|_{\alpha,in} \leq \|A\|_{\beta,in}$ for all $A \in V$ if and only if $\|A\|_{\alpha,in} = \|A\|_{\beta,in}$ for all $A \in V$.

4.77. If $Q$ is unitary (or orthogonal), then:

(a) $\|Qx\|_2 = \|x\|_2$.

(b) $\|Q\|_{2,in} = 1$.

Definition 4.15. A matrix norm $\| \cdot \|$ on the class of $n \times n$ matrices is a minimal matrix norm if the only matrix norm $N(\cdot)$ such that $N(A) \leq \|A\|$ for all $A$ is $N(\cdot) = \| \cdot \|$.

4.78. Every induced norm is minimal and every minimal norm is induced.

Definition 4.16. If $A$ is $m \times n$, the Frobenius norm is defined to be

$$\|A\|_F = \left( \sum_i \sum_j |a_{ij}|^2 \right)^{1/2} = \sqrt{\text{trace}(A^*A)^{1/2}} = \|A^*\|_F.$$

When $m \neq n$, this norm is a generalized matrix norm, while if $m = n$, it is a matrix norm. However, it is not an induced norm. It is often referred to as the Euclidean norm.
matrix norm as \( \|A\|_F \), like \( \|A\|_{2,in} \), uses an \( L_2 \) vector norm. For this reason, Graybill [1983], for example, uses \( E \), but we shall follow the general trend and use the subscript \( F \) to avoid confusion. Harville [1997] refers to the Frobenius norm as the “usual norm.” Even when \( m \neq n \), the following result shows that the norm satisfies a result like (4) of Definition 4.13.

4.79. If \( A \) is \( m \times n \) and \( B \) is \( n \times p \), then \( \|AB\|_F \leq \|A\|_F \cdot \|B\|_F \).

4.80. If \( A \) is \( m \times n \) of rank \( r \) with singular values \( \sigma_i = \sigma_i(A) \), then

\[
\|A\|_F^2 = \text{trace}(A^*A) = \text{trace}(AA^*) = \sum_{i=1}^{r} \sigma_i^2.
\]

4.81. Given real symmetric \( A \) and real skew-symmetric \( B \), both \( n \times n \), then

\[
\|A + B\|_F^2 = \|A\|_F^2 + \|B\|_F^2.
\]

4.82. \( \|A\|_{2,in} \leq \|A\|_F \leq \sqrt{n}\|A\|_{2,in} \).

4.83. If \( A \) and \( U \) are \( n \times n \) and \( U \) is unitary, then

\[
\|A\|_{2,in} = \|UA\|_{2,in} = \|AU\|_{2,in} = \|U^*AU\|_{2,in}.
\]

The above also holds for \( \|\cdot\|_F \).

Proofs. Section 4.6.2.

4.63. Rao and Rao [1998: 363]. The results follow by applying (4.55) to \( \text{vec} A \).

4.64. We see that \( \|Ax + Ay\|_v \leq \|Ax\|_v + \|Ay\|_v \) implies that \( \max \|Ax + Ay\|_v \leq \max \{\|Ax\|_v, \|Ay\|_v\} \leq \max \|Ax\|_v + \max \|Ay\|_v \).

4.65. Quoted by Golub and van Loan [1996: 55].

4.66. Horn and Johnson [1985: 294–295, the proofs hold for \( m \neq n \)] and Meyer [2000a: 281–284].


4.68b. Horn and Johnson [1985: 290].


4.68e. Horn and Johnson [1985: 296].


4.69b. Horn and Johnson [1985: 292].
4.70. Horn and Johnson [1985: 323].
4.71. Horn and Johnson [1985: 301]. See also (19.16a) using an infinite series.
4.73a–c. Horn and Johnson [1985: 293] and Rao and Bhimasankaram [2000: 259; see the solution to exercise 15].
4.73d. Since \( \|Ax\|_v = \| -Ax\|_v \).
4.73e. From \( \sup(a + b) \leq \sup a + \sup b \).
4.73f. Follows from (d).
4.73g. Rao and Bhimasankaram [2000: 259; see the solution to exercise 15].
4.76. Horn and Johnson [1985: 303–305, further results are given there in section 5.6].
4.78. Horn and Johnson [1985: 306].
4.80. From the singular value decomposition of \( A \), \( \sigma_i^2 \) is the \( i \)th ordered eigenvalue of \( AA^* \) and the trace is the sum of the eigenvalues.
4.82. Since \( A^*A \) is non-negative definite it has non-negative eigenvalues \( \lambda_i \) and \( \text{trace}(A^*A) = \sum \lambda_i \). The result then follows from \( \lambda_{\max} \leq \sum \lambda_i \leq n\lambda_{\max} \) and taking square roots.

### 4.6.3 Unitarily Invariant Norms

**Definition 4.17.** A real-valued function \( \| \cdot \| \) on the vector space \( V \) of \( m \times n \) complex matrices is said to be a **unitarily invariant (generalized matrix) norm**, and denoted by \( \| \cdot \|_u \), if it has the following properties. We shall drop the words “generalized matrix” below.

1. \( \| A \| \geq 0 \) for all \( A \in V \) and \( \| A \| = 0 \) if and only if \( A = 0 \).
2. \( \| \alpha A \| = |\alpha| \| A \| \) for every \( \alpha \in \mathbb{C} \) and \( A \in V \).
(3) \(|A + B| \leq |A| + |B|\) for all \(A\) and \(B\) in \(V\).

(4) \(\|UAV\| = |A|\) for all \(A \in V\) and unitary matrices \(U\) and \(V\) of orders \(m \times m\) and \(n \times n\), respectively.

Thus a generalized matrix norm, which satisfies the first three conditions, is unitarily invariant if it satisfies (4) as well. If \(m = n\) and \(\|AB\| \leq |A||B|\) for all \(n \times n\) matrices, then \(\|\cdot\|\) is a matrix norm that we denote by \(\|\cdot\|_{ui}\).

If \(V\) is the space of real matrices, then we use the term orthogonally invariant norm.

**4.84.** Let \(\|\cdot\|_{ui}\) be a unitarily invariant norm defined on \(V\), the space of \(m \times n\) matrices. Then:

(a) \(\|AB^*\|_{ui} \leq \sigma_1(A)\|B\|_{ui}\) for all \(A, B \in V\).

(b) If \(E_{11}\) is the matrix with 1 in the \((1,1)\) position and zeros elsewhere, then \(\|A\|_{ui} \geq \sigma_1(A)\|E_{11}\|_{ui}\) for all \(A \in V\).

Here \(\sigma_1(A)\) is the maximum singular value of \(A\).

**4.85.** A unitarily invariant norm \(\|\cdot\|_{ui}\) on the space \(V\) of \(n \times n\) matrices is a matrix norm if and only if \(\|A\|_{ui} \geq \sigma_1(A) (= \|\|A\|\|_{2,in})\) for all \(A \in V\). An equivalent condition from (4.84b) above is \(\|E_{11}\|_{ui} \geq 1\). Note that Bhatia [1997: 91] uses the sufficient condition \(\|E_{11}\|_{ui} = 1\) in his definition of matrix norm, which leads to a slightly different norm.

**Definition 4.18.** We define the term general square root of the \(m \times n\) complex matrix \(A\) to be the unique non-negative definite matrix \((A^*A)^{1/2}\) (cf. 10.8), and denote it by \(|A|\).

**4.86.** Let \(A\) be an \(m \times n\) matrix. Since \((A^*A)^{1/2}\) has the same singular values as \(A\), which are the same as those of \(A^*\) (cf. 16.34d), then from (4.87) below we have

\[\|A\|_{ui} = \|A\|_{ui}\]

for all unitarily invariant norms.

**4.87.** Let \(A = P\Sigma Q^*\) be the singular value decomposition of an \(m \times n\) matrix \(A\), where \(\Sigma\) is diagonal and \(P\) and \(Q\) are unitary \(m \times m\) and \(n \times n\) matrices, respectively. Then

\[\|A\|_{ui} = \|P^*P\Sigma Q^*Q\|_{ui} = \|\Sigma\|_{ui}\]

which is a function of the singular values of \(A\). The nature of this function is discussed below.

**4.88.** Let \(A\) be an \(m \times n\) matrix.

(a) The Frobenius norm \(\|A\|_F = (\sum_{i=1}^m \sum_{j=1}^n |a_{ij}|^2)^{1/2}\) and \(\|A\|_{2,in} = \sigma_{max}\) (the maximum singular value of \(A\)) are both unitarily invariant generalized matrix norms. When \(m = n\) they are both unitarily invariant matrix norms.

(b) \(\|A\|_{2,in}\) is the only unitarily invariant norm that is also an induced norm.
Two other classes of unitarily invariant norms that seem to be of particular interest are the Ky Fan $k$-norms and the Schatten $p$-norms (Bhatia [1997: 92] and Horn and Johnson [1985: 441, 445]).

4.89. Suppose $A$ and $B$ belong to the vector space $V$ of $m \times n$ matrices and let $p = \min\{m, n\}$. In order that $\|A\|_{ui} \leq \|B\|_{in}$ for every unitarily invariant norm $\| \cdot \|_{ui}$ on $V$, it is sufficient that

$$\sigma_i(A) \leq \sigma_i(B) \quad \text{for all} \quad i = 1, 2, \ldots, p,$$

and it is necessary and sufficient that

$$\sigma_1(A) + \cdots + \sigma_i(A) \leq \sigma_1(B) + \cdots + \sigma_i(B), \quad i = 1, 2, \ldots, p.$$

We now introduce a function, called a symmetric gauge function, which is intimately related to the unitarily invariant matrix norm. In fact, $\|A\|$ is a unitarily invariant norm if and only it is a symmetric gauge function of the singular values of $A$ (cf. (4.87) and (4.92)).

**Definition 4.19.** A real-valued function $\phi$ from $\mathbb{R}^n$ to $\mathbb{R}$ is said to be a **symmetric gauge function** if it has the following properties.

1. $\phi(x) > 0$ for all $x \in \mathbb{R}^n$ with $x \neq 0$.
2. $\phi(\alpha x) = |\alpha| \phi(x)$ for all $x \in \mathbb{R}^n$ and $\alpha \in \mathbb{R}$.
3. $\phi(x + y) \leq \phi(x) + \phi(y)$ for all $x$ and $y$ in $\mathbb{R}^n$.
4. $\phi(x_{\pi}) = \phi(x)$ for all $x \in \mathbb{R}^n$ and all permutations $x_{\pi}$ of the elements of $x$.
5. $\phi(Jx) = \phi(x)$ for all $x \in \mathbb{R}^n$ and all diagonal matrices $J$ with diagonal elements $+1$ or $-1$. This is equivalent to $\phi(x) = \phi(\text{mod } x)$, where $\text{mod } x = (|x_i|)$.

4.90. The following hold.

(a) From (1) to (3) above, $\phi$ is a vector norm on $\mathbb{R}^n$.

(b) A symmetric gauge function is continuous.

(c) The sum of two symmetric gauge functions is a symmetric gauge function.

(d) A positive multiple of a symmetric gauge function is a symmetric gauge function.

(e) The $L_p$ vector norm ($p \geq 1$) on $\mathbb{R}^n$ is a symmetric gauge function.

For some examples of symmetric gauge functions, their properties, and some inequalities see Bhatia [1997: chapter 4].

4.91. Let $\phi$ be a symmetric gauge function, and let $x = (x_i) \in \mathbb{R}^n$.

(a) If $y = (y_i) = (p_i x_i)$, where $0 \leq p_i \leq 1$ for all $i$, then

$$\phi(y_1, \ldots, y_n) \leq \phi(x_1, \ldots, x_n).$$
(b) If \(0 \leq x_i \leq y_i\) for all \(i\), then
\[
\phi(x_1, \ldots, x_n) \leq \phi(y_1, \ldots, y_n).
\]

(c) \(k(\max_{1 \leq i \leq n} |x_i|) \leq \phi(x_1, \ldots, x_n) \leq k(\sum_{i=1}^{n} |x_i|)\), where \(k = \phi(1, 0, 0, \ldots, 0)\).

4.92. Let \(\|\cdot\|_{ui}\) be any unitarily invariant norm on the vector space \(V\) of \(m \times n\) real matrices, and let \(p = \min\{m, n\}\). For each \(x = (x_i) \in \mathbb{R}^m\) let \(X_{m \times n} = \text{diag}(x)\) and \(\phi(x_1, \ldots, x_m) = \|X\|_{ui}\). Then \(\phi\) is a symmetric gauge function. Thus from (4.87), with \(\Sigma\) replacing \(X\), we have that \(\|A\|_{ui} = \phi(\sigma_1(A), \sigma_2(A), \ldots, \sigma_p(A))\), where \(\phi\) is a symmetric gauge function and \(\sigma_i(A)\) is the \(i\)th singular value of \(A\).

Conversely, if \(\phi\) is a symmetric gauge function on \(\mathbb{R}^p\), then the function defined by
\[
\|A\| = \phi(\sigma_1(A), \sigma_2(A), \ldots, \sigma_p(A))
\]
is a unitarily invariant norm on \(V\).

Unitarily invariant norms and gauge functions have been found useful in multivariate analysis in relation to monotone properties of power functions and simultaneous confidence intervals (Mudholkar [1965, 1966] and Wijsmann [1979]).

4.93. The \(n \times n\) matrix \(A\) has the same singular values as \(A^*\) so that by (4.86) above, \(\|A\|_{ui} = \|A^*\|_{ui}\) for all \(A\) and all unitarily invariant norms. Such a norm is called a self-adjoint norm.

4.94. (Ky Fan) If \(\phi\) is a symmetric gauge function on \(\mathbb{R}^p\) and \(\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_p \geq 0\) and \(\sigma'_1 \geq \sigma'_2 \geq \cdots \geq \sigma'_p \geq 0\) are two sets of values, then
\[
\phi(\sigma_1, \ldots, \sigma_p) \geq \phi(\sigma'_1, \ldots, \sigma'_p)
\]
if and only if
\[
\sigma_1 + \ldots + \sigma_i \geq \sigma'_1 + \ldots + \sigma'_i, \quad i = 1, 2, \ldots, p.
\]

Proofs. Section 4.6.3.

4.84. Horn and Johnson [1991: 206].
4.85. Horn and Johnson [1985: 450; 1991: 211, exercise 3].
4.88b. Horn and Johnson [1985: 308].
4.94. Fan [1951].
4.6.4 $M, N$-Invariant Norms

**Definition 4.20.** Let $M$ be a given positive definite $m \times m$ matrix and $N$ a given $n \times n$ positive definite matrix. A generalized matrix norm on the space $V$ of $m \times n$ matrices is said to be an $M, N$-invariant norm if, in addition to conditions (1), (2), and (3) of Definition 4.17 in the previous section, it satisfies the following condition

$$\|VAU\| = \|A\| \quad \text{for every} \quad A \in V,$$

and any $m \times m$ matrix $V$ and any $n \times n$ matrix $U$ such that $V^*MV = M$ and $U^*NU = N$. This norm was introduced by Rao [1979, 1980] to deal with dimension-reducing techniques in multivariate analysis. When $M$ and $N$ are the identity matrices, the $M, N$-invariant norm becomes the unitarily invariant norm.

4.95. Using the above notation, let $M^{1/2}, M^{-1/2}, N^{1/2}$ and $N^{-1/2}$ be the respective positive definite square roots of $M, M^{-1}, N$ and $N^{-1}$ (cf. 10.32). Then the following hold.

(a) If $\|A\|_\alpha$ is a unitarily invariant norm of $A$, then $\|M^{1/2}AN^{1/2}\|_\alpha$ is an $M, N$-invariant norm of $A$.

(b) If $\|A\|_\beta$ is an $M, N$-invariant norm of $A$, then $\|M^{-1/2}AN^{-1/2}\|_\beta$ is a unitarily invariant norm of $A$.

**Proofs.** Section 4.6.4.


4.6.5 Computational Accuracy

An important question in computing is: How do errors both in the data and in the round-off affect the computation of expression—for example, the inverse of a nonsingular matrix? Suppose $A$ is $n \times n$ and, instead of computing $A^{-1}$, we actually compute $(A + \delta A)^{-1}$. Then, assuming that a particular matrix norm of the error $\|\delta A\|$ is small enough, Horn and Johnson [1985: 335–338] show that if $\|\delta A\| \|A^{-1}\| < 1$, then

$$\frac{\|A^{-1} - (A + \delta A)^{-1}\|}{\|A^{-1}\|} \leq \frac{\kappa(A)}{1 - \kappa(A)\|\delta A\|/\|A\|} \cdot \|\delta A\|,$$

where $\kappa(A) = \|A\|\|A^{-1}\|$. The above expression bounds the relative error in the inverse in terms of the relative error in the data. For $\|\delta A\|$ small, the right-hand side of the above expression is of the order of $\kappa(A)\|\delta A\|/\|A\|$. Therefore if $\kappa(A)$ is not large, the relative error in the inverse is of the same order as the relative error of the data.

One can obtain a similar result in computing an eigenvalue. For example, if $\lambda$ is an eigenvalue of $A + \delta A$, where $A$ is diagonalizable (e.g., symmetric) with $A = R\Lambda R^{-1}$ and $\Lambda = \text{diag}(\lambda_1, \ldots, \lambda_n)$, then there is some eigenvalue $\lambda_i$ of $A$ such that, for an appropriate matrix norm,

$$|\lambda - \lambda_i| \leq \|R\|\|R^{-1}\|\|\delta A\| = \kappa(R)\|\delta A\|.$$
Horn and Johnson [1985: section 6.3] derive a number of perturbation results like the one above for different properties of $A$ and $\delta A$.

Finally, we look at a corresponding result in relation to solving linear equations. For example, consider

$$(A + \delta A)(x + \delta x) = b + \delta b.$$  

Duff et al. [1986: 89–90] show that if $\|\delta A\|\|A^{-1}\| < 1$, then

$$\frac{\|\delta x\|}{\|x\|} \leq \frac{\kappa(A)}{1 - \kappa(A)} \left( \frac{\|\delta A\|}{\|A\|} + \frac{\|\delta b\|}{\|b\|} \right).$$

In introducing $\kappa(A)$ in the above discussion, we have not specified the norm $\| \cdot \|$. Furthermore, in deriving the above expression it transpires that we only require the norm to be an induced one. Also, the definition of $\kappa(A)$ used above is only appropriate for nonsingular matrices. By choosing an appropriate norm, we now generalize the definition to include nonsingular and rectangular matrices.

**Definition 4.21.** The *condition number* of an $m \times n$ real matrix $A$, denoted by $\kappa_2(A)$, is the ratio of the largest singular value to the smallest nonzero singular value. Thus,

$$\kappa_2(A) = \left( \frac{\lambda_{\text{max}}}{\lambda_{\text{min}}} \right)^{1/2},$$

where $\lambda_{\text{max}}$ is the largest and $\lambda_{\text{min}}$ is the smallest nonzero eigenvalue of $A'A$. Unfortunately, this condition number is not easy to compute, and for further details see Gentle [1998: 115–116].

4.96. When $A$ is positive definite, its eigenvalues are positive, $A'A = A^2$, and

$$\kappa_2(A) = \frac{\lambda_{\text{max}}}{\lambda_{\text{min}}}.$$

The same is true for a Hermitian positive definite $A$, as we replace $A'A$ by $A^*A$.

4.97. If $A$ is nonsingular, then

$$\kappa_2(A) = \frac{\|\|A\|\|_{2,in} \cdot \|\|A^{-1}\|\|_{2,in}}{\|\|A\|\|_{2,in}},$$

where $\|\| \cdot \|\|_{2,in}$ is the induced matrix norm corresponding to the $L_2$ vector norm (cf. 4.74b).

We can also define $\kappa_1(A)$ and $\kappa_\infty(A)$ corresponding to the $L_1$ and $L_\infty$ norms.

4.98. If $v = 1, 2, \text{ or } \infty$, then:

(a) $\kappa_v(A) = \kappa_v(A^{-1})$.

(b) $\kappa_v(cA) = \kappa_v(A)$ for $c \neq 0$.

(c) $\kappa_v(A) \geq 1$.

(d) $\kappa_1(A) = \kappa_\infty(A)$.

(e) $\kappa_2(A) = \kappa_2(A')$.

(f) $\kappa_2(A'A) = \kappa_2(A) \geq \kappa_2(A)$.

**Proofs.** Section 4.6.5.

4.98. Gentle [2000: 78].
Although complex matrices have been referred to in previous chapters, it seems appropriate to have a chapter that looks more closely at complex matrices. Complex matrices arise, for example, in time series and the related topic of signal processing, and in experimental designs. We shall initially list some general properties of complex matrices before looking at Hermitian matrices. The related matrices that are considered are the skew-Hermitian, complex symmetric, real symmetric, skew-symmetric, complex orthogonal, and normal matrices. Factorizations and decompositions for these matrices are given in Chapter 16, while results about eigenvalues and eigenvectors for these matrices are located in Chapter 6. Unitary and real orthogonal matrices are considered in greater detail in Section 8.1, and Fourier matrices are covered in Section 8.12.2. At the end of this chapter we briefly consider quaternions, which are used, for example, in nuclear physics.

5.1 COMPLEX MATRICES

Definition 5.1. Given a complex number \( x = x_1 + ix_2 \), where \( x_1 \) and \( x_2 \) are both real, then its complex conjugate is defined to be \( \bar{x} = x_1 - ix_2 \), and its modulus or absolute value is defined to be \( |x| = (x_1^2 + x_2^2)^{1/2} \). If \( A \) is complex, it can be expressed in the form \( A = A_1 + iA_2 \), where \( A_1 \) and \( A_2 \) are real matrices, and its complex conjugate is \( \bar{A} = A_1 - iA_2 \). We also define the conjugate transpose of \( A \) to be \( A^* = \bar{A}' \).
**Definition 5.2.** An \( n \times n \) matrix \( A \) is said to be a **Hermitian matrix** if \( A^* = A \) and **skew-Hermitian (anti-Hermitian)** if \( A = -A^* \).

A real or complex matrix \( A \) is symmetric if \( A = A' \).

A complex orthogonal \( n \times n \) matrix \( T \) is a complex matrix such that \( T'T = I_n \).

We omit the word "complex" if \( T \) is real.

An \( n \times n \) matrix \( U \) is called a **unitary matrix** if \( U^*U = I_n \).

**5.1.1 Some General Results**

5.1. For complex scalars \( x \) and \( y \) we have:

(a) \( |xy| = |x||y| \).

(b) \( |x + y| \leq |x| + |y| \).

(c) \( |x|^2 + |y|^2 \geq 2\Re(xy) \), where \( \Re \) is the "real part."

5.2. A complex orthogonal matrix \( T \) need not be unitary.

5.3. (Isomorphism Between Complex and Real Matrices) Let \( Z = Z_1 + iZ_2 \) be an \( n \times n \) complex matrix with \( Z_i \) \((i = 1, 2)\) real matrices. Let

\[
Z^R = \begin{pmatrix} Z_1 & -Z_2 \\ Z_2 & Z_1 \end{pmatrix},
\]

and define \( X^R \) and \( Y^R \) in a similar fashion.

(a) If \( Z = X + Y \), then \( Z^R = X^R + Y^R \).

(b) If \( Z = XY \), then \( Z^R = X^RY^R \).

(c) If \( W = Z^{-1} \), then \( W^R = (Z^R)^{-1} \).

(d) \( \det Z^R = |\det Z|^2 \).

(e) If \( Z \) is Hermitian, then \( Z^R \) is symmetric.

(f) If \( Z \) is unitary, then \( Z^R \) is orthogonal.

(g) Suppose the eigenvalues and eigenvectors of \( Z \) are \( \lambda_j \) and \( \alpha_j = \alpha_{1j} + i\alpha_{2j} \), \( j = 1, 2, \ldots, n \), where the \( \alpha_{rj} \) are real for \( r = 1, 2 \), and all \( j \). Then those of \( Z^R \) are, respectively,

\[
\lambda_j, \begin{pmatrix} \alpha_{1j} \\ \alpha_{2j} \end{pmatrix}; \quad \lambda_j, \begin{pmatrix} -\alpha_{2j} \\ \alpha_{1j} \end{pmatrix}, \quad j = 1, 2, \ldots, n.
\]

This result could be useful for carrying out numerical computations involving complex matrices.

5.4. Let \( x = (x_1, x_2, \ldots, x_n)' \) be a complex vector with \( |\sum_{i=1}^n x_i| = \sum_{i=1}^n |x_i| \). Then \( x_i = \theta|x_i|, \ i = 1, 2, \ldots, n \), for some complex number \( \theta \) satisfying \( |\theta| = 1 \).

5.5. If \( A \) is a square complex matrix and \( x^*Ax = 0 \) for all complex \( x \), then \( A = 0 \). Thus if \( x^*Ax = x^*Bx \) for all complex \( x \), then \( A = B \). However, these results do not necessarily hold if the matrices are real and the equalities hold for all real \( x \).
5.6. If $\mathbf{A}$ is an $n \times n$ real or complex matrix, then there exists a nonsingular matrix $\mathbf{S}$ such that $\mathbf{SAS}^{-1}$ is symmetric. There also exists a nonsingular matrix $\mathbf{R}$ such that $\mathbf{A}' = \mathbf{RAR}^{-1}$.

5.7. Let $\mathbf{A}$ be an $n \times n$ real or complex matrix. Then every product of $n$ entries of $\mathbf{A}$ taken from distinct rows and columns equals 0 (i.e., $a_{11}, a_{22}, \ldots, a_{nn} = 0$), with distinct $i_j$, if and only if $\mathbf{A}$ contains an $r \times s$ zero submatrix, where $r + s = n + 1$.

5.8. Let $\mathbf{A} = (a_{ij})$ be an $n \times n$ real or complex matrix with eigenvalues $\lambda_i$ ($i = 1, 2, \ldots, n$), then

$$\sum_{i=1}^{n} |\lambda_i|^2 \leq \sum_{i=1}^{n} \sum_{j=1}^{n} |a_{ij}|^2.$$ 

Equality occurs if and only if $\mathbf{A}$ is normal (cf. Section 5.6).

Proofs. Section 5.1.1.

5.1. Abadir and Magnus [2005: 12].

5.2. For a $2 \times 2$ counterexample see Horn and Johnson [1985: 71, exercise 8].

5.3. Quoted by Brillinger [1975: 71] with a corrected sign change. All the results except (c) and (d) can be verified directly, while (c) amounts to showing that if $\mathbf{WZ} = \mathbf{I}$ then $\mathbf{W}^R \mathbf{Z}^R = \mathbf{I}$; (d) follows from (5.10).

5.4. Bapat and Raghavan [1997: 19].

5.5. Davis [1979: 61–62]. For a counter example see (5.25).


5.1.2 Determinants

5.9. Let $\mathbf{A} = \mathbf{A}_1 + i\mathbf{A}_2$, where $\mathbf{A}_1$ and $\mathbf{A}_2$ are real $n \times n$ matrices. If $\det \mathbf{A} = a + ib$ and $|\cdot|$ represents the modulus, then:

- (a) $\det \mathbf{A} = a - ib$.
- (b) $\det \mathbf{A}' = \det \mathbf{A}$.
- (c) $|\det \mathbf{A}|^2 = |\det \mathbf{A}|^2 = a^2 + b^2 = |\det \mathbf{A} \det \mathbf{A}| = \det \mathbf{A} \det \mathbf{A}$.
- (d) $|\det \mathbf{A} \det \mathbf{A}| = |\det \mathbf{A} \det \mathbf{A}^T| = |\det(\mathbf{A} \mathbf{A}^T)|$.

5.10. Let

$$\mathbf{A} = \mathbf{A}_1 + i\mathbf{A}_2, \quad \mathbf{B} = \begin{pmatrix} \mathbf{A}_1 & \mathbf{A}_2 \\ -\mathbf{A}_2 & \mathbf{A}_1 \end{pmatrix} \quad \text{and} \quad \mathbf{C} = \begin{pmatrix} \mathbf{A}_1 & -\mathbf{A}_2 \\ \mathbf{A}_2 & \mathbf{A}_1 \end{pmatrix},$$

where \( A_1 \) and \( A_2 \) are real matrices. Then, for \( \det A_1 \neq 0 \),
\[
\det B = \det C \quad \text{and} \quad |\det A| = |\det B|^{1/2} = |\det C|^{1/2}.
\]

**Proofs.** Section 5.1.2.

5.9. The results (a)–(c) follow from the definition and the product rule for determinants, and (d) follows from the expansion of a determinant.


### 5.2 HERMITIAN MATRICES

5.11. An \( n \times n \) matrix \( A \) is Hermitian if and only if one (and therefore all) of the following five conditions hold.

1. \( x^*Ax \) is real for all \( x \in \mathbb{C}^n \).
2. \( A^2 = A^*A \).
3. \( \text{trace}(A^2) = \text{trace}(A^*A) \).
4. \( A \) is normal and all the eigenvalues of \( A \) are real.
5. \( S^*AS \) is Hermitian for all \( n \times n \) \( S \).

5.12. Suppose \( A \) is an \( n \times n \) Hermitian matrix. Then the following hold.

(a) \( A^k \) is Hermitian for \( k = 1, 2, \ldots \).
(b) \( iA \) is skew-Hermitian.
(c) If \( A \) is nonsingular, then \( A^{-1} \) is Hermitian.
(d) The diagonal elements of \( A \) are real.
(e) The eigenvalues of \( A \) are real (see Section 6.1.6 for further details).

5.13. Let \( A \) be an \( n \times n \) matrix.

(a) \( A \) can be expressed uniquely in the form \( A = S + iT \), where \( S \) and \( T \) are Hermitian.
(b) \( A \) can be expressed uniquely in the form \( A = B + C \), where \( B \) is Hermitian and \( C \) is skew-Hermitian.

5.14. (Complex Householder Matrix) If \( A = I_n - 2bb^* \), where \( b \) is a complex \( n \times 1 \) vector such that \( b^*b = 1 \), then \( A \) is Hermitian, unitary (i.e., \( A^*A = I_n \)), and involutionary (i.e., \( A^2 = I_n \)).

5.15. (Trace) If \( A \) is \( n \times n \), then:

(a) \( \text{trace}(AX) = 0 \) for all Hermitian matrices \( X \) if and only if \( A = 0 \).
(b) \( \text{trace}(AX) \) is real for all Hermitian \( X \) if and only if \( A \) is Hermitian.
5.16. A square matrix $A$ is a product of two Hermitian matrices if and only if it is similar to $A^*$.  

Proofs. Section 5.2.


5.13a. Horn and Johnson [1985: 170]. We set $A = \frac{1}{2}(A+A^*)+i\frac{1}{2}(A-A^*)$, and assume two such representations.

5.13b. Set $A = \frac{1}{2}(A+A^*) + \frac{1}{2}(A-A^*)$.


5.3 SKEW-HERMITIAN MATRICES

5.17. $A - A^*$ is skew-Hermitian for all square matrices $A$.

5.18. Let $A$ be skew-Hermitian.

(a) $iA$ is Hermitian.

(b) The diagonal elements of $A$ are all purely imaginary.

(c) Since the eigenvalues of an Hermitian matrix are real, the eigenvalues of $A$ (and therefore of a real skew-symmetric matrix) are purely imaginary or zero.

(d) $(I_n + A)$ is nonsingular.

5.19. Suppose $A$ is a skew-Hermitian $n \times n$ matrix. Then, using (5.18d) above, we have:

(a) $U = (I_n - A)(I_n + A)^{-1} = (I_n + A)^{-1}(I_n - A)$ is unitary as $U^*U = I_n$.

This follows from $(I_n - A)(I_n + A) = (I_n + A)(I_n - A)$.

(b) $U = [2I_n - (I_n + A)](I_n + A)^{-1}$.

(c) From (a) we see that $I_n - A$ and $(I_n + A)^{-1}$ commute.

(d) $I_n + U$ is nonsingular because, by (b), it equals $2(I_n + A)^{-1}$.

(e) The matrices $U$ and $A$ are in $(1,1)$-correspondence on account of the pair of equations

\[
U = 2(I_n + A)^{-1} - I_n, \\
A = 2(I_n + U)^{-1} - I_n.
\]

Thus $A$ is skew-Hermitian if and only if $U$ is unitary.
These results hold if $A$ is (real) skew-symmetric and $U$ is real orthogonal. Apparently the above results were first applied to statistics by Hsu [1953].

Proofs. Section 5.3.

5.18a. $(iA)^* = iA^* = (-i)(-A) = iA$.

5.18b. Use (a) and (5.12d).

5.18c. Use (5.12e).

5.18d. The determinant of a matrix is the product of its eigenvalues. Also, $\lambda(I_n + A) = 1 + \lambda(A) = 1 + ia \neq 0$, as from (c) $a$ is real or zero.

5.4 COMPLEX SYMMETRIC MATRICES

Although real symmetric matrices play a fundamental role in statistics, we shall first consider some results that hold for both real and complex symmetric matrices. Note that real symmetric matrices are also Hermitian (Section 5.2), normal (Section 5.6), and diagonalizable (Section 16.1), so that the results in those sections also apply to symmetric matrices.

5.20. We assume that $A$ is an $n \times n$ real or complex matrix.

(a) $A$ is symmetric if and only if there exists an $n \times n$ matrix $S$ such that $A = SS^\prime$.

We may choose $S = UD$, where $U$ is unitary,

$$D = \text{diag}(\sqrt{\sigma_1}, \sqrt{\sigma_2}, \ldots, \sqrt{\sigma_n}),$$

and the $\sigma_i$ are the singular values of $A$, in which case $\text{rank } S = \text{rank } A$.

(b) If $A$ is symmetric, then $A$ is diagonalizable (cf. Definition 16.3) if and only if it is complex orthogonally diagonalizable. Thus $A = SAS^{-1}$ for a diagonal matrix $\Lambda$ of eigenvalues of $A$ (cf. 16.17a) if and only if $A = QAQ^\prime$, where $Q$ is an $n \times n$ complex orthogonal matrix (i.e., $Q^\prime Q = I_n$).

5.21. If $A$ and $B$ are real or complex symmetric $n \times n$ matrices, then there exists a nonsingular $n \times n$ matrix $R$ such that $A = RBR^\prime$ if and only if $\text{rank } A = \text{rank } B$.

5.22. By considering a $2 \times 2$ matrix, we see that the eigenvalues values of a complex symmetric matrix are not necessarily real.

Proofs. Section 5.4.

5.20a. Horn and Johnson [1985: 207].

5.20b. Horn and Johnson [1985: 211–212].

5.21. Horn and Johnson [1985: 225]

5.22. For a counterexample, Abadir and Magnus [2005: 175] consider

$$\begin{pmatrix} 1 & i \\ i & 1 \end{pmatrix},$$

which has eigenvalues $1 \pm i$. 

5.5 REAL SKEW-SYMMETRIC MATRICES

**Definition 5.3.** A matrix $A$ is said to be *skew-symmetric* if $A' = -A$. Note that a complex matrix like

$$A = \begin{pmatrix} 0 & a \\ -a & 0 \end{pmatrix},$$

where $a$ is complex, is skew-symmetric. However, my focus is on real matrices as they are a special case of skew-Hermitian matrices; some of the properties in Section 5.3 will then apply for real matrices. For a factorization of a real skew-symmetric matrix see (16.46b(ii)).

5.23. The diagonal elements of a real skew-symmetric matrix are all zero.

5.24. Let $A$ be an $n \times n$ real skew-symmetric matrix.

(a) From (5.18c), the eigenvalues $\lambda_i(A)$ of $A$ are zero or purely imaginary and occur in conjugate pairs, as the characteristic polynomial has real coefficients. Hence the eigenvalues take the form $\pm ia_i$ with $a_i$ real ($i = 1, 2, \ldots, p$), along with $(n - 2p)$ zeros. Thus:

(i) If $n$ is odd, $\det(A) = 0$.

(ii) If $n$ is even, $\det(A) \geq 0$.

(iii) $\det(I_n + A) = \prod_{i=1}^{n}(1 + \lambda_i(A)) \geq 1$ with equality if and only if $A = 0$.

(b) Let $n = 2m$, then $\det(A)$ is the square of a polynomial of degree $m$ in the matrix entries (e.g., (4.45)). The polynomial is called the *pfaffian* of $A$ and is denoted by $Pf(A)$. There are two ways of defining a pfaffian and a helpful resource is [http://en.wikipedia.org/wiki/Pfaffian](http://en.wikipedia.org/wiki/Pfaffian). We have:

(i) $\det(A) = [\text{Pf}(A)]^2$.

(ii) $\text{Pf}(BAB') = \det(B)\text{Pf}(A)$.

(iii) $\text{Pf}(cA) = c^n\text{Pf}(A)$.

(iv) $\text{Pf}(A') = (-1)^n\text{Pf}(A)$.

(v) For an arbitrary $m \times m$ matrix $C$,

$$\text{Pf} \left( \begin{array}{cc} 0 & C \\ -C' & 0 \end{array} \right) = (-1)^{m(m-1)/2}\det(C).$$

For further references see Halton [1966b], Mehta [2004: 543-545, examples of computation] and Northcott [1984].

5.25. Let $A$ be a real square matrix and $x$ a real vector, then $x'Ax = 0$ for all $x$ if and only if $A$ is skew-symmetric.

**Proofs.** Section 5.5.

5.23. Follows from (5.18b).

5.24a(i). The determinant of a matrix is the product of its eigenvalues.

5.24a(ii). $(ia)(-ia) = a^2$, where $a$ may be zero.
5.24a(iii). Use (5.18d) and \((1 + ia)(1 - ia) = 1 + a^2\).


5.25. Davis [1979: 60–61].

5.6 NORMAL MATRICES

Definition 5.4. A square matrix \(A\) is said to be normal if \(AA^* = A^*A\). Note that Hermitian, skew-Hermitian, and unitary matrices are all normal, as are their real counterparts.

5.26. An \(n \times n\) matrix \(A\) with eigenvalues \(\lambda_1, \lambda_2, \ldots, \lambda_n\) is normal if and only if there exists a unitary matrix \(Q\) such that

\[ Q^*AQ = \text{diag}(\lambda_1, \lambda_2, \ldots, \lambda_n). \]

We say that \(A\) is unitarily diagonalizable. Note that this applies to Hermitian and unitary matrices (see also (16.46)).

5.27. If \(A\) is a commuting family of \(n \times n\) normal matrices (i.e., \(A_1A_2 = A_2A_1\) for all \(A_1, A_2 \in A\)), then every member of \(A\) is unitarily diagonalizable by the same unitary matrix.

5.28. In addition to being unitarily diagonalizable, normal matrices have many unique properties, some of which are listed below. The following statements are equivalent.

1. \(A\) is normal.

2. There exists a polynomial \(p(x)\) of degree at most \(n - 1\) such that \(A^* = p(A)\).

3. The singular values of \(A\) are \(|\lambda_1(A)|, |\lambda_2(A)|, \ldots, |\lambda_n(A)|\).

4. \(A = R + iS\), where \(R\) and \(S\) are real, symmetric, and commute (i.e., \(RS = SR\)).

5. Every eigenvector of \(A\) is an eigenvector of \(A^*\)

6. There exists a set of eigenvectors of \(A\) that form an orthonormal basis for \(\mathbb{C}^n\).

7. \(\sum_i \sum_j |a_{ij}|^2 = \sum_i |\lambda_i(A)|^2\).

5.29. If \(A\) is normal and \(p(z)\) is a polynomial, then \(p(A)\) is normal.

5.30. An upper-triangular matrix is normal if and only if it is diagonal.

5.31. A normal matrix is unitary if and only if its eigenvalues have absolute value 1.
5.32. If $A$ and $B$ are normal, then so is their Kronecker product $A \otimes B$.

5.33. If $A$ and $B$ are $n \times n$ normal matrices and $AB = BA$, then $AB$ is normal.

5.34. A normal matrix is Hermitian if and only if its eigenvalues are real, and it is skew-Hermitian if and only if its eigenvalues have zero real part.

**Proofs.** Section 5.6.


5.27. Horn and Johnson [1985: 103].

5.28. For these and further properties see Horn and Johnson [1985: 100–111] and Zhang [1999: 241–242].


5.31. From (5.26), $I = AA^* = UAU^*U\bar{A}U^* = U\bar{A}AU^*$ and $\bar{A}A = I$.

5.32. From (11.1f),

$$(A \otimes B)^*(A \otimes B) = (A^* \otimes B^*)(A \otimes B) = A^*A \otimes B^*B = AA^* \otimes BB^*,$$

which, by reversing the argument, is $(A \otimes B)(A \otimes B)^*$.

5.33. Using (5.27), we have $A = U\Lambda A^*, B = U\Lambda B^*$, and $AB = U\Lambda A\Lambda B U^* = UAU^*$. Then $AB(AB)^* = U\Lambda A\Lambda B U^* = U\Lambda A U^* = (AB)^*AB$. Also $A = -A^*$ if and only if $\Lambda = \bar{\Lambda}$.

5.34. If $A = UAU^*$, then $A = A^*$ if and only if $\Lambda = \bar{\Lambda}$.

### 5.7 QUATERNIONS

**Definition** 5.5. Just as a complex number has two components, a *quaternion number* has four components

$$q = q^{(0)} + q^{(1)}e_1 + q^{(2)}e_2 + q^{(3)}e_3 = q_0 + q \cdot e,$$

where the $e_i$ are quantities (not ordinary numbers) satisfying the symbolic rules

$$e_1^2 = e_2^2 = e_3^2 = -1, \quad e_1e_2 = -e_2e_1 = e_3, \quad e_2e_3 = -e_3e_2 = e_1, \quad e_3e_1 = -e_1e_3 = e_2,$$

where "1" is a particular unit identity. This 1 and the $e_i$ can be expressed as the matrices $C(1) = I_2$, and the so-called *Pauli matrices*

$$C(e_1) = \begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix}, \quad C(e_2) = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \quad \text{and} \quad C(e_3) = \begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix},$$

where $i = \sqrt{-1}$. Then

$$C(q) = \begin{pmatrix} q^{(0)} + iq^{(1)} & q^{(2)} + iq^{(3)} \\ -q^{(2)} + iq^{(3)} & q^{(0)} - iq^{(1)} \end{pmatrix}.$$
is a matrix representation of the quaternion \( q \). For any \( 2 \times 2 \) complex matrix we have

\[
\begin{pmatrix}
a & b \\
c & d
\end{pmatrix} = \frac{1}{2}(a + d)C(1) - \frac{i}{2}(a - d)C(e_1) + \frac{1}{2}(b - c)C(e_2) - \frac{i}{2}(b + c)C(e_3).
\]

Thus \( q^{(0)} = \frac{1}{2}(a + d) \), \( q^{(1)} = \frac{1}{2}(a - d) \), and so on.

The \( q^{(i)} \) can be real or complex. If they are all real, then we call the quaternion real, though \( C(q) \) isn’t necessarily real. The notation for quaternions is a little different from the usual for complex numbers. For example, the *conjugate quaternion* of a complex quaternion \( q = q^{(0)} + q \cdot e \) is

\[
\bar{q} = q^{(0)} - q \cdot e,
\]

which is different from its *complex conjugate quaternion*

\[
q^* = q^{(0)*} + q^* \cdot e.
\]

A quaternion with \( q^* = q \) is real. Applying both types of conjugation together, we obtain the *Hermitian conjugate*

\[
q^\dagger = \bar{q}^* = q^{(0)*} - q^* \cdot e.
\]

When \( q^\dagger = q \), \( q \) is called a *Hermitian quaternion*, and it can be shown directly after some algebra that \( C(q) \) is a \( 2 \times 2 \) Hermitian matrix. If \( q^\dagger = -q \), then it is called an *anti-Hermitian quaternion* and the corresponding matrix \( C(q) \) is skew-Hermitian.

For further information about quaternions see Carmeli [1983: chapters 8 and 9], Kantor and Solodovnikov [1989], Mehta [2004: 39], and, particularly, Zhang [1997]; for a geometrical perspective see Hanson [2006].

Since any \( 2n \times 2n \) complex matrix \( Q \) can be expressed in terms of \( n^2 \) blocks of \( 2 \times 2 \) matrices, we can write \( Q = (q_{ij}) \) for \( i, j = 1, 2, \ldots, n \), where \( q_{ij} \) is a quaternion with matrix representation \( C(q_{ij}) \). We call \( Q \) an \( n \times n \) *quaternion matrix*. Using quaternion arithmetic, we can define certain matrix properties for quaternion matrices, namely transposition

\[
(Q^\dagger)_{ij} = -e_2 \bar{q}_{ij} e_2,
\]

Hermitian conjugation

\[
(Q^\dagger)_{ij} = q^\dagger_{ji},
\]

and dual

\[
(Q^R)_{ij} = e_2 (Q^\dagger)_{ij} e_2^{-1} = \bar{q}_{ji}.
\]

If \( Q = Q^R \), the matrix is said to be *self-dual*. For further matrix details see Mehta [1989].

5.35. Let \( Q \) be a quaternion matrix. Then:

(a) \( Q^R = Q^\dagger \) is necessary and sufficient for the elements of \( Q \) to be real quaternions. When this holds we call such a matrix *quaternion real*.

(b) If \( Q \) is both Hermitian and self-dual, then it is also quaternion real. Furthermore, since \( q^\dagger_{ij} = \bar{q}_{ij} = q_{ji} \) for all \( i, j \), the \( 2 \times 2 \) corresponding matrix \( q_{ij}^{(0)} \)
must form a real symmetric matrix, whereas \(q_{ij}^{(1)}, q_{ij}^{(2)},\) and \(q_{ij}^{(3)}\) must lead to real skew-symmetric matrices. Self-dual Hermitian quaternion matrices have an important role in nuclear physics and are related to random matrices (cf. Section 21.10). The corresponding \(2n \times 2n\) Hermitian matrix is called a self-dual Hermitian matrix.

**Definition 5.6.** Let \(Z_1 = C(e_2) \otimes I_n = \begin{pmatrix} 0 & I_n \\ -I_n & 0 \end{pmatrix}\), a \(2n \times 2n\) matrix, where \(\otimes\) is the Kronecker product. A real \(2n \times 2n\) matrix \(A\) is said to be Hamiltonian if \((Z_1A)' = Z_1A\). Note that \(Z_1\) is skew-symmetric. Hamiltonian matrices are used in classical mechanics for the study of Hamiltonian dynamical systems.

5.36. \([C(e_2)]^{-1} = [C(e_2)]' = -C(e_2)\). Also \(C(e_2)^2 = -I_2\).

5.37. \(Z_1^2 = C(e_2)^2 \otimes I_n = -I_2 \otimes I_n = -I_{2n}\) and \(Z_1^{-1} = -Z_1 = Z_1'\).

5.38. Let \(A\) be an \(2n \times 2n\) Hamiltonian matrix. Then:

(a) Since \(Z_1A\) is symmetric, \(Z_1A + A'Z_1 = 0\) and, by (5.37), \(A = -Z_1^{-1}A'Z_1 = Z_1A'Z_1\).

(b) \(A'\) is Hamiltonian.

(c) \(\text{trace } A = 0\).

5.39. Let

\[
A = \begin{pmatrix} C & D \\ E & F \end{pmatrix},
\]

where all matrices are \(n \times n\), \(D\) and \(E\) are symmetric, and \(C + F' = 0\). Then \(A\) is Hamiltonian.

**Definition 5.7.** A real or complex \(2n \times 2n\) matrix \(B\) is said to be symplectic if \(B'ZB = Z\), where \(Z\) is a nonsingular, skew-symmetric matrix. Typically, \(Z = Z_1\), as defined above, or \(Z = Z_2\), where

\[
Z_2 = I_n \otimes C(e_2) = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & \cdots & 0 & 0 \\ -1 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & \cdots & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & 0 & \cdots & -1 & 0 \end{pmatrix},
\]

a matrix used in nuclear physics. In this case, \(Z_2\) can expressed as an \(n \times n\) quaternion matrix \(e_2I_n\) (Mehta [2004: 38-41]).

5.40. \(Z_2\) has the same properties as \(Z_1\) in (5.37).

5.41. If \(B\) is symplectic, then (i) \(B^{-1} = Z^{-1}B'Z\) and (ii) \(\det(B) = 1\).

5.42. The matrix \(Z_i\) \((i = 1, 2)\) is symplectic.

5.43. Let \(H\) be any quaternion real \(2n \times 2n\) matrix. Then there exist a symplectic matrix \(B\) such that \(H = B^{-1}DB\), where \(D\) is a real, scalar, and diagonal matrix. Here scalar means that \(D = \text{diag}(d_1, d_1, d_2, d_2, \ldots, d_n, d_n)\) so that the eigenvalues of \(H\) consist of equal pairs. For further extensions see Carmeli [1983: 70-71].
Proofs. Section 5.7.

5.36-5.37. These are straightforward; we use (11.1e), (11.1i), and (11.11).

5.38b. Taking transposes in (a) and using (5.37), we have $A' = Z_1 AZ_1$.

5.38c. Using (a), $\text{trace } A = -\text{trace}(Z_1^{-1} A' Z_1) = -\text{trace } A'$.

5.39. Show that $Z_1 A$ is symmetric.

5.40. $Z_2^2 = I_n \otimes C(e_2)^2 = -I_n \otimes I_2 = -I_{2n}$.

5.41. The result (i) follows from the definition by multiplying on the left by $Z^{-1}$ and on the right by $B^{-1}$, and (ii) follows from (5.24b(ii)).

5.42. $(Z_i' Z_i) Z_i = (Z_i^{-1} Z_i) Z_i = Z_i$.

5.43. Carmeli [1983: 70].
EIGENVALUES, EIGENVECTORS, AND SINGULAR VALUES

Eigenvalues, eigenvectors, and singular values play an important role in statistics, and they arise in most of the chapters in this book. In this chapter we deal with these topics in a general sense. They also occur in a number of important inequalities in this chapter, in Chapter 14, and in Chapter 23 on majorization, and they underlie many of the factorizations and decompositions in Chapter 16. For those relating to specific matrices and some patterned matrices, the reader will need to refer to the index for those matrices. This chapter closes with a brief introduction to antieigenvalues and antieigenvectors, which are becoming of increasing interest to statisticians in recent years.

6.1 INTRODUCTION AND DEFINITIONS

Definition 6.1. Let $A$ be an $n \times n$ matrix, which we assume to have elements in $F$ (i.e., either $\mathbb{R}$ or $\mathbb{C}$, unless otherwise stated). The polynomial $c(\lambda) = \det(A - \lambda I_n)$ is called the characteristic polynomial. The equation $c(\lambda) = 0$ is called the characteristic equation, and its roots are called the eigenvalues (characteristic roots, latent roots) of $A$. Many authors use $f(\lambda) = \det(\lambda I_n - A) = (-1)^n \det(A - \lambda I_n)$ for the characteristic polynomial, as the coefficient of $\lambda^n$ is now 1. This alternative version is sometimes more convenient, so both $c(\cdot)$ and $f(\cdot)$ are used below.

Eigenvalues may be real, complex, or a mixture of both. We shall order the eigenvalues by their modulus values, i.e., $|\lambda_1| \geq |\lambda_2| \geq \cdots \geq |\lambda_n| \geq 0$. If $\lambda_1$ is unique, we shall call it the dominant eigenvalue. In this case there exists a unique
right eigenvector $x_1$ of unit length such that $Ax_1 = \lambda_1 x_1$, called the dominant eigenvector.

The $s$ distinct eigenvalues are denoted by $\mu_1, \mu_2, \ldots, \mu_s$ (or $\mu_j(A)$, $j = 1, 2, \ldots, s$), where $|\mu_1| > |\mu_2| > \cdots > |\mu_s| \geq 0$. The set of $\mu_j$ is called the spectrum of $A$, and $\rho(A) = |\lambda_1|$ is called the spectral radius. We can therefore write $f(\lambda) = \prod_{j=1}^{s} (\lambda - \mu_j)^{m_j}$, where $\sum_{j=1}^{s} m_j = n$. Here $m_j$ (or $m(\mu_j)$) is called the algebraic multiplicity of the eigenvalue $\mu_j$. If $m_j = 1$, $\mu_j$ is called a simple eigenvalue, while if $m_j > 1$, $\mu_j$ is called a multiple eigenvalue.

For every $\mu_j$ there exists a nonzero solution $x$ such that $Ax = \mu_j x$, and $x$ is called an eigenvector associated with $\mu_j$. The set of all such $x$ together with $0$, namely $\mathcal{N}(A - \mu_j I_n)$ the null space of $A - \mu_j I_n$, is called the eigenspace of $\mu_j$. The dimension $g_j$ (or $g(\mu_j)$) of this space is called the geometric multiplicity of $\mu_j$. To avoid ambiguity, we shall refer to such an $x$ as a right eigenvector. There similarly exists a nonzero $y$ such that $y^T A = \mu_j y'$ called the left eigenvector of $A$ associated with $\mu_j$.

If $m(\mu_j) = g(\mu_j)$, then $\mu_j$ is said to be a semisimple eigenvalue.

6.1. (Multiplicities). Let $A$ be an $n \times n$ matrix.

(a) $g(\mu_j) \leq m(\mu_j)$; that is, the geometric multiplicity is no greater than the algebraic multiplicity.

(b) $\text{rank}(A - \mu_j I_n) = n - g(\mu_j) \geq n - m(\mu_j)$ for all $j$.

(c) If $m(\mu_j) = 1$ so that $\mu_j$ is a simple eigenvalue, then $g(\mu_j) = 1$ and $\text{rank}(A - \mu_j I_n) = n - 1$. Conversely, if $\text{rank}(A - \mu_j I_n) = n - 1$, then $\mu_j$ is an eigenvalue, but not necessarily a simple eigenvalue.

Proofs. Section 6.1


6.1b. From (3.3a), $\text{dim} \mathcal{C}(B) + \text{dim} \mathcal{N}(B) = n$ for $B = A - \mu_j I_n$, as $\text{dim} \mathcal{C}(A^*) = \text{rank} A^* = \text{rank} A = \text{dim} \mathcal{C}(A)$.

6.1c. Magnus and Neudecker [1999: 20].

6.1.1 Characteristic Polynomial

Definition 6.2. (Symmetric Functions) Given a set of constants $\lambda_1, \ldots, \lambda_n$, we define the elementary symmetric functions as

\[
S_1 = \sum_{i=1}^{n} \lambda_i, \\
S_2 = \sum_{1 < j} \lambda_i \lambda_j, \\
S_r = \sum_{i_1 < i_2 < \cdots < i_r} \lambda_{i_1} \lambda_{i_2} \cdots \lambda_{i_r}, \\
S_n = \lambda_1 \lambda_2 \cdots \lambda_n.
\]
Also, let \( c(\lambda) = (-1)^n(\lambda^n + a_1\lambda^{n-1} + \cdots + a_{n-1}\lambda + a_n) = (-1)^nf(\lambda) \) be the characteristic polynomial.

6.2. If the characteristic polynomial has real coefficients, then any complex eigenvalues must come in conjugate pairs.

6.3. (Cayley–Hamilton theorem) \( f(A) = 0 \).

6.4. The coefficient \( a_r \) \((r = 1, 2, \ldots, n)\) is \((-1)^r\) times the sum of all the \( r \times r \) principal minors of \( A \). These are obtained by striking out \( n - r \) rows and the same numbered columns of \( A \) and taking the determinant of the remaining submatrix.

(a) \( a_r = (-1)^rS_r \) \((r = 1, 2, \ldots, n)\) with \( a_n = (-1)^n\det A \).

(b) From (a), \( S_r \) is the sum of all the \( r \times r \) principal minors of \( A \).

(c) If \( t_r = \lambda_1^r + \lambda_2^r + \cdots + \lambda_n^r \) for \( r = 1, 2, \ldots, n \) and we define \( 0 \equiv a_{n+1} \equiv a_{n+2} \equiv \ldots \), then \( t_r + t_{r-1}a_1 + \cdots + t_1a_{r-1} + ra_r = 0 \) \((r = 1, 2, \ldots)\). These expressions for the \( a_r \) are known as Newton’s identities (Hunter [1983a: 156–157]).

6.5. If \( A \) is \( n \times n \), and \( \mu \) is not an eigenvalue of \( A \), then \( A - \mu I_n \) is nonsingular as its determinant is nonzero.

6.6. If \( A, B, \) and \( R \) are \( n \times n \) matrices, and \( B = RAR^{-1} \) (i.e., \( A \) and \( B \) are similar), then \( A \) and \( B \) have the same characteristic polynomial. Note that having the same eigenvalues is a necessary but not sufficient condition for similarity.

6.7. If \( A \) and \( B \) are real \( n \times n \) matrices, then the eigenvalues of

\[
C = \begin{pmatrix} A & B \\ B & A \end{pmatrix}
\]

are those of \( A + B \) and \( A - B \).

**Definition 6.3.** If \( f \) is a polynomial such that \( f(A) = 0 \), we say that \( f \) annihilates \( A \). A polynomial is said to be **monic** if the coefficient of the highest power is unity.

6.8. If \( A \) is \( n \times n \), there exists a unique monic polynomial of minimum degree no greater than \( n \) that annihilates \( A \).

**Definition 6.4.** The monic polynomial \( q(\lambda) \) of the least degree that annihilates \( A \) is called the **minimal polynomial**.

6.9. Every monic polynomial is both the minimal polynomial and the characteristic polynomial \((f(\lambda) \text{ version})\) of its companion matrix (cf. 6.14).

6.10. The minimal polynomial divides every polynomial that annihilates \( A \). It therefore divides the characteristic polynomial \( f(\lambda) \) (by 6.3).

6.11. If \( q(\lambda) \) is the minimal polynomial of \( A \), then \( \lambda \) is a root \( q(\lambda) = 0 \) if and only if it is an eigenvalue of \( A \). Thus every root of the characteristic equation is a root of \( q(\lambda) = 0 \).

6.12. If \( A, B, \) and \( R \) are \( n \times n \) matrices, then \( A \) and the similar matrix \( B = RAR^{-1} \) have the same minimal polynomial.
6.13. Let \( A \) be an \( n \times n \) matrix, and let \( A^k \) be the first matrix for which the set \( \{ I_n, A, A^2, \ldots, A^t \} \) is linearly independent, that is, \( A^k = \sum_{i=0}^{k-1} a_i A^i \). Then the minimum polynomial of \( A \) is \( x_k - \sum_{i=0}^{k-1} a_i x^i \).

6.14. (Companion Matrix) Consider the polynomial \( p_n(x) = x^n + a_{n-1}x^{n-1} + \cdots + a_1x + a_0 \). The matrix

\[
A = \begin{pmatrix}
0 & 0 & \cdots & 0 & -a_0 \\
1 & 0 & \cdots & 0 & -a_1 \\
\vdots & \vdots & \ddots & \vdots & \vdots \\
0 & 0 & \cdots & 0 & -a_{n-2} \\
0 & 0 & \cdots & 0 & -a_{n-1}
\end{pmatrix}
\]

is called the companion matrix of the polynomial \( p_n \) (Golub and Van Loan [1996: 348] and Horn and Johnson [1985: 146]). However, variations on the above matrix are also called the companion matrix, such as the transpose of \( A \) (e.g., Abadir and Magnus [2005: 173–174] and Rao and Bhimasankaram [2000: 283, solution to exercise 3]). Some authors take the transpose, then move the bottom row to the top and shift the other rows down one.

If \( A \) is defined above, then:

(a) \( \det(xI_n - A) = \det(xI_n - A^t) = p_n(x) \).

(b) \( p_n(x) \) is also the minimal polynomial of \( A \).

A version of the companion matrix can be used to find various upper and lower bounds on the roots of \( f_n(\lambda) = 0 \), as in Horn and Johnson [1985: 316–320]. Boshnakov [2002] extends the above concept to multi-companion matrices.

**Proofs.** Section 6.1.1


6.4b. Horn and Johnson [1985: 42].


6.6. Horn and Johnson [1985: 45].

6.7. Let \( (A + B)u = \lambda u \) and \( (A - B)v = \mu v \). Then \( C \) has eigenvectors \( (u', u')' \) and \( (v', -v')' \).


6.9. Horn and Johnson [1985: 147].


6.11. Horn and Johnson [1985: 143].
295].


6.1.2 Eigenvalues

We assume that $A$ is $n \times n$.

6.15. For every $j$, and $A$ real or complex:

(a) $\lambda_j(A') = \lambda_j(A)$.

(b) $\lambda_j(A) = \bar{\lambda}_j(A)$.

(c) $\lambda_j(A^*) = \bar{\lambda}_j(A)$.

(d) $\lambda_j(K^{-1}AK) = \lambda_j(A)$ for all $j$.

6.16. If $A$ has $r$ nonzero eigenvalues, then:

(a) $\text{rank } A \geq r$

(b) It is possible to have $r = 0$, but have $\text{rank } A = n - 1$.

6.17. We have the following:

(a) If $k$ is a positive integer, then

$$\text{trace } A^k = \sum_{i=1}^{n} \lambda_i^k.$$ 

(b) Taking $k = 1$, $\text{trace } A = \sum_{i=1}^{n} \lambda_i$.

(c) $\det(A) = \prod_{i=1}^{n} \lambda_i$.

6.18. $A$ is nonsingular if and only if $\lambda_j(A) \neq 0$ for all $j$ (cf. 6.17c).

6.19. If $A$ is triangular, then, since the determinant of the upper-triangular matrix

$A - \lambda I_n$ is the product of its diagonal elements, the eigenvalues are the diagonal

elements of $A$.

6.20. If $\lambda_n = 0$ is the only zero eigenvalue, then

$$\text{trace}(\text{adj } A) = \prod_{i=1}^{n-1} \lambda_i,$$

where $\text{adj } A$ is the adjoint matrix of $A$. 
6.21. (Bounds Using Traces) Let $A$ be an $n \times n$ real or complex matrix with real eigenvalues $\lambda_i$; for example, $A$ is Hermitian or symmetric. Define

$$m = \frac{1}{n} \sum_{i=1}^{n} \lambda_i = \frac{1}{n} \text{trace}(A)$$

and

$$s^2 = \frac{1}{n} \left( \sum_{i=1}^{n} \lambda_i^2 \right) - m^2 = \frac{1}{n} \text{trace}(A^2) - m^2.$$

(a) Then

$$m - s(n - 1)^{1/2} \leq \lambda_{\min}(A) \leq m - s(n - 1)^{-1/2},$$

$$m + s(n - 1)^{-1/2} \leq \lambda_{\max}(A) \leq m + s(n - 1)^{1/2}.$$  

Equality on the left (respectively right) of the first equation holds if and only if equality holds on the left (respectively right) of the second equation, if and only if the $n - 1$ largest (respectively smallest) eigenvalues are equal. When $n = 2$ we have $\lambda_{\min}(A) = m - s$ and $\lambda_{\max}(A) = m + s$.

(b) (Bounds on the Condition Number) Let $A$ be Hermitian positive definite with condition number $\kappa_2(A) = \lambda_{\max}(A)/\lambda_{\min}(A)$ (cf. 4.96).

(i) When $n$ is even,

$$1 + \frac{2s}{m - s(n - 1)^{-1/2}} \leq \kappa_2(A).$$

When $n > 2$, equality holds if and only if $A = cI_n$, where $c$ is a real constant.

(ii) When $n$ is odd, (i) holds along with

$$1 + \frac{2sn(n^2 - 1)^{-1/2}}{m - s(n - 1)^{-1/2}} \leq \kappa_2(A).$$

When $n = 3$, equality holds if and only if the two smallest eigenvalues are equal. When $n > 3$, equality holds if and only if $A = cI_n$.

(iii) In general,

$$\kappa_2(A) \leq 1 + \frac{(2n)^{1/2}s[m + s(n - 1)^{-1/2}]^{n-1}}{\det A}.$$  

When $n > 2$, equality holds if and only if $A = cI_n$.

(iv) If $A$ is Hermitian, $\text{trace } A > 0$, and $(\text{trace } A)^2 > (n - 1)\text{trace}(A^2)$, then $A$ is positive definite, (i) holds, and

$$\kappa_2(A) \leq 1 + \frac{(2n)^{1/2}s}{m - s(n - 1)^{1/2}}.$$  

When $n > 2$, equality holds if and only if $A = cI_n$.  

(c) Suppose \( A \) has real eigenvalues with \( f \) eigenvalues of \( A \) positive and \( g \) negative. Let \( \text{trace}(A^2) > 0 \).

(i) When \( \text{trace} A \geq 0 \), then

\[
(\text{trace} A)^2 / \text{trace}(A^2) \geq f,
\]

with equality if and only if all the positive eigenvalues are equal and all the nonpositive eigenvalues are equal.

(ii) When \( \text{trace} A \leq 0 \), then

\[
(\text{trace} A)^2 / \text{trace}(A^2) \leq g,
\]

with equality if and only if all the negative eigenvalues are equal and all the non-negative eigenvalues are equal.

(d) Let \( \lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n \).

(i) Then

\[
\lambda_k - \lambda_l \leq s \left( \frac{1}{k} + \frac{1}{n-l+1} \right)^{1/2}, \quad 1 \leq k \leq l \leq n.
\]

Equality occurs if and only if

\[
\lambda_1 = \lambda_2 = \cdots = \lambda_k,
\]

\[
\lambda_{k+1} = \lambda_{k+2} = \cdots = \lambda_{l-1} = m,
\]

\[
\lambda_l = \lambda_{l+1} = \cdots = \lambda_n.
\]

(ii) From (i) we have

\[
\lambda_1 - \lambda_n \leq (2n)^{1/2} s.
\]

When \( n > 2 \), equality holds if and only if

\[
\lambda_2 = \lambda_3 = \cdots = \lambda_{n-1} = \frac{1}{2} (\lambda_1 + \lambda_n).
\]

(iii) If \( n = 2q \) is even, then

\[
2s \leq \lambda_1 - \lambda_n,
\]

with equality if and only if

\[
\lambda_1 = \lambda_2 = \cdots = \lambda_q \quad \text{and} \quad \lambda_{q+1} = \lambda_{q+2} = \cdots = \lambda_n.
\]

(iv) If \( n = 2q \pm 1 \) is odd, the previous inequality (iii) holds and

\[
2sn(n^2 - 1)^{-1/2} \leq \lambda_1 - \lambda_n,
\]

with equality if and only if the conditions for the equality of (iii) hold.

(v)

\[
\frac{(\text{trace } A)^2}{\text{trace}(A^2)} \leq n - 2 + \frac{(\lambda_1 + \lambda_n)^2}{\lambda_1^2 + \lambda_n^2}.
\]
When $n > 2$, equality holds if and only if $\lambda_1 + \lambda_n \neq 0$ and
\[
\lambda_2 = \lambda_3 = \cdots = \lambda_{n-1} = \frac{\lambda_1^2 + \lambda_n^2}{\lambda_1 + \lambda_n}.
\]

(e) The above results can be extended to complex matrices with complex eigenvalues. For example, if $A$ now has complex eigenvalues $|\lambda_1| \geq |\lambda_2| \geq \cdots \geq |\lambda_n|$ and we define
\[
m = \frac{1}{n} \text{trace } A \quad \text{and} \quad s_n^2 = \frac{1}{n} \text{trace}(A^*A) - |m|^2,
\]
then:

(i) $|m| - s_n(n-1)^{1/2} \leq |\lambda_n| \leq |\text{trace}(A^*A)/n|^{1/2}$.

Equality holds on the left if and only if $A$ is normal, $\lambda_1 = \lambda_2 = \cdots = \lambda_{n-1}$, and $\lambda_n = cm$ for some real non-negative scalar $c \leq 1$. Equality holds on the right if and only if $A$ is normal and $|\lambda_1| = |\lambda_2| = \cdots = |\lambda_n|$.

(ii) $|m| \leq |\lambda_1| \leq |m| + s_n(n-1)^{1/2}$.

Equality holds on the left if and only if $\lambda_1 = \lambda_2 = \cdots = \lambda_n$. Equality holds on the right if and only if $A$ is normal, $\lambda_2 = \lambda_3 = \cdots = \lambda_n$, and $\lambda_1 = cm$ for scalar $c \geq 1$.

(iii) If $A$ has $k$ nonzero eigenvalues, then
\[
|\text{trace } A|^2 / \text{trace}(A^*A) \leq k \leq \text{rank } A.
\]

Equality holds on the left if and only if $A$ is normal and $|\lambda_1| = |\lambda_2| = \cdots = |\lambda_k|$. Equality holds on the right if and only if rank $A = \text{rank}(A^2)$.

Further extensions are given by Wolkowicz and Styan [1980].

Additional results relating to sums of eigenvalues are given by Wolkowicz and Styan [1980]. Extensions are given by Merikoski and Virtanen [2004] and are used to give a lower bound for the Perron root of a non-negative matrix.

6.22. Let $A = (a_{ij})$ and $B = (b_{ij})$ be $n \times n$ matrices with eigenvalues $\lambda_i$ and $\gamma_i$, respectively. Define
\[
M = \max_{1 \leq i \leq n, 1 \leq j \leq n} (|a_{ij}|, |b_{ij}|) \quad \text{and} \quad \delta(A, B) = \frac{1}{n} \sum_{i=1}^{n} \sum_{j=1}^{n} |a_{ij} - b_{ij}|,
\]
then
\[
\max_{1 \leq i \leq n} \min_{1 \leq j \leq n} |\lambda_i - \gamma_j| \leq (n + 2)M^{1-n-1}[\delta(A, B)]^{1/n}.
\]

6.23. Let $A$ and $B$ be real $n \times n$ symmetric matrices with $C(A) \subseteq C(B)$. Suppose that $B$ is non-negative definite, and let $X$ be an $n \times k$ matrix. Then:

(a) $C(X'AX) \subseteq C(X'BX)$.

(b) Consider the eigenvalues of $(X'BX)^{-1}X'AX$ for any weak inverse $(X'BX)^{-1}$.
(i) The eigenvalues are all real and do not depend on the choice of generalized inverse.
(ii) The eigenvalues are the generalized eigenvalues of \( X'AX \) with respect to \( X'BX \) (cf. Section 6.1.8).

(c) \( \text{In}[(X'AX)'X'AX] = \text{In}(X'AX) \), where \( \text{In}(\cdot) \) is the inertia.

6.24. For each \( i, \lambda_i \) is a continuous function of the elements of \( A \).

6.25. (Quadratic Inequalities) Suppose \( A \) is an \( n \times n \) Hermitian matrix and \( x_i \) \( (i = 1, 2, \ldots, n) \) are a set of mutually orthonormal vectors, i.e., \( x_i^*x_j = \delta_{ij} \), then:

(a) \( \sum_{i=1}^{k} x_i^*Ax_i \leq \sum_{i=1}^{k} \lambda_i(A), \quad k = 1, 2, \ldots, n - 1. \)
(b) \( \sum_{i=1}^{n} x_i^*Ax_i = \sum_{i=1}^{n} \lambda_i(A). \)

6.26. (Hirsch and Bendixson) Let \( A = (a_{ij}) \) be an \( n \times n \) complex matrix with eigenvalues \( \lambda_i \), and define the Hermitian matrices \( B = (A + A^*)/2 \) and \( C = (A - A^*)/(2i) \). Then:

(a) \( |\lambda_i| \leq n \max_{i,j} |a_{ij}|. \)
(b) \( |\Re(\lambda_i)| \leq n \max_{i,j} |b_{ij}|. \)
(c) \( |\Im(\lambda_i)| \leq n \max_{i,j} |c_{ij}|. \)

Here \( \Re \) and \( \Im \) denote the “real” and “imaginary” parts, respectively. When \( A \) is Hermitian, the three results all reduce to (a).

6.27. (Schur) If \( A = (a_{ij}) \) is an \( n \times n \) complex matrix with eigenvalues \( \lambda_i \), then

\[
\sum_{i=1}^{n} |\lambda_i|^2 \leq \sum_{i} \sum_{j} |a_{ij}|^2,
\]

with equality if and only if \( A \) is a normal matrix.

6.28. If \( A \) is any \( n \times n \) matrix, then, given \( \varepsilon > 0 \), there exists an \( n \times n \) matrix \( B \) with distinct eigenvalues such that

\[
\sum_{i=1}^{n} \sum_{j=1}^{n} |a_{ij} - b_{ij}| < \varepsilon.
\]

6.29. (Geršgorin) Let \( A = (a_{ij}) \) be an \( n \times n \) matrix, and let

\[
R_i = \sum_{j=1; j \neq i}^{n} |a_{ij}|, \quad i = 1, 2, \ldots, n.
\]

(a) All the eigenvalues of \( A \) are located in the union of \( n \) discs (called Geršgorin discs)

\[
\cup_{i=1}^{n} \{ z \in \mathbb{C} : |z - a_{ii}| \leq R_i \}.
\]
Furthermore, if the union of \( k \) of these discs forms a connected region that is disjoint from the remaining \( n - k \) discs, then there are precisely \( k \) eigenvalues in this region.

(b) Since \( A \) and \( A' \) have the same eigenvalues, a similar result holds with \( R_i \) replaced by

\[
C_j = \sum_{i=1:i\neq j}^{n} |a_{ij}|, \quad j = 1, 2, \ldots, n
\]

and the union of discs by

\[
\bigcup_{j=1}^{n} \{ z \in \mathbb{C} : |z - a_{jj}| \leq C_j \}.
\]

(c) The eigenvalues of \( A \) lie in the intersection of the above two regions.

(d) \( \max_i |\lambda_i(A)| \leq \max_i \sum_{j=1}^{n} |a_{ij}| \).

Some generalizations of the above results are given by Horn and Johnson [1985: section 6.4]:

6.30. (Commuting Matrices) Let \( A \) be an \( n \times n \) matrix with distinct eigenvalues, and let \( B \) be an \( n \times n \) matrix that commutes with \( A \), that is, \( AB = BA \). Then \( B \) can be expressed uniquely as a polynomial in \( A \) with degree no more than \( n - 1 \).

6.31. (Perturbations) Suppose that a Hermitian \( n \times n \) matrix with (real) eigenvalues \( \lambda_1 \geq \cdots \geq \lambda_n \) is perturbed by a Hermitian matrix \( E \) with ranked eigenvalues \( \epsilon_i \) to give \( B = A + E \) with ranked eigenvalues \( \beta_i \). Then

\[
\lambda_i + \epsilon_1 \geq \beta_i \geq \lambda_i + \epsilon_n, \quad i = 1, 2, \ldots, n.
\]

Proofs. Section 6.1.2


6.16b. For a counter example see Abadir and Magnus [2005: 165, exercise 7.19].


6.20. If \( A \) has nonzero eigenvalues, then \( \text{trace}(\text{adj}A) = \text{trace}[(\text{det} A)A^{-1}] = \prod_i \lambda_i \sum_i \lambda_i^{-1} \). Let \( \lambda_n \to 0 \).

6.21. Wolkowicz and Styan [1980: (a), 474–476; (b) 484–485; (c) 480–481; (d) 482–483; and (e) 491, 495].


6.1.3 Singular Values

**Definition 6.5.** Suppose $B$ is an $m \times n$ real or complex matrix of rank $r$, where $r \leq p = \min(m,n)$. The $p$ largest eigenvalues of $B^*B$, which are the same as those for $BB^*$ (by 6.54c) are non-negative (by 10.10 and 10.2), as $B^*B$ is non-negative definite. Their positive square roots are called the *singular values* of $B$. Denote these by $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_p = 0$; we shall use the notation $\sigma_i = \sigma_i(B)$. (See Section 16.3 for further details and the singular value decomposition of a matrix.) Some interesting historical comments are given by Horn and Johnson [1991: section 3.0].

6.32. Suppose that $B$ is an $m \times n$ matrix with singular values $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_p \geq 0$, and $p = \min\{m,n\}$. Let

$$A = \begin{pmatrix} 0 & B^* \\ B & 0 \end{pmatrix}.$$ 

Then $A$ is an $(m + n) \times (m + n)$ Hermitian matrix with eigenvalues

$$\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_p \geq 0 = \cdots = 0 \geq -\sigma_p \geq -\sigma_{p-1} \geq \cdots \geq -\sigma_1,$$

with $|m - n|$ zeros in the middle.

6.33. Suppose $B \in \mathcal{B}$, the set of all $m \times n$ matrices. Then, for every $\epsilon > 0$, there exists $B_\epsilon \in \mathcal{B}$ with distinct singular values such that $\|B - B_\epsilon\| < \epsilon$, where $\| \cdot \|$ is any generalized matrix norm on $\mathcal{B}$.

6.34. Let $A$ be an $n \times n$ matrix with $\lambda_i(A)$ and $\sigma_i(A)$ the ordered eigenvalues and singular values, respectively, in decreasing order of magnitude.

(a) $\prod_{i=1}^k |\lambda_i(A)| \leq \prod_{i=1}^k \sigma_i(A)$ for $k = 1,2,\ldots,n$, with equality for $k = n$.

(b) $\sum_{i=1}^k |\lambda_i(A)| \leq \sum_{i=1}^k \sigma_i(A)$ for $k = 1,2,\ldots,n$.

(c) $|\text{trace } A| \leq \sigma_1(A) + \sigma_2(A) + \cdots + \sigma_n(A)$. Equality holds if and only if $A = uC$ for some non-negative definite matrix $C$ and some complex scalar $u$ with unit modulus. When equality holds, $A$ is a normal matrix.
(d) \(\sigma_i(A) = \sigma_i(UAV)\) (i = 1, 2, \ldots, n) for all \(n \times n\) unitary matrices \(U\) and \(V\).

(e) \(\lim_{n \to \infty} [\sigma_i(A^n)]^{1/n} = |\lambda_i(A)|\) for \(i = 1, 2, \ldots, n\).

6.35. If \(A\) is an \(n \times n\) matrix and \(H(A)\) is the Hermitian matrix \(\frac{1}{2}(A + A^*)\), then, for \(i = 1, 2, \ldots, n\), the following results hold.

(a) \(\sigma_i(A) \geq \lambda_i(H(A))\).

(b) \(\sigma_i(A) \geq \lambda_i[H(UAV)]\) for all \(n \times n\) unitary \(U\) and \(V\).

6.36. If \(A\) is an \(m \times n\) matrix, \(p = \min\{m, n\}\), and \(\sigma_i = \sigma_i(A)\), then:

(a) \(\sum_{i=1}^{k} a_{ii}^2 \leq \sum_{i=1}^{k} \sigma_i^2\), \(k = 1, 2, \ldots, p\).

(b) \(\sum_{i=1}^{k} a_{ii} \leq \sum_{i=1}^{k} \sigma_i\), \(k = 1, 2, \ldots, p\).

Equality in (a) holds if and only if the leading \(k \times k\) principal submatrix of \(A\) is diagonal and \(|a_{ii}| = \sigma_i\) (i = 1, 2, \ldots, \(k\)). Equality in (b) occurs when equality in (a) holds and \(a_{ii} \geq 0\) (i = 1, 2, \ldots, \(k\)).

6.37. (Bilinear Inequalities) Let \(A\) be an \(m \times n\) matrix, and let \(p = \min\{m, n\}\). For \(i = 1, 2, \ldots, p\), let \(z_i = (x_i, y_i')\) be any mutually orthonormal vectors, where \(x_i\) is \(m \times 1\) and \(y_i\) is \(n \times 1\). Then

\[\sum_{i=1}^{k} 2x_i^*Ay_i \leq \sum_{i=1}^{k} \sigma_i(A), \quad k = 1, 2, \ldots, p.\]

Equality is attained when \(x_i\) and \(y_i\) are, respectively, the left and right singular vectors of \(A\) associated with \(\sigma_i\) (cf. Section 16.3).

6.38. Let \(A\) be a real or complex square matrix with numerical radius

\[w(A) = \sup_{\|x\| = 1} |x^*Ax|.\]

Then \(\rho(A) \leq w(A) \leq \sigma_{\text{max}} \leq 2w(A)\), where \(\rho(A)\) is the spectral radius of \(A\).

Proofs. Section 6.1.3


6.34d. Horn and Johnson [1991: 146].

6.34e. Horn and Johnson [1991: 180].

6.35. Horn and Johnson [1991: 151].


6.1.4 Functions of a Matrix

6.39. If \( Ax = \lambda x \) and \( k \) is a positive integer, then \( A^k x = \lambda^k x \), so that \( A^k \) has eigenvalues \( \lambda_i^k \) and the same eigenvectors as \( A \).

If \( A^t = 0 \) for some positive integer \( t \), then \( \lambda_i(A) = 0 \) for all \( i \).

6.40. If \( A \) has eigenvalues \( \lambda_i(A) \), a polynomial \( g(A) \) has eigenvalues \( g(\lambda_i) \) (\( i = 1, 2, \ldots, n \)) and the same eigenvectors as \( A \).

6.41. If \( A \) is nonsingular with eigenvalues \( \lambda_j \), then \( A^{-1} \) has eigenvalues \( \lambda_j^{-1} \).

6.42. Let \( A \) be an \( n \times n \) matrix. If \( a_0, a_1, \ldots, a_m \) are real or complex numbers, and

\[
B = a_0 I_n + a_1 A + \cdots + a_m A^m,
\]

then the eigenvalues of \( B \) are

\[
a_0 + a_1 \mu_1(A) + a_2 \mu_2^2(A) + \cdots + a_m \mu_m^m(A) \quad \text{for} \quad j = 1, 2, \ldots, s,
\]

where the \( \mu_i(A) \) are the distinct eigenvalues. If \( B = 0 \), then any eigenvalue \( \lambda \) of \( A \) must satisfy the equation

\[
a_0 + a_1 \lambda + a_2 \lambda^2 + \cdots + a_m \lambda^m = 0.
\]

Proofs. Section 6.1.4


6.42. Quoted by Marcus and Minc [1964: 23].

6.1.5 Eigenvectors

6.43. Right (left) eigenvectors associated with distinct eigenvalues \( \mu_j \) are linearly independent.

6.44. The eigenspace corresponding to a distinct eigenvalue \( \mu_j \), say, is a vector subspace.

6.45. Let \( A \) be a real or complex square matrix, and let \( x \) be any \( n \times 1 \) nonzero vector. Then there exists an eigenvector \( y \) of \( A \) belonging to the span of \( \{x, Ax, A^2 x, \ldots\} \).

6.46. (Left and Right Eigenvectors) Suppose \( A \) is a complex square matrix.

(a) If \( Ax = \lambda x \), \( y^* A = \mu y^* \), and \( \lambda \neq \mu \), then \( x \) is orthogonal to \( y \) (i.e., \( x^* y = 0 \)).

(b) \( A^* y = \bar{\mu} y \).

Proofs. Section 6.1.5


6.44. Schott [2005: 88].


6.1.6 Hermitian Matrices

Hermitian matrices are also discussed in Sections 5.2.

6.47. Suppose $A$ is an $n \times n$ Hermitian matrix. Then the following hold.

(a) The eigenvalues of $A$ are real.

(b) Eigenvectors corresponding to different eigenvalues are orthogonal (with respect to the inner product $\langle x, y \rangle = x^* y$). A right eigenvalue is also a left eigenvalue, and vice versa.

(c) There is a complete set of $n$ orthonormal eigenvectors.

(d) $\sum_{i=1}^{n} \sum_{j=1}^{n} |a_{ij}|^2 = \sum_{i=1}^{n} |\lambda_i|^2$.

(e) There exists a unitary matrix $U$ (i.e., $U^* U = I_n$) such that $U^* A U = \Lambda$, where $\Lambda$ is a diagonal matrix of the eigenvalues of $A$ (cf. 16.44).

(f) Since $A$ is also normal, the results relating to normal matrices apply.

6.48. (Real Symmetric Matrices) If $A$ is an $n \times n$ real symmetric matrix, then it is also Hermitian and all the results for Hermitian matrices in (6.47) above apply here. However, we collect some of the results below for easy reference.

(a) The eigenvalues $\lambda_i$ are all real and the corresponding eigenvectors can be chosen to be real.

(b) If $\text{rank} A = r$, there are $r$ nonzero eigenvalues and $\lambda = 0$ has algebraic multiplicity $(n - r)$.

(c) Since $x' A = \lambda x'$ if and only if $A x = \lambda x$, right eigenvectors are also left eigenvectors.

(d) Eigenvectors corresponding to different eigenvalues are orthogonal so that the corresponding eigenspaces are orthogonal.

(e) There exist $n$ mutually orthogonal eigenvectors.

(f) $\text{rank}(A - \lambda_i I_n) = n - m_i$, where $m_i$ is the algebraic multiplicity of $\lambda_i$.

(g) There exists an orthogonal matrix $T$ such that (cf. Section 16.6)

$$T^* A T = \text{diag}(\lambda_1, \lambda_2, \ldots, \lambda_n).$$

(h) $\sum_{i=1}^{n} \sum_{j=1}^{n} a_{ij}^2 = \text{trace}(A^2) = \sum_{i=1}^{n} \lambda_i^2$.

(i) If $x$ is any nonzero vector, then, for some $r \geq 1$, the vector space spanned by the vectors $x, A x, \ldots, A^{r-1} x$ contains an eigenvector of $A$.

Proofs. Section 6.1.6

6.47. Horn and Johnson [1985: 169–172]. For the second part of (b), if $y^* A = \lambda y^*$, then $A y = A^* y = \overline{\lambda} y = \lambda y$.


6.48i. Schott [2005: 96].
6.1.7 Computational Methods

6.49. (Power Method) Let $A$ be an $n \times n$ real diagonalizable matrix with real eigenvalues and a dominant eigenvalue $\lambda_1$ (i.e., $|\lambda_1| > |\lambda_2| \geq \cdots \geq |\lambda_n|$). Since $A$ is diagonalizable, there exist $n$ real right eigenvectors $u_1, u_2, \ldots, u_n$, with $u_i$ corresponding to $\lambda_i$, which are scaled to have unit length and are linearly independent.

(a) Let $y = \sum_{i=1}^{n} a_i u_i$, where $a_1 > 0$. Set $y_0 = y$ and define $z_k$ and $y_k$ inductively by the following: $z_k = Ay_{k-1}$ and $y_k = (1/\|z_k\|)z_k$ for $k = 1, 2, \ldots$. Then $\|z_k\| \rightarrow |\lambda_1|$ as $k \rightarrow \infty$, and $y_{2m} \rightarrow u_1$ as $m \rightarrow \infty$. Also $y_{2m+1}$ converges to $u_1$ or $-u_1$ according as $\lambda_1$ is positive or negative. One can determine the sign of $\lambda_1$ by considering successive iterations. See also Golub and Van Loan [1996: 406].

(b) If $R$ is any nonsingular matrix with $u_1$ as the first column, then

$$R^{-1}AR = \begin{pmatrix} \lambda_1 & a' \\ 0 & B \end{pmatrix}$$

for some $a$ and $B$, and the eigenvalues of $A$ are those of $B$ together with $\lambda_1$. If $\mu \neq \lambda_1$ is an eigenvalue of $B$ with $v$ as a corresponding eigenvector, then, setting $b = (a'v)/(\mu - \lambda_1)$, we find that $R^{(b)}_v$ is an eigenvector of $A$ corresponding to $\mu$. This approach can be used to obtain the eigenvalues and corresponding eigenvectors if $|\lambda_1| > |\lambda_2| > \cdots > |\lambda_n|$.

(c) Suppose $|\lambda_i| > |\lambda_j|$ and let $v_i$ and $v_j$ be the real, left unit eigenvectors corresponding to $\lambda_i$ and $\lambda_j$, respectively. Then, since $A'v_j = \lambda_j v_j$ and $Au_i = \lambda_i u_i$, we have:

(i) $(Au_i)'v_j = u_i' A' v_j = \lambda_j u_i' v_j$ and $(Au_i)'v_j = \lambda_i u_i' v_j$, so that $u_i \perp v_j$ as $\lambda_i \neq \lambda_j$.

(ii) If $B = A - \lambda_i v_i u_i'$, then $Bv_j = \lambda_j v_j$. As in (b), this method can be also be used for finding other eigenvalues.

6.50. (Jacobi’s Method) Let $A$ be a real symmetric matrix. Jacobi’s method is based on the spectral decomposition of $A$ (cf. 16.44), and the method may be described broadly as follows. Let $Q_k$ be an orthogonal matrix, and consider the iteration process $A^{(k+1)} = Q_k' A^{(k)} Q_k = P_{k+1}' A P_{k+1}$, where $P_{k+1} = Q_1 Q_2 \cdots Q_k$ is orthogonal. The starting values are $A^{(1)} = A$ and $P_1 = I_n$. Each $Q_i$ is a Givens rotation matrix that reduces a current off-diagonal element to zero, thus reducing the sum of squares of the off-diagonal elements. We then find that $A^{(k)}$ tends towards a diagonal matrix so that

$$\lim_{k \rightarrow \infty} P_k' A P_k = \Lambda \quad \text{and} \quad \lim_{k \rightarrow \infty} P_k = P,$$

where $\Lambda$ is a diagonal matrix consisting of the eigenvalues of $A$, and the columns of $P$ are corresponding eigenvectors. Some theory is provided by Rao and Bhimasankaram [2000: 323–324] and a good description of the method along with further computational details are given by Gentle [1998: section 4.2].

6.51. (QR Method) This seems to be the most common method, and it can be used for both symmetric and nonsymmetric matrices $A = (a_{ij})$, though the symmetric
case is easier, since the eigenvalues are now real. The first step is to transform \( \mathbf{A} \) into upper Hessenberg form using Householder or Givens transformations. When \( \mathbf{A} \) is symmetric, the upper Hessenberg form is tridiagonal. For some details see Gentle [1998: section 4.3] and Golub and Van Loan [1996: section 7.4]).

**Proofs.** Section 6.1.7


6.49b. Rao and Bhimasankaram [2000: 327 and exercise 3 for a correction].


### 6.1.8 Generalized Eigenvalues

**Definition 6.6.** If \( \mathbf{A} \) and \( \mathbf{B} \) are \( n \times n \) matrices, we say that \( \lambda \) is an **eigenvalue of \( \mathbf{A} \) with respect to \( \mathbf{B} \)** if there exists a nonzero \( \mathbf{x} \) that does not belong to both \( \mathcal{N}(\mathbf{A}) \) and \( \mathcal{N}(\mathbf{B}) \) such that \( \mathbf{A}\mathbf{x} = \lambda\mathbf{B}\mathbf{x} \). Here \( \lambda \) is one of the \( n \) roots of \( \det(\mathbf{A} - \lambda\mathbf{B}) \), and these roots are also called the **generalized eigenvalues**. As \( \mu \) varies over \( \mathbb{R} \), the matrix \( \mathbf{A} - \mu\mathbf{B} \) is called a **matrix pencil**.

Generalized eigenvalues are used extensively in multivariate analysis—for example, in dimension-reducing techniques and for hypothesis testing in multivariate analysis of variance (Chapter 21). In this regard, some computational aspects using Cholesky decompositions are discussed by Maindonald [1984: section 6.5].

**6.52.** Let \( \mathbf{A} \) and \( \mathbf{B} \) be real \( n \times n \) matrices with \( \mathbf{B} \) nonsingular.

(a) The generalized eigenvalues are the eigenvalues of \( \mathbf{B}^{-1}\mathbf{A} \), which are the same as those of \( \mathbf{AB}^{-1} \).

(b) Suppose \( \mathbf{A} \) is symmetric and \( \mathbf{B} \) is positive definite.

(i) The eigenvalues of \( \mathbf{AB}^{-1} \) are real.

(ii) From (6.54a), \( \lambda(\mathbf{B}^{-1/2}\mathbf{AB}^{-1/2}) = \lambda(\mathbf{B}^{-1}\mathbf{A}) \), where \( \mathbf{B}^{1/2} \) is the unique positive definite square root of \( \mathbf{B} \) (cf. 10.32).

(c) The \( \lambda(\mathbf{B}^{-1}\mathbf{A}) \) can be computed using a Schur decomposition (cf. 16.37).

For further details see Harville [1997: section 21.14], and some computational aspects of the problem are discussed by Golub and Van Loan [1996: section 7.7].

**Proofs.** Section 6.1.8

6.52a. This follows from \( \det(\mathbf{A} - \lambda\mathbf{B}) = 0 \) if and only if \( \det\mathbf{B}\det(\mathbf{B}^{-1}\mathbf{A} - \lambda\mathbf{I}) = 0 \) if and only if \( \det(\mathbf{AB}^{-1} - \lambda\mathbf{I})\det\mathbf{B} = 0 \).

6.1.9 Matrix Products

6.53. If \( A \) and \( B \) are real symmetric \( n \times n \) matrices, then the eigenvalues of \( AB \) are real if either \( A \) or \( B \) is non-negative definite.

6.54. Suppose \( A \) is \( m \times n \) and \( B \) is \( n \times m \) (\( m \leq n \)), both complex matrices.

(a) \( \lambda^{n-m} \det(\lambda I_m - AB) = \det(\lambda I_n - BA) \),
and \( AB \) and \( BA \) have the same nonzero eigenvalues, counting algebraic multiplicities.

(b) If \( \lambda \) is a nonzero eigenvalue of \( AB \), then \( \lambda \) is an eigenvalue of \( BA \) with the same geometric multiplicity. Also, if \( x_1, \ldots, x_r \) are linearly independent eigenvectors of \( AB \) corresponding to \( \lambda \), then \( Bx_1, \ldots, Bx_r \) are linearly independent eigenvectors of \( BA \) corresponding to \( \lambda \).

(c) If \( A \) is \( m \times n \), then \( AA^* \) and \( A^*A \) have the same nonzero eigenvalues.

6.55. If \( A \) and \( B \) are \( n \times n \) matrices and \( A \) is nonsingular, then \( AB \) and \( BA \) have the same eigenvalues.

6.56. (Frobenius) Let \( A \) and \( B \) be \( n \times n \) matrices that commute with \( AB - BA \). Let \( f(x_1,x_2) \) be any polynomial in \( x_1 \) and \( x_2 \) with possibly complex coefficients. Then there exists an ordering of the eigenvalues of \( A \) and \( B \), namely \((\alpha_i, \beta_i)\) for \( i = 1, 2, \ldots, n \), such that the eigenvalues of \( f(A,B) \) are \( f(\alpha_i, \beta_i) \) for \( i = 1, 2, \ldots, n \).

6.57. (Von Neumann) Let \( A \) be \( m \times n \) and \( B \) be \( n \times m \) matrices such that \( AB \) and \( BA \) are Hermitian non-negative definite. Let \( p = \min\{m,n\} \) and \( q = \max\{m,n\} \). If we define \( \sigma_j(A) = \sigma_j(B) = 0 \) for \( p + 1 \leq j \leq q \), where \( \sigma(\cdot) \) is a singular value, then there exists a permutation \( \tau \) of \( \{1, 2, \ldots, q\} \) such that

\[
\text{trace}(AB) = \text{trace}(BA) = \sum_{i=1}^{q} \sigma_i(A)\sigma_{\tau(i)}(B).
\]

where \( \tau(i) \) is the \( i \)th element of permutation \( \tau \).

Proofs. Section 6.1.9


6.54c. This follows from (a) with \( B = A^* \).

6.55. This follows from (6.54a) with \( m = n \).

6.56. Quoted by Marcus and Minc [1964: 25].

6.2 VARIATIONAL CHARACTERISTICS FOR HERMITIAN MATRICES

A common statistical problem is that of finding the maximum or minimum of a ratio of two quadratic forms subject to some linear constraints—for example, in multivariate analysis. As we shall see below, eigenvalues and eigenvectors feature prominently in the theory. We shall work mainly with the more general complex quadratics as real quadratics follow as a special case. In following up proofs of the following results, the reader should note that we rank the eigenvalues \( \lambda_i \) in decreasing order of magnitude, whereas some authors such as Horn and Johnson [1985] and Magnus and Neudecker [1999] do the reverse. In the latter case, we change the sign of the suffix and add \( n + 1 \) to get corresponding results; thus \( \lambda_i \) becomes \( \lambda_{n+1-i} \). However, Horn and Johnson [1985: 419] do not reverse the order of the singular values, but rank them in decreasing order.

6.58. Let \( A \) be an \( n \times n \) Hermitian matrix with (real) eigenvalues \( \lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_n \) and a corresponding set of orthonormal eigenvectors \( u_1, u_2, \ldots, u_n \) (i.e., \( u_i^*u_j = \delta_{ij} \)) in \( \mathbb{C}^n \) such that \( Au_i = \lambda_i u_i \). For \( k = 1, 2, \ldots, n \), let \( U_k = (u_1, u_2, \ldots, u_k) \) and \( V_k = (u_k, u_{k+1}, \ldots, u_n) \). Define \( U = U_n = V_1 \). In what follows, we assume that \( x \in \mathbb{C}^n \) and \( x \neq 0 \). We shall give properties of the ratio \( r(x) = x^*Ax/x^*x \), which is sometimes called the \textit{Raleigh (Ritz) ratio} (quotient). (In what follows some authors use "sup" and "inf" instead of "max" and "min," respectively. However, these expressions are equivalent as the extrema are attained.)

The results below immediately follow for real symmetric matrices by replacing * by '. We note that \( r(x) \) does not depend on \( ||x||_2 \) so that if \( x \neq 0 \) we can scale \( x \) to satisfy \( ||x||_2 = 1 \); the denominator of \( r(x) \) becomes 1. This alternative representation will be mentioned only once below, but it holds in all the following results. For general references see Horn and Johnson [1985: 176–180], Magnus and Neudecker [1999: 203–207], Rao and Rao [1998: 332–335], Schott [2005: 104–110], and Seber [1984: 525–526].

(a) \( \text{(Raleigh--Ritz Theorem)} \)

(i) \( \lambda_n \leq r(x) \leq \lambda_1 \).

(ii) \( \max_{||x||_2 = 1} x^*Ax = \max_{x \neq 0} r(x) = \lambda_1 \), and the maximum occurs when \( x = u_1 \).

(iii) \( \min_{x \neq 0} r(x) = \lambda_n \), and the minimum occurs when \( x = u_n \).

(b) The following hold for \( k = 2, \ldots, n - 1 \).

(i) \( \max_{x \neq 0: U_{k-1}^*x = 0} r(x) = \lambda_k \), and the maximum is attained when \( x = u_k \). Note that \( U_{k-1}^*x = 0 \) implies that \( x \perp \{u_1, u_2, \ldots, u_{k-1}\} \), i.e., \( x \in S(u_k, u_{k+1}, \ldots, u_n) \), where \( S \) is the span.

(ii) \( \min_{x \neq 0: V_{k+1}^*x = 0} r(x) = \lambda_k \), and the minimum is attained when \( x = u_k \). Note that \( V_{k+1}^*x = 0 \) implies that \( x \perp \{u_{k+1}, u_{k+2}, \ldots, u_n\} \), i.e., \( x \in S(u_1, u_2, \ldots, u_k) \).
(c) $\min_{C^*x=0} r(x) \leq \lambda_k \leq \max_{B^*x=0} r(x)$

for every $n \times (k-1)$ matrix $B$ and $n \times (n-k)$ matrix $C$.

(d) (Courant-Fischer Min-Max Theorem) Let $B$ be any $n \times (k-1)$ complex matrix. Then for $k = 2, \ldots, n$ we have the following:

(i) $\min_{B \neq 0: B^*x = 0} \max_{x \neq 0} r(x) = \lambda_k,$

and the result is attained when $B = U_{k-1}$ and $x = u_k$.

(ii) $\max_{B \neq 0: B^*x = 0} \min_{x \neq 0} r(x) = \lambda_{n-k+1},$

and the result is attained when $B = V_{n-k+1}$ and $x = u_{n-k+1}$.

Since $U_{k-1}^* U_{k-1} = V_{n-k+1}^* V_{n-k+1} = I_{k-1}$, we can impose the restriction $B^*B = I_{k-1}$ without changing the above two results. Some authors use this formulation of the Courant-Fischer theorem (e.g., Schott [2005: 108–110]). Rao [1973a: 62], Seber [1984: 525–526], and Magnus and Neudecker [1999: 205–208, with the labeling $\lambda_1 \leq \cdots \leq \lambda_n$] prove the above for real matrices and Horn and Johnson [1985: 176] for the complex case. The complex case follows directly from proofs for the real case by simply replacing $2i$ by $|x_i|^2$.

The reader should note that there is a confusing variation in the proofs depending on how the constraints are defined (in our case by $B^*x = 0$). For example, if $B$ is replaced by an $n \times (n-k)$ matrix $C$ in (ii), then $\lambda_{n-k+1}$ is replaced by $\lambda_k$ (Abadir and Magnus [2005: 346] and Schott [2005: 108]). Furthermore, if $C$ is used in (i) and $B$ in (ii), then $\lambda_k$ now refers to the $k$th largest eigenvalue rather than the $k$th smallest (Horn and Johnson [1985: 179] and Magnus and Neudecker [1999: 207]). One can also replace $B$ by a general vector space, as in Meyer [2000a: 550] and Rao and Rao [1998: 332].

(e) The min–max theorem extends to singular values by replacing $A$ by $A^*A$, as $\sigma_i(A)^2 = \lambda_i(A^*A)$, and by noting that

$$ \left( \frac{x^*A^*Ax}{x^*x} \right) = \left( \frac{\|Ax\|_2}{\|x\|_2} \right)^2,$$

where $\|\cdot\|_2$ is the Euclidean vector norm. For example, let $B$ be any $n \times (k-1)$ complex matrix. Then, for $k = 2, \ldots, n$, we have the following.

(i) $\min_{B \neq 0: B^*x = 0} \max_{x \neq 0} \left( \frac{\|Ax\|_2}{\|x\|_2} \right) = \sigma_k.$

(ii) $\max_{B \neq 0: B^*x = 0} \min_{x \neq 0} \left( \frac{\|Ax\|_2}{\|x\|_2} \right) = \sigma_{n-k+1}.$

(f) The min–max theorem also extends to the eigenvalues of the product of two non-negative definite matrices. For details see Mäkeläinen [1970: 33].

6.59. Let $A$ be a real $n \times n$ symmetric matrix, and let $B$ be any $n \times n$ positive definite matrix. Let $\gamma_1 \geq \gamma_2 \geq \cdots \geq \gamma_n$ be the eigenvalues of $B^{-1}A$—that is, $\gamma_i = \lambda_i(B^{-1}A)$—with corresponding right eigenvectors $v_1, v_2, \ldots, v_n$, all of which are real by (6.52b(i)). Then
EIGENVALUES, EIGENVECTORS, AND SINGULAR VALUES

(a) \( \max_{x \neq 0} \frac{x'Ax}{x'Bx} = \gamma_1 \) and \( \min_{x \neq 0} \frac{x'Ax}{x'Bx} = \gamma_n \),

with the bounds being attained when \( x = v_1 \) and \( x = v_n \), respectively.

In particular, for any \( a \) we have

\[
\max_{x \neq 0} \frac{(a'x)^2}{x'Bx} = a'B^{-1}a,
\]

and the maximum occurs when \( x \propto B^{-1}a \). The result for \( \gamma_1 \) applies to hypothesis testing for multivariate linear hypotheses and to the dimension reduction technique of discriminant coordinate analysis (cf. 21.49b)).

(b) Let \( U_i = (v_1, \ldots, v_i) \) and \( W_i = (v_i, \ldots, v_n) \). Then, for \( x \neq 0 \) and \( i = 2, 3, \ldots, n-1 \),

\[
\max_{U_i', Bx=0} \frac{x'Ax}{x'Bx} = \gamma_i \quad \text{and} \quad \min_{W_{i+1}, Bx=0} \frac{x'Ax}{x'Bx} = \gamma_i.
\]

6.60. Let \( A \) be a real \( n \times n \) symmetric matrix, and let \( B \) be any \( n \times n \) positive definite matrix. For \( i = 1, 2, \ldots, n \), let \( B_i \) be any \( n \times (i-1) \) matrix and \( C_i \) be any \( n \times (n-i) \) matrix satisfying \( B_i'B_i = I_{i-1} \) and \( C_i'C_i = I_{n-i} \), respectively. Then

\[
\min_{B_i} \max_{x \neq 0: B_i'x=0} \frac{x'Ax}{x'Bx} = \lambda_i(B^{-1}A)
\]

and

\[
\max_{C_i} \min_{x \neq 0: C_i'x=0} \frac{x'Ax}{x'Bx} = \lambda_i(B^{-1}A),
\]

where the inner min and max are over all \( x \neq 0 \) when \( i = 1 \) and \( i = n \), respectively. The results will hold for Hermitian matrices with ‘ replaced by *.

6.61. Let \( A \) and \( B \) be positive definite \( n \times n \) matrices. Then

\[
\max_{x \neq 0, y \neq 0} \left\{ \frac{(x'Ly)^2}{x'Ax \cdot y'y} \right\} = \theta_{\max},
\]

where \( \theta_{\max} \) is the largest eigenvalue of \( A^{-1}LB^{-1}L' \), and also of \( B^{-1}L'A^{-1}L' \). The maximum occurs when \( x \) is a right eigenvector of \( A^{-1}LB^{-1}L' \) corresponding to \( \theta_{\max} \), and \( y \) is a right eigenvector of \( B^{-1}L'A^{-1}L \) corresponding to \( \theta_{\max} \). This result is used, for example, in applying the union–intersection method to testing hypotheses relating to variance matrices in multivariate analysis (Seber [1984: 89]).

6.62. Let \( A \) be a real \( m \times n \) matrix of rank \( r \) \( (r \leq \min\{m, n\}) \), and let \( \sigma_1^2 \geq \sigma_2^2 \geq \cdots \geq \sigma_r^2 > 0 \) be the nonzero eigenvalues of the symmetric matrix \( AA' \) (and of \( A'A \)), where \( \sigma_i \) is the \( i \)th singular value of \( A \). Referring to the singular value decomposition of \( A \) (Section 16.3), let \( t_1, t_2, \ldots, t_r \) be the corresponding orthogonal right eigenvectors of \( AA' \), and let \( w_1, w_2, \ldots, w_r \) be the corresponding orthogonal right eigenvectors of \( A'A \). Define \( T_k = (t_1, t_2, \ldots, t_k) \) and \( W_k = (w_1, w_2, \ldots, w_k) \) \((k < r)\), and assume \( x \neq 0 \) and \( y \neq 0 \). Then

(a) \( \max_{x \neq 0, y \neq 0} \left\{ \frac{(x'Ay)^2}{x'x \cdot y'y} \right\} = \sigma_1^2 \).

The maximum occurs when \( x = t_1 \) and \( y = w_1 \).
The above results are sometimes expressed in a square root version—for example,
\[ \dfrac{x' Ay}{\sqrt{x' x \cdot y' y}} = \sigma_1, \]
and so on. Another way of expressing this result is
\[ \max_{\|x\|=1, \|y\|=1} x' Ay = \sigma_1, \]
and the $t_i$ and $w_i$ are now scaled to have unit norms. The above results are used
in the multivariate technique of canonical correlation analysis (Seber [1984: 259]).

6.63. (Some Matrix Extensions) Let $A$ be an $n \times n$ positive definite matrix, and
let $X$ be an $n \times T$ matrix of rank $r$. Then
\[ \max_{X'X=I_r} \det(X'AX) = \prod_{i=1}^{r} \lambda_i(A) \quad \text{and} \quad \min_{X'X=I_r} \det(X'AX) = \prod_{i=1}^{r} \lambda_{n-r+i}(A). \]

Proofs. Section 6.2

6.58b. Meyer [2000a: 549] and Seber [1984: 525, with $\lambda_{n-k}$ changed to $\lambda_k$].
6.58c. Abadir and Magnus [2005: 345].
6.60. Schott [2005: 123].

6.3 SEPARATION THEOREMS

In this section we follow our usual practice and rank the eigenvalues of an $n \times n$
matrix $C$ as $\lambda_1(C) \geq \lambda_2(C) \geq \cdots \geq \lambda_n(C)$.

6.64. Let $A$ be an $n \times n$ Hermitian or real symmetric matrix, and let $A_k$ be the
leading principal $k \times k$ submatrix of $A$, that is, $A_k = (a_{rs})$, $r, s = 1, 2, \ldots, k$
for $k = 1, 2, \ldots, n - 1$; we define $A_n = A$. Let $\lambda_1(A_k) \geq \lambda_2(A_k) \geq \cdots \geq \lambda_k(A_k)$
for each $k$ (including $k = n$), and let $\sigma_1(A_k) \geq \cdots \geq \sigma_k(A_k)$ be the singular values.
(a) (Sturmian Separation Theorem) From the Courant-Fisher theorem we obtain the inequality

$$\lambda_{i+1}(A_{k+1}) \leq \lambda_i(A_k) \leq \lambda_i(A_{k+1}), \quad i = 1, 2, \ldots, k.$$  

(b) (Interlacing Theorem for Eigenvalues) From the left- and right-hand sides of (a) we get

(i) 

$$\lambda_{n-k+i}(A_n) \leq \lambda_{n-k+i-1}(A_{n-1}) \leq \cdots \leq \lambda_i(A_k)$$

$$\lambda_i(A_k) \leq \lambda_i(A_{k+1}) \leq \cdots \leq \lambda_i(A_n).$$

(ii) From (i) we get

$$\lambda_{n-k+i}(A) \leq \lambda_i(A_k) \leq \lambda_i(A), \quad i = 1, 2, \ldots, k.$$  

(iii) If we reverse the order of listing the above inequalities in (i), we get the alternative expression

$$\lambda_{n-i+1}(A) \leq \lambda_i(A_{k-i+1}) \leq \lambda_{k-i+1}(A), \quad i = 1, 2, \ldots, k.$$  

(c) (Interlacing Theorems for Singular Values) Let $A$ be $m \times n$ with singular values $\sigma_1(A) \geq \sigma_2(A) \geq \cdots \geq \sigma_r(A)$, where $r = \min\{m, n\}$.

(i) Let $B$ be a $p \times q$ submatrix of $A$ with singular values $\sigma_1(B) \geq \sigma_2(B) \geq \cdots \geq \sigma_s(B)$, where $s = \min\{p, q\}$. Then

$$\sigma_i(A) \geq \sigma_i(B), \quad i = 1, 2, \ldots, s.$$  

(ii) Assume $m \geq n$. If $B$ is a submatrix obtained from $A$ by deleting one of the columns, then

$$\sigma_1(A) \geq \sigma_1(B) \geq \sigma_2(A) \geq \sigma_2(B) \geq \cdots \geq \sigma_{n-1}(A) \geq \sigma_{n-1}(B) \geq \sigma_n(A).$$  

(iii) Assume $m < n$. If $B$ is a submatrix obtained from $A$ by deleting one of the columns, then

$$\sigma_1(A) \geq \sigma_1(B) \geq \sigma_2(A) \geq \sigma_2(B) \geq \cdots \geq \sigma_m(A) \geq \sigma_m(B),$$  

which we now combine with (ii).

(iv) Suppose we extend the definition of singular values so that $\sigma_j(A) = 0$ for $j > r$. Let $A_s$ be any matrix obtained from $A$ by deleting a total of $s$ rows and columns (i.e., $s - k$ rows and $k$ columns for some $0 \leq k \leq s$), then

$$\sigma_i(A) \geq \sigma_i(A_s) \geq \sigma_{i+s}(A), \quad i = 1, 2, \ldots, \min\{m, n\}.$$  

Note that since $\sigma_i(A') = \sigma(A)$, we can obtain the result for deleting a single row by interchanging the two cases (ii) and (iii). Also (i)-(iii) follow from (iv).
6.65. (Eigenvalue Inequalities)

(a) (Poincaré’s Separation Theorems) Let \( A \) be be an \( n \times n \) Hermitian matrix, and let \( B_k \) be any \( n \times k \) matrix such that \( B_k^* B_k = I_k \). Then:

\[
\lambda_{n-k+i}(A) \leq \lambda_i(B_k^* A B_k) \leq \lambda_i(A), \quad i = 1, 2, \ldots, k.
\]

The first equalities on the left are attained if and only if \( B_k = V_k U \), where \( U \) is unitary and the \( k \) columns of \( V_k \) are any set of right eigenvectors corresponding to the \( k \) smallest eigenvalues, while the second equalities on the right are attained if and only if \( B_k = W_k U \), where \( W_k \) has \( k \) columns consisting of any set of right eigenvectors corresponding to the largest \( k \) eigenvalues. Scott and Styan [1985: 213–214] give some historical remarks on the history of the above result and use it to obtain bounds on the distribution of chi-square statistics used in sample surveys. Such inequalities are also used for the Durbin–Watson bounds test for serial correlation in regression.

The left-hand side can also be written in the form

\[
\lambda_{n-j}(A) \leq \lambda_{k-j}(B_k^* A B_k), \quad j = 0, 1, \ldots, k - 1.
\]

By setting \( B_k = (I_k, 0)' \), we can obtain the left-hand side of (6.64b(ii)).

(ii) Summing \( i = 1, \ldots, k \) in (i), we get, for \( k = 1, 2, \ldots, n \),

\[
\min_{B_k^* B_k = I_k} \text{trace}(B_k^* A B_k) = \sum_{i=1}^{k} \lambda_{n-k+i}(A),
\]

\[
\max_{B_k^* B_k = I_k} \text{trace}(B_k^* A B_k) = \sum_{i=1}^{k} \lambda_i(A).
\]

The bounds are achieved by a suitable choice of \( B_k \).

By setting \( B_k = (I_k, 0)' \), we have \( \lambda_n \leq a_{ii} \leq \lambda_1 \) (\( i = 1, 2, \ldots, n \)),

\[
\lambda_{n-1} + \lambda_n \leq a_{ii} + a_{jj} \leq \lambda_1 + \lambda_2, \quad (i, j = 1, 2, \ldots, n; \ i \neq j),
\]

and so on. In particular,

\[
\sum_{i=1}^{k} \lambda_{n-k+i}(A) \leq \sum_{i=1}^{k} a_{ii} \leq \sum_{i=1}^{k} \lambda_i(A).
\]

(iii) If \( P \) is an \( n \times n \) idempotent Hermitian matrix (i.e., \( P^2 = P \)) of rank \( k \), then

\[
\lambda_{n-k+i}(A) \leq \lambda_i(PAP) \leq \lambda_i(A), \quad i = 1, 2, \ldots, k.
\]

(b) Let \( A \) and \( B \) be real \( n \times n \) matrices with \( A \) symmetric and \( B \) non-negative definite with Moore–Penrose inverse \( B^+ \). Also, let \( T \) be an \( n \times k \) matrix of rank \( k \) such that \( C(T) \subseteq C(B) \) and \( T' B T = I_k \), and let \( \lambda_i = \lambda_i(B^+ A) \). Then the following maxima and minima with respect to \( T \) hold.

(i) \( \max\{\text{trace}(T' A T)\} = \lambda_1 + \cdots + \lambda_k \).

(ii) \( \min\{\text{trace}(T' A T)\} = \lambda_{n-k+1} + \cdots + \lambda_n \).
(iii) \( \max \{ \text{trace}[(T'AT)^2] \} = \lambda_1^2 + \cdots + \lambda_k^2 \).

(iv) \( \min \{ \text{trace}[(T'AT)^2] \} = \lambda_{n-k+1}^2 + \cdots + \lambda_n^2 \).

(v) \( \max \{ \text{trace}[(T'AT)^{-1}] \} = \lambda_{r-k+1}^{-1} + \cdots + \lambda_r^{-1} \), for \( A \) positive definite and \( \text{rank } B = r \).

(vi) \( \min \{ \text{trace}[(T'AT)^{-1}] \} = \lambda_1^{-1} + \cdots + \lambda_k^{-1} \) for \( A \) positive definite.

The optimum values are reached when \( T = (t_1, \ldots, t_k) \), where \( B^{1/2}t_i \) are orthonormal right eigenvectors of \((B^+)^{1/2}A(B^+)^{1/2}\) associated with the eigenvalues \( \lambda_i \) \((i = 1, 2, \ldots, k)\).

(c) If \( A \) and \( B \) are \( n \times n \) positive definite matrices, then:

(i) \( \lambda_1(A^sB^t) \leq \lambda_1^s(AB) \) for \( 0 \leq s \leq t \).

(ii) \( [\lambda_1(AB)]^t \leq \lambda_1(A^tB^t) \) for \( t \geq 1 \).

6.66. (Singular Values) Let \( A \) be an \( m \times n \) matrix with singular values \( \sigma_i(A) \). Let \( B = U^*AV \), where \( U \) and \( V \) are \( m \times p \) and \( n \times q \), respectively, such that \( U^*U = I_p \) and \( V^*V = I_q \).

(a) If \( r = (m - p) + (n - q) \),

\[ \sigma_{i+r}(A) \leq \sigma_i(B) \leq \sigma_i(A), \quad i = 1, 2, \ldots, \min\{m, n\}. \]

(b) If \( p = q = k \),

\[ |\det B|^2 = \det(BB^*) = \prod_i \lambda_i(BB^*) = \prod_i \sigma_i^2(B), \]

so that

\[ |\det B| \leq \sigma_1(A) \cdots \sigma_k(A). \]

(c) If \( p = q = k \), we can sum in (a) and obtain, for \( k = 1, 2, \ldots, \min\{m, n\} \),

\[ \max_{U^*U = I_p, V^*V = I_q} |\text{trace } B| = \sum_{i=1}^k \sigma_i(A). \]

6.67. Let \( A \) be an \( n \times n \) real symmetric matrix, and let \( B \) be an \( n \times n \) positive definite matrix. If \( F \) is any \( n \times k \) matrix of rank \( k \), then for \( i = 1, 2, \ldots, k \),

\[ \lambda_i[(F^*BF)^{-1}(F^*AF)] \leq \lambda_i(B^{-1}A), \]

and

\[ \max_F \lambda_i[(F^*BF)^{-1}(F^*AF)] = \lambda_i(B^{-1}A). \]

6.68. Let \( A \) and \( B \) be \( n \times n \) non-negative definite matrices satisfying \( C(A) \subseteq C(B) \), and let \( X \) be an \( n \times k \) real matrix with

\[ b = \text{rank } B \quad \text{and} \quad r = \text{rank}(BX). \]

Then

\[ \lambda_{b-r+i}(B^{-1}A) \leq \lambda_i([(X'BX)^{-1}X'AX]) \leq \lambda_i(B^{-1}A), \quad i = 1, 2, \ldots, r. \]
In the above equation, any choices of the weak inverses $B^{-}$ and $(X'BX)^{-}$ may be made. Equality occurs on the left simultaneously for all $i = 1, 2, \ldots, r$ if and only if there exists a real $n \times r$ matrix $Q_{0}$ such that

$$Q_{0}'BQ_{0} = I_{r}, \quad AQ_{0} = BQ_{0}A_{o}, \quad \text{and} \quad C(BQ_{0}) = C(BX).$$

Here $A_{0}$ is an $r \times r$ diagonal matrix containing the $r$ smallest, not necessarily zero, generalized eigenvalues of $A$ with respect to $B$. Equality holds on the right simultaneously for all $i = 1, 2, \ldots, r$ if and only if there exists a real $r \times r$ matrix $Q_{1}$ such that

$$Q_{1}'BQ_{1} = I_{r}, \quad AQ_{1} = BQ_{1}A_{1}, \quad \text{and} \quad C(BQ_{1}) = C(BX).$$

Here $A_{1}$ is an $r \times r$ diagonal matrix containing the $r$ largest generalized eigenvalues of $A$ with respect to $B$. Scott and Styan [1985] give an application to finding distributional bounds on two standard asymptotic hypothesis tests in multiway contingency tables.

6.69. A product version of (6.65a(ii)) is as follows. If $A$ is a Hermitian positive definite matrix and $B$ is an $n \times k$ matrix, then

$$\min_{B_{k}'B_{k} = I_{k}} \det(B_{k}'AB_{k}) = \prod_{i=1}^{k} \lambda_{n-k+i}(A),$$

$$\max_{B_{k}'B_{k} = I_{k}} \det(B_{k}'AB_{k}) = \prod_{i=1}^{k} \lambda_{i}(A).$$

By setting $B_{k} = (I_{k}, 0)'$ and defining $A_{k}$ as in (6.64), we have

$$\prod_{i=1}^{k} \lambda_{n-k+i}(A) \leq \det A_{k} \leq \prod_{i=1}^{k} \lambda_{i}(A).$$

**Proofs.** Section 6.3

6.64a. Rao and Bhimasankaram [2000: 347–348, real symmetric case with $i$ and $k$ interchanged; the proof is identical for Hermitian matrices].

6.64b(ii). Rao and Rao [1998: 328, with $A_{k}$ replaced by $B$] and Zhang [1999: 222–225].

6.64b(iii). Schott [2005: 112].


6.65a(i). For the real case see Abadir and Magnus [2005: 347], Schott [2005: 111], and Rao and Bhimasankaram [2000: 348].

6.65a(iii). Abadir and Magnus [2005: 348].
6.68. Scott and Styan [1985].

6.4 INEQUALITIES FOR MATRIX SUMS

6.70. (Eigenvalues) Let \( A \) and \( B \) be \( n \times n \) Hermitian or real symmetric matrices, and let \( C = A + B \), with corresponding eigenvalues 

\[
\alpha_1 \geq \alpha_2 \geq \cdots \geq \alpha_n; \quad \beta_1 \geq \beta_2 \geq \cdots \geq \beta_n \quad \text{and} \quad \gamma_1 \geq \gamma_2 \geq \cdots \geq \gamma_n,
\]

respectively. Then:

(a)
(b) It follows from (a) that
\[ \gamma_i \leq \alpha_j + \beta_{i-j+1}, \quad \text{for } j = 1, 2, \ldots, i; \quad i = 1, 2, \ldots, n, \]
and \[ \gamma_i \geq \alpha_j + \beta_{n-j+i}, \quad \text{for } j = i, i+1, \ldots, n; \quad i = 1, 2, \ldots, n. \]

(c) (Weyl’s Theorem) From (b) we have:

(i) For \( i, j \leq n \)
\[ \lambda_i(A + B) \leq \lambda_j(A) + \lambda_{i-j+1}(B) \quad \text{for } j \leq i, \]
\[ \lambda_i(A + B) \geq \lambda_j(A) + \lambda_{n+i-j}(B) \quad \text{for } j \geq i. \]

(ii) If in (i) we make the subscript substitution \( j = a \) and \( i - j + 1 = b \) so that \( i = a + b - 1 \), and then relabel, we get from the first equation
\[ \lambda_{a+b-1}(A + B) \leq \lambda_a(A) + \lambda_b(B), \quad a + b - 1 \leq n, \ b \geq 1. \]

(iii) Setting \( j = i \) in (i) we have, for \( i = 1, 2, \ldots, n \),
\[ \lambda_i(A) + \lambda_n(B) \leq \lambda_i(A + B) \leq \lambda_i(A) + \lambda_1(B). \]

(iv) (Monotonicity of Eigenvalues) If \( B \) is real non-negative definite and \( A \) is real symmetric, then \( \lambda_i(B) \geq 0 \) for all \( i \) and, from (iii),
\[ \lambda_i(A) \leq \lambda_i(A + B), \quad i = 1, 2, \ldots, n. \]
If \( B \) is positive definite, then the inequality is strict.

(d) (i) (Lidskii) Let \( i_1, i_2, \ldots, i_k \) be integers satisfying \( 1 \leq i_1 < \cdots < i_k \leq n \). Then for \( k = 1, 2, \ldots, n \),
\[ \sum_{j=1}^{k} \{ \lambda_{i_j}(A) + \lambda_{n-k+j}(B) \} \leq \sum_{j=1}^{k} \lambda_{i_j}(A + B) \leq \sum_{j=1}^{k} \{ \lambda_{i_j}(A) + \lambda_j(B) \}. \]

(ii) (Sum of the \( k \) largest eigenvalues) For \( k = 1, 2, \ldots, n \),
\[ \sum_{i=1}^{k} \lambda_i(A) + \sum_{i=1}^{k} \lambda_{n-k+i}(B) \leq \sum_{i=1}^{k} \lambda_i(A + B) \leq \sum_{i=1}^{k} \{ \lambda_i(A) + \lambda_i(B) \}. \]

(e) Suppose \( B \) is a real symmetric matrix with \( \text{rank} B \leq r \) and \( A \) is real symmetric. For \( i = 1, 2, \ldots, n - r \) we have:
\[ \lambda_{i+r}(A) \leq \lambda_i(A + B), \]
\[ \lambda_{i+r}(A + B) \leq \lambda_i(A). \]

6.71. (Convexity) For any two real symmetric \( n \times n \) matrices \( A \) and \( B \), and \( 0 \leq \alpha \leq 1 \),
\[ \lambda_1[\alpha A + (1 - \alpha)B] \leq \alpha \lambda_1(A) + (1 - \alpha)\lambda_1(B), \]
\[ \lambda_n[\alpha A + (1 - \alpha)B] \geq \alpha \lambda_n(A) + (1 - \alpha)\lambda_n(B). \]
Hence, $\lambda_1$ is convex and $\lambda_n$ is concave on the space of real symmetric matrices. Putting $\alpha = 1/2$ gives us

$$\lambda_1(A + B) \leq \lambda_1(A) + \lambda_1(B),$$
$$\lambda_n(A + B) \geq \lambda_n(A) + \lambda_n(B).$$

6.72. (Singular Values) Let $A$ and $B$ be $m \times n$ matrices, and let $p = \min\{m, n\}$. Then:

(a) 
$$\sigma_i(A + B) \leq \sigma_j(A) + \sigma_{i-j+1}(B), \quad j = 1, 2, \ldots, i; \quad i = 1, 2, \ldots, p.$$ 
$$\sigma_{i+j-1}(A + B) \leq \sigma_i(A) + \sigma_j(B), \quad 1 \leq i, j \leq p; \quad i + j \leq p + 1.$$ 

(b) In particular,

(i) $\sigma_1(A + B) \leq \sigma_1(A) + \sigma_1(B)$.

(ii) $\sigma_p(A + B) \leq \min\{\sigma_p(A) + \sigma_1(B), \sigma_1(A) + \sigma_p(B)\}$.

(iii) $\sigma_i(A) + \sigma_n(B) \leq \sigma_i(A + B) \leq \sigma_i(A) + \sigma(B)$.

(c) $|\sigma_i(A + B) - \sigma_i(A)| \leq \sigma_1(B)$ for $i = 1, 2, \ldots, p$.

(d) $\sum_{i=1}^{k} \sigma_i(A + B) \leq \sum_{i=1}^{k} [\sigma_i(A) + \sigma_i(B)], \quad k = 1, 2, \ldots, p.$

Proofs. Section 6.4


6.70c(i). Bhatia [1997: 62, with $i$ and $j$ interchanged].

6.70c(ii). Schott [2005: 114, real case].


6.70d(i). Wielandt [1955] and Dùmbgen [1995].


6.70e. Schott [2005: 112–114].

6.71. Abadir and Magnus [2005: 344–345] and Magnus and Neudecker [1999: 205, $\lambda_1$ and $\lambda_n$ are interchanged].


6.72b(iii). Zhang [1999: 228].


6.72d. Horn and Johnson [1991: 196].
6.5 INEQUALITIES FOR MATRIX DIFFERENCES

6.73. Let $A$, $B$, and $A - B$ be Hermitian non-negative definite $n \times n$ matrices with rank $B \leq k$. Then

$$\lambda_i(A - B) \geq \lambda_{k+i}(A)$$

for all $i$ $(k + i \leq n)$ with equality for all $i$ if and only if

$$B = \sum_{i=1}^{k} \lambda_i(A)u_iu_i^\prime,$$

where $u_1, u_2, \ldots, u_k$ are the first $k$ orthonormal eigenvectors of $A$ (i.e., those corresponding to the $\lambda_i(A)$, $i = 1, 2, \ldots, k$).

6.74. Let $A$ and $B$ be $m \times n$ matrices with ranks $r$ and $s$, respectively. Then:

(a) \[ \sigma_i(A - B) \geq \sigma_{i+s}(A), \quad i + s \leq r, \]

\[ \geq 0, \quad i + s > r. \]

(b) The equalities in (a) are attained if and only if $s \leq r$ and

$$B = \sum_{i=1}^{s} \sigma_i(B)u_iu_i^\prime,$$

where the singular value decomposition of $A$ is $A = \sum_{i=1}^{r} \sigma_i(A)u_iu_i^\prime$.

Proofs. Section 6.5

6.73. Quoted by Rao and Rao [1998: 382], though the proof is similar to that of (6.74).


6.6 INEQUALITIES FOR MATRIX PRODUCTS

6.75. Let $A$ be an $n \times n$ non-negative definite matrix, and let $B$ be an $n \times n$ positive definite matrix. If $i, j, k = 1, 2, \ldots, n$ such that $j + k \leq i + 1$, then:

(a) $\lambda_i(AB) \leq \lambda_j(A)\lambda_k(B)$.

(b) $\lambda_{n-i+1}(AB) \geq \lambda_{n-j+1}(A)\lambda_{n-k+1}(B)$.

The case when $A$ is symmetric and $B$ is non-negative definite is discussed in detail by Mäkeläinen [1970].

6.76. If $A$ and $B$ are $n \times n$ Hermitian non-negative definite matrices, then

$$\lambda_i(A)\lambda_n(B) \leq \lambda_i(AB) \leq \lambda_i(A)\lambda_1(B), \quad i = 1, 2, \ldots, n.$$
6.77. (von Neumann) (Trace) If $A$ and $B$ are $n \times n$ Hermitian matrices, then

$$\sum_{i=1}^{n} \lambda_i(A) \lambda_{n-i+1}(B) \leq \text{trace}(AB) \leq \sum_{i=1}^{n} \lambda_i(A) \lambda_i(B).$$

Equality holds on the right when $B = \sum_{i=0}^{n} \lambda_i(B) u_i u_i^*$, and equality holds on the left when $B = \sum_{i=0}^{n} \lambda_{n-i+1}(B) u_i u_i^*$. Here $u_i$ is a right eigenvector of $A$ for the eigenvalue $\lambda_i(A)$, $i = 1, 2, \ldots, n$. 

6.78. Let $A$ and $B$ be $n \times n$ non-negative definite matrices. If $1 \leq i_1 < \cdots < i_k \leq n$, then

$$\prod_{j=1}^{k} \lambda_{i_j}(AB) \leq \prod_{j=1}^{k} \lambda_{i_j}(A) \lambda_{j}(B), \quad k = 1, 2, \ldots, n,$$

with equality for $k = n$. 

6.79. (Partial Sum) Let $A$ and $B$ be $n \times n$ (real) non-negative definite matrices. Then

$$\sum_{i=1}^{k} \lambda_i(A) \lambda_{n-i+1}(B) \leq \sum_{i=1}^{k} \lambda_i(AB), \quad k = 1, 2, \ldots, n.$$ 

6.80. Let $A$ be an $m \times n$ and $B$ an $n \times m$ real or complex matrices. Then

$$\sigma_i(A) \sigma_m(B) \leq \sigma_i(AB) \leq \sigma_i(A) \sigma_1(B), \quad i = 1, 2, \ldots, m.$$ 

6.81. Let $A$ be an $m \times n$ and $B$ an $n \times m$ real or complex matrices, and let $p = \min\{m, n\}$. Then, for singular values $\sigma(\cdot)$,

$$-\sum_{i=1}^{p} \sigma_i(A) \sigma_i(B) \leq \text{trace}(AB) \leq \sum_{i=1}^{p} \sigma_i(A) \sigma_i(B).$$

Equality holds on the right when $B = \sum_{i=1}^{p} \sigma_i(B) q_i p_i^*$, and equality on the left holds when $B = \sum_{i=1}^{p} \sigma_i(B) (-q_i) p_i^*$, where $p_i$ and $q_i$ are the singular vectors of $A$ for $\sigma_i(A)$, $i = 1, 2, \ldots, p$ (cf. Section 16.3). 

6.82. (Horn) Let $A$ be an $m \times p$ and $B$ an $p \times n$ real or complex matrices, and let $q = \min\{m, n, p\}$.

(a) $\prod_{j=1}^{i} \sigma_j(AB) \leq \prod_{j=1}^{i} \sigma_j(A) \sigma_j(B), \quad i = 1, 2, \ldots, q.$

If $A$ and $B$ are square matrices of the same order (i.e., $m = n = p$), then equality holds in the above equation for $i = n$. 

(b) $\sum_{j=1}^{i} [\sigma_j(AB)]^p \leq \sum_{j=1}^{i} [\sigma_j(A) \sigma_j(B)]^p$ for $i = 1, 2, \ldots, q$ and any $p > 0$.

Horn and Johnson [1991: 177] give some extensions to functions of the singular values.
6.83. Let $A$ and $B$ be real $n \times n$ symmetric matrices, and let $T$ be an $n \times n$ orthogonal matrix. Then

$$\max_T \text{trace}(TAT'B) = \sum_{i=1}^{n} \lambda_i(A)\lambda_i(B) \quad \text{and}$$

$$\min_T \text{trace}(TAT'B) = \sum_{i=1}^{n} \lambda_i(A)\lambda_{n+1-i}(B).$$

Setting

$$B = \begin{pmatrix} I_k & 0 \\ 0 & 0 \end{pmatrix},$$

we have

$$\max_{R'AR=I_k} \text{trace}(R'AR) = \sum_{i=1}^{k} \lambda_i(A).$$

6.84. Let $X_i$ be an $n \times p_i$ matrix of rank $p_i$ ($i = 1, 2$). Then the eigenvalues of $(X_2'X_2)^{-1}X_2'X_1(X_1'X_1)^{-1}X_1'X_2$ are less than or equal to one. This result arises in the correspondence analysis of a contingency table.

6.85. If $A$ and $B$ are $n \times n$ real or complex matrices of which at least one is nonsingular, then

$$\lambda_{\min}(AA^*)\lambda_{\min}(BB^*) \leq \lambda_i(AB)\lambda_i(AB) \leq \lambda_{\max}(AA^*)\lambda_{\max}(BB^*)$$

for all $i$. If $A$ and $B$ are both Hermitian, one is positive definite (say $A$), and the other is non-negative definite, then

$$\lambda_{\min}(A)\lambda_{\min}(B) \leq \lambda_i(AB) \leq \lambda_{\max}(A)\lambda_{\max}(B).$$

Proofs. Section 6.6


6.79. Quoted by Schott [2005: 128; see also 137, exercise 3.57].


6.82b. Horn and Johnson [1991: 177].


6.84. Bénasséni [2002].

6.7 ANTEIGENVALUES AND ANTEIEIGENVECTORS

If \( A \) is an \( n \times n \) positive definite matrix, then the cosine of the angle \( \theta \) between \( n \times 1 \) real vectors \( \mathbf{x} \) and \( A\mathbf{x} \) is (cf. Definition 2.12 in Section 2.2.1)

\[
\cos \theta = \frac{\mathbf{x}'A\mathbf{x}}{\sqrt{(\mathbf{x}'\mathbf{x})(\mathbf{x}'A^2\mathbf{x})}},
\]

which has the value of unity when \( \mathbf{x} \) is an eigenvalue of \( A \), that is \( A\mathbf{x} = \lambda \mathbf{x} \) for some \( \lambda \). This raises the question of what value of \( \mathbf{x} \) minimizes \( \cos \theta \), or equivalently maximises the angle between \( \mathbf{x} \) and \( A\mathbf{x} \). This question motivates the following definitions.

**Definition 6.7.** Let \( \lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n > 0 \) be the eigenvalues of positive definite \( A \) and \( \mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_n \) be the corresponding right eigenvectors. Referring to the above introduction, \( \cos \theta \) takes its minimum value of

\[
\mu_1 = \frac{2\sqrt{\lambda_1 \lambda_n}}{\lambda_1 + \lambda_n}
\]

by the Kantorovich inequality (12.2a) (with \( \mathbf{x} = A^{1/2} \mathbf{y} \)), and the minimum is attained at

\[
\mathbf{x} = \frac{\sqrt{\lambda_n} \mathbf{x}_1 \pm \sqrt{\lambda_1} \mathbf{x}_n}{\sqrt{\lambda_1 + \lambda_n}} = (u_1, u_2), \text{ say.}
\]

The vectors \((u_1, u_2)\) are called the first antieigenvectors and \( \mu_1 \) the first antieigenvalue. The angle \( \theta \) is called the angle of the operator of \( A \). We then define

\[
\mu_2 = \min_{\mathbf{x} \perp \mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_n} \frac{\mathbf{x}'A\mathbf{x}}{\sqrt{(\mathbf{x}'\mathbf{x})(\mathbf{x}'A^2\mathbf{x})}} = \frac{2\sqrt{\lambda_2 \lambda_{n-1}}}{\lambda_2 + \lambda_{n-1}},
\]

which is attained at

\[
\mathbf{x} = \frac{\sqrt{\lambda_{n-1}} \mathbf{x}_2 \pm \sqrt{\lambda_2} \mathbf{x}_{n-1}}{\sqrt{\lambda_2 + \lambda_{n-1}}} = (u_3, u_4), \text{ say.}
\]

We call \( \mu_2 \) the second antieigenvalue of \( A \) and \((u_3, u_4)\) the second antieigenvectors. We then find the third set by minimizing \( \cos \theta \) subject to \( \mathbf{x} \perp \{\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_{n-1}, \mathbf{x}_n\} \), and carry on this process until we have \( \mu_1 \leq \mu_2 \leq \cdots \leq \mu_r \ (r = [p/2]) \), where

\[
\mu_i = \frac{2\sqrt{\lambda_i \lambda_{n-i+1}}}{\lambda_i + \lambda_{n-i+1}}
\]

are the ordered antieigenvalues and \((u_1, u_2), (u_3, u_4), \ldots, (u_{2r-1}, u_{2r})\) are the corresponding pairs of antieigenvectors. When \( p \) is odd, the antieigenvalue of order \((n+1)/2\) is unity, with the corresponding antieigenvector \( \mathbf{x}_{(p+1)/2} \).

The above terminology and concepts were introduced by Gustafson [1968] under the umbrella of **operator trigonometry**. The theory was extended to arbitrary non-singular matrices by Gustafson [2000]. He also applied the theory to the question...
of one measure of efficiency of the ordinary least squares estimator (OLSE) with respect to the best linear unbiased estimator (BLUE) in Gustafson [2002, 2005]. Rao [2005] also discussed this question in detail.

6.86. If $A$ is an $n \times n$ positive definite matrix, then

$$\frac{A^2x}{x'Ax} - \frac{2Ax}{x'Ax} + x = 0$$

is called the Euler Equation. This equation is satisfied by all the eigenvectors $x_i$ of $A$, and the only other solutions are the antieigenvectors

$$\frac{\sqrt{\lambda_j}x_k \pm \sqrt{\lambda_k}x_j}{\sqrt{\lambda_j + \lambda_k}}.$$

This topic has links with canonical correlations (Gustafson [2005: 116]).

6.87. Let $A$ be a positive definite $n \times n$ matrix. Then

$$\max_{x'x=1} [x'Ax - (x'A^{-1}x)^{-1}] = (\sqrt{\lambda_1} - \sqrt{\lambda_n})^2,$$

with the maximum occurring at

$$x = \left(\frac{\sqrt{\lambda_1}}{\sqrt{\lambda_1} + \sqrt{\lambda_n}}\right)^{1/2} x_1 \pm \left(\frac{\sqrt{\lambda_n}}{\sqrt{\lambda_1} + \sqrt{\lambda_n}}\right)^{1/2} x_n,$$

where $x_1$ and $x_n$ are the eigenvectors corresponding to $\lambda_1$ and $\lambda_n$, the maximum and minimum eigenvalues of $A$. Rao [2005: 64–65] uses the above result to define the first of another series of antieigenvalues that he calls the SM–antieigenvalues, with corresponding antieigenvectors.

Proofs. Section 6.7


CHAPTER 7

GENERALIZED INVERSES

When a matrix is not square, or square and singular, then an inverse does not exist. However, a type of inverse does exist for these matrices called a generalized inverse that functions very much like an inverse. Such inverses are very useful in statistics for finding explicit solutions for a variety of problems such as the solution of linear equations so that this chapter has close links with Chapter 13. The reader should also consult Chapter 14 on partitioned matrices. A summary of some computational aspects of generalized inverses, along with references, is given by Ben-Israel and Greville [2003: chapter 7].

7.1 DEFINITIONS

Definition 7.1. A weak inverse of an $m \times n$ matrix $A$ is defined to be any $n \times m$ matrix $G$ that satisfies the condition

$$ AGA = A. $$

Such a matrix always exists (by 7.1 below), but it is not unique. We shall write $G = A^{-}$. Many of the results below are proved by verifying, or finding conditions, that (1) is true.

Note that the name "generalized inverse" is fairly common but not universal. Other terms used include conditional inverse (cf. Graybill [1983: chapter 6]), pseudo-inverse, $g$-inverse, and weak inverse. I shall use the term weak inverse to avoid confusion.
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If \( A \) is real and \( G \) also satisfies

1. \( GAG = A \),
2. \( AG \) is symmetric,
3. \( GA \) is symmetric,

then we call \( G \) the Moore–Penrose inverse and write \( G = A^+ \). The above definition applies to complex matrices \( A \) if we replace "symmetric" by "Hermitian."

There are other matrices \( G \) that satisfy just one or more of the above four conditions, and we shall use subscripts to identify the conditions. For example, if \( G \) satisfies at least (1) and (2) we shall call \( G \) a \( g_{12} \)-inverse and write \( G = A^{-}_{(1,2)} \).

Similarly we can write \( A^{-} = A^{-}_{(1)} \) and refer to \( A^{-} \) as a \( g_{1} \)-inverse. We shall only use the subscript notation if there is any danger of ambiguity. For one list of the various inverses see Rao and Rao [1998: 294).

We shall also define \( A_{\{i,j,\ldots,p\}} \) to be the set of all matrices \( G \) which satisfy at least the conditions \( (i) \), \( (j), \ldots, (p) \). Thus \( A_{(1,2)}^{-} \in A_{\{1,2\}}^{-} \), \( A^{-} \in A_{\{1\}}^{-} \), and so on. We shall discuss these inverses later.

If \( A \) is square, then a generalized inverse \( G \) that satisfies (1), (2), and \( AG = GA \) is called the group inverse, which we denote by \( A^{\#} \).

7.2 WEAK INVERSES

7.2.1 General Properties

Let \( A \) be an \( m \times n \) real or complex matrix of rank \( r \). Many of the following results can be proved by simply checking that condition (1) above holds.

7.1. (Existence) From (16.33) there exist conformable nonsingular matrices \( B \) and \( C \) such that

\[
BAC = \begin{pmatrix} I_r & 0 \\ 0 & 0 \end{pmatrix}, \quad \text{or} \quad A = B^{-1} \begin{pmatrix} I_r & 0 \\ 0 & 0 \end{pmatrix}C^{-1}.
\]

Then \( A^{-} = C \begin{pmatrix} I_r & X \\ Y & Z \end{pmatrix}B \) for arbitrary \( X, Y, \) and \( Z \) of appropriate sizes. Although a weak inverse always exists, we see that it is not unique. Another version based on the singular value decomposition is given in (7.82).

7.2. (Basic Properties)

(a) Taking the transpose of both sides of \( AA^{-}A = A \), we see that \( A^{-}' \) is a weak inverse of \( A' \). Although we shall write \( (A^{-})' = (A')^{-} \), what we mean, technically, is that \( A^{-}' \in A_{\{1\}}^{-} \). This idea underlies all the results below.

(b) For \( k \neq 0 \), \( k^{-1}A^{-} \) is a weak inverse \( kA \).

(c) \( A^{-}A \) and \( AA^{-} \) are each idempotent. Also, since \( P_{C(A)} = AA^{-} \) is not generally symmetric, it represents a nonorthogonal (oblique) projection onto \( C(A) \). Similarly, \( P_{C(A')} = (A^{-}A)' = A'A^{-} \) represents an oblique projection onto \( C(A') \).
WEAK INVERSES

(d) \( \text{rank}(\mathbf{AA}^{-}) = \text{trace}(\mathbf{AA}^{-}) = \text{trace}(\mathbf{A}^{-}\mathbf{A}) = \text{rank}(\mathbf{A}^{-}\mathbf{A}) = \text{rank}(\mathbf{A}) \leq \text{rank}(\mathbf{A}^{-}). \)

(e) \( \mathcal{C}(\mathbf{AA}^{-}) = \mathcal{C}(\mathbf{A}), \mathcal{N}(\mathbf{AA}^{-}) = \mathcal{N}(\mathbf{A}), \) and \( \mathcal{C}[(\mathbf{A}^{-}\mathbf{A})^*] = \mathcal{C}(\mathbf{A}^*). \)

(f) Taking conjugate transposes of \( \mathbf{AA}^{-} = \mathbf{A} \) we get \( (\mathbf{A}^*)^{-} = (\mathbf{A}^{-})^*. \)

(g) \( \text{rank} \mathbf{A} = m \) if and only if \( \mathbf{AA}^{-} = \mathbf{I}_m \) (i.e., \( \mathbf{A}^{-} \) is a right inverse of \( \mathbf{A} \)).

(h) \( \text{rank} \mathbf{A} = n \) if and only if \( \mathbf{A}^{-}\mathbf{A} = \mathbf{I}_n \) (i.e., \( \mathbf{A}^{-} \) is a left inverse of \( \mathbf{A} \)).

(i) \( \mathbf{A}(\mathbf{A}^*\mathbf{A})^{-}\mathbf{A}^*\mathbf{A} = \mathbf{A} \) and \( \mathbf{A}^*\mathbf{A}(\mathbf{A}^*\mathbf{A})^{-}\mathbf{A}^* = \mathbf{A}^* \). This means that \( (\mathbf{A}^*\mathbf{A})^{-}\mathbf{A}^* \) is a weak inverse of \( \mathbf{A} \), and \( \mathbf{A}(\mathbf{A}^*\mathbf{A})^{-} \) is a weak inverse of \( \mathbf{A}^* \).

(j) \( \mathbf{A}(\mathbf{A}^*\mathbf{A})^{-}\mathbf{A}^* \) is Hermitian, idempotent, and invariant for any choice of the weak inverse \( (\mathbf{A}^*\mathbf{A})^{-} \).

(k) \( \mathbf{A}^*\mathbf{A}\mathbf{G}\mathbf{A} = \mathbf{A}^*\mathbf{A} \) if and only if \( \mathbf{G} \) is a weak inverse of \( \mathbf{A} \).

7.3. The following conditions are equivalent.

(1) \( \mathbf{G} \) is a weak inverse of \( \mathbf{A} \).

(2) \( \mathbf{AG} \) is idempotent and \( \text{rank}(\mathbf{AG}) = \text{rank} \mathbf{A} \).

(3) \( \mathbf{GA} \) is idempotent and \( \text{rank}(\mathbf{GA}) = \text{rank} \mathbf{A} \).

(4) \( \text{rank}(\mathbf{I}_n - \mathbf{GA}) = n - \text{rank} \mathbf{A} \).

7.4. (Symmetric and Hermitian Matrices)

(a) A Hermitian matrix has a Hermitian weak inverse, namely \( \frac{1}{2}(\mathbf{A}^{-} + (\mathbf{A}^{-})^*). \)

(b) A Hermitian matrix \( \mathbf{A} \) has a non-negative definite weak inverse if and only if \( \mathbf{A} \) is non-negative definite.

7.5. (Rank of Inverse)

(a) Taking \( \mathbf{X} = \mathbf{0} \) and \( \mathbf{Y} = \mathbf{0} \) in (7.1) and noting that the rank is unchanged by multiplying by a nonsingular matrix, we see that

\[
\text{rank}(\mathbf{A}^{-}) = \text{rank} \mathbf{A} + \text{rank} \mathbf{Z}.
\]

Since \( \mathbf{Z} \) is arbitrary, there exists an \( \mathbf{A}^{-} \) having any specified rank between \( \text{rank} \mathbf{A} \) and \( \min\{m,n\} \) (Rao and Mitra [1971: 31]). In particular, we can choose \( \mathbf{Z} \) such that \( \mathbf{A}^{-} \) has full row or column rank (i.e., the rows or columns are linearly independent).

(b) \( \text{rank}(\mathbf{A}^{-}) = \text{rank} \mathbf{A} \) if and only if \( \mathbf{A}^{-} \) is also a \( g_{1,2} \)-inverse

7.6. (Representation of \( \mathbf{A}^{-1} \)) Let \( \mathbf{A}^{-} \) be any weak inverse of \( \mathbf{A} \). Then we have the following representations.

(a) \( \mathbf{A}^- = \{ \mathbf{X} : \mathbf{X} = \mathbf{A}^{-} + \mathbf{H} - \mathbf{A}^{-}\mathbf{AH}\mathbf{A}^{-}; \mathbf{H} \text{ arbitrary} \}. \)

(ii) \( \mathbf{A}^- = \{ \mathbf{X} : \mathbf{X} = \mathbf{A}^{-} + (\mathbf{I} - \mathbf{A}^{-}\mathbf{A})\mathbf{F} + \mathbf{G}(\mathbf{I} - \mathbf{AA}^{-}); \mathbf{F}, \mathbf{G} \text{ arbitrary} \}. \)
(b) Let $A_1^-$, $A_2^-$, and $A_3^-$ be any (not necessarily the same) fixed weak inverses of $A$. Then $B_1$ and $B_2$ are also weak inverses of $A$, where

$$B_1 = A_1^- + F - A_2^- AFAA_3^-,$$

$$B_2 = A_1^- + (I - A_3^- A)F + G(I - AA_3^-).$$

Here $F$ and $G$ are arbitrary matrices of appropriate sizes. Also, any weak inverse of $A$ can be written as $B_1$ and as $B_2$ for some matrices $F$ and $G$. If we consider the special case of $A_1^-$, $A_2^-$, and $A_3^-$ being all the same, we see that $B_1$ and $B_2$ reduce to (a)(i) and (a)(ii), respectively.

(c) If $A$ and $B$ are $m \times n$ matrices with $A \{1\} = B \{1\}$, that is every weak inverse of $A$ is a weak inverse of $B$, and vice-versa, then $A = B$.

7.7. (Rank and Products)

(a) $\text{rank}(ABC) = \text{rank} B$ implies that $C(ABC)^-A$ is a weak inverse of $B$. We can set $A = I$ or $C = I$.

(b) Let $V$ be a matrix such that $\text{rank}(A^*VA) = \text{rank} A$ (which is automatically satisfied if $A$ is Hermitian positive definite), then:


(ii) $A(A^*VA)^-A^*$ is invariant for any choice of $(A^*VA)^-$ and is of the same rank as $A$. If $A^*VA$ is Hermitian, then so is $A(A^*VA)^-A^*$.

7.8. If $A$ is $m \times n$ and $D$ is $m \times m$, and both are of rank $m$, then

$$D^{-1} = A(A'DA)^-A'.$$

7.9. (Hermite Form)

(a) If $A$ is $n \times n$ and $B$ is nonsingular such that $BA = H_A$, where $H_A$ is in Hermite form (Section 16.2.4), then $B$ is weak inverse of $A$.

(b) Let $A$ be an $m \times n$ ($m > n$) matrix, and let $A_0 = (A, 0_{m \times (m-n)})$. Let $B_0$ be a nonsingular matrix such that $B_0A_0 = H$, where $H$ is in Hermite form. Suppose $B_0$ is partitioned as

$$B_0 = \begin{pmatrix} B \\ B_1 \end{pmatrix}$$

where $B$ is $n \times m$. Then $B$ is a weak inverse of $A$.

A similar result holds for $m < n$.

7.10. Let $A$ and $B$ be $m \times n$ complex matrices. Then the following statements are equivalent:

1. The nonzero eigenvalues of $B^{-}A$ are invariant with respect to $B^{-}$.
2. $\text{trace}(B^{-}A)$ is invariant with respect to $B^{-}$.
3. $\mathcal{C}(A) \subseteq \mathcal{C}(B)$ and $\mathcal{C}(A^*) \subseteq \mathcal{C}(B^*)$. 
Proofs. Section 7.2.1.


7.2b. The result follows from the definition of a weak inverse.

7.2c. $A^{-}A^{-}A = A^{-}A$ and $AA^{-}AA^{-} = AA^{-}$. Also $P_{C(A)}A = A$ and then take the transpose of $AP_{C(A)}^{'} = A$.


7.2e. Ben-Israel and Greville [2003: 43].

7.2g–7.2h. Ben-Israel and Greville [2003: 43] and Schott [2005: 204].


7.4b. Arguing as in (7.21) for Hermitian matrices, we have $A = UAU^*$, where $U$ is unitary and $A$ is a diagonal matrix of non-negative eigenvalues. We then set $A^{-} = UA^{-}U^{*}$, which is Hermitian non-negative definite.


7.6a(ii). Rao and Mitra [1971: 26].

7.6b. Graybill [1983: 137]


7.8. This follows from (7.7a) by noting that $\text{rank}(A'DA) = \text{rank}D$, since $D$ is nonsingular.


7.2.2 Products of Matrices

7.11. (Invariance Properties)

(a) The matrix $BA^-C$ is invariant for any choice of $A^-$ if and only if $C(B') \subseteq C(A')$ and $C(C) \subseteq C(A)$.

(b) From (a), if $A$ is a real symmetric matrix, then $B'A^-B$ is invariant for any choice of $A^-$ if and only if $C(B) \subseteq C(A)$.

(c) From (a), if $A$ is any $n \times n$ matrix with $c \subseteq C(A)$ and $c \subseteq C(A')$, then $c'A^-c$ is invariant with respect to $A^-$.

(d) (Regression) Let $X$ be any real matrix and let $G = (X'X)^-$ be any weak inverse of $X'X$.

(i) If $c \subseteq C(X')$, then $c'(X'X)^-X'$ is invariant for any weak inverse of $X'X$.

(ii) $X(X'X)^-X' = XX^+$ is invariant and symmetric, being the orthogonal projector onto $C(X)$. Here $X^+$ is the Moore–Penrose inverse of $X$.

(iii) $G'$ is also a weak inverse of $X'X$.

(iv) $(X'X)^-X'$ is a weak inverse of $X$.

(e) If rank$(CAB) = rank C = rank B$, then $B(CAB)^-C$ is invariant for any choice of $(CAB)^-.$

7.12. If $P$ is idempotent, then $P(PAP)^-P$ is a weak inverse of $PAP$.

7.13. Noting that $FF^-$ and $(F^-F)' = F'F'^-$, being idempotent, represent (oblique) projections onto $F$ and $F'$, respectively (cf. 7.2c), we have the following for conformable matrices.

(a) $BA^-A = B$ if and only if $C(B') \subseteq C(A')$, that is, if and only if there exists a matrix $D$ such that $B = DA$.

(b) $AA^-B = B$ if and only if $C(B) \subseteq C(A)$, that is, if and only if there exists a matrix $D$ such that $B = AD$.

(c) $(CAB)(CAB)^-C = C$ if and only if rank$(CAB) = rank C$.

(d) $B(CAB)^-(CAB) = B$ if and only if rank$(CAB) = rank B$.

7.14. Let $A$ be an $m \times n$ matrix, $B$ be an $m \times m$ matrix, and $C$ be an $n \times n$ matrix.

(a) If $B$ and $C$ are nonsingular, $(BAC)^- = C^{-1}A^{-1}B^{-1}$ for some weak inverse $A^-$ of $A$.

(b) If $A$ has rank $m$ and $B$ is nonsingular, then $(A'BA)^- = A^{-1}B^{-1}A'$.

(c) $(AB)^- = B^-A^-$ if and only if $P = A^-ABB^-$ is idempotent.

7.15. Let $A$, $B$, and $C$ be $m \times n$, $p \times m$, and $n \times q$ matrices, respectively. If $B$ has full column rank $m$, and $C$ has full row rank $n$, then $(BAC)^- = C^-A^-B^-$. 
We can also get special cases by setting one of the matrices equal to the identity matrix.

7.16. If \((A'A)^-\) is a weak inverse of \(A'A\), then so is \((A'A)^-\).

7.17. The following hold for weak inverses \(A^-\) and \(B^-\).

(a) \((I - AA^-)B^-BA = -(I - AA^-)(I - B^-B)A\).

(b) \(BAA^-(I - B^-B) = -B(I - AA^-)(I - B^-B)\).

(c) \((BA)^- = A^-B^- - A^-(I - B^-B)(I - AA^-)(I - B^-B)B^-\).

(d) Let \(A\) be an \(m \times n\) matrix and \(B\) be an \(n \times p\) matrix. If rank \(B = n\), then \((AB)^- = B^-A^-\).

(e) \(C(A) \cap C(B) = 0\) if and only if \((AA' + BB')^-\) is a weak inverse of \(AA'\).

**Proofs.** Section 7.2.2.

7.11a. Graybill [1983: 134-135], with the notation change \(A^c \rightarrow A^-\) and \(A^- \rightarrow A^\dagger\) and Rao and Mitra [1971: 21]. An alternative proof using the idea of extremal ranks is given by Tian [2006a: 95]. He also gives necessary and sufficient conditions for rank\((BA^-C)\) to be invariant with respect to \(A^-\).

7.11d(i). Graybill [1983: 135].


7.12. Follows from the definition of a weak inverse.


7.14b. From (7.2g) we have \(AA^- = I_m\), and then use the definition of weak inverse.

7.14c. Harville [2001: 51, exercise 8]. If \(P^2 = P\), then \(AP^2B = APB\), which implies that \((AB)^- = B^-A^-\). The converse is straightforward.

7.15. We use the fact that \(B^-B = I_m\) and \(CC^- = I_n\) from (7.2g) and (7.2h).


7.17. Isotalo et al. [2005b: chapter 12] and (a)–(c) quoted by Searle [1982: 226]. For (d) we have \(AB(B^-A^-)AB = AB\) since \(BB^- = I_n\).
7.2.3 Sums and Differences of Matrices

7.18. The following conditions are equivalent for any weak inverse \((A + B)^-\).

1. \[
    \begin{pmatrix}
        A \\
        B
    \end{pmatrix} (A + B)^- (A, B) = \begin{pmatrix}
        A & 0 \\
        0 & B
    \end{pmatrix}.
\]

2. \((A + B)^-\) is a weak inverse of both \(A\) and \(B\).

3. \(C(A) \cap C(B) = 0\) and \(C(A') \cap C(B') = 0\).

7.19. Let \(A, B, C,\) and \(V\) be real conformable matrices with \(V\) positive definite, and \(C(C) = C(A') \cap C(B')\). Let \(Q_B = I - P_B\), where \(P_B = B(B'B)^{-1}B'\).

(a) \[
    A(A'VA)^{-1}A' - AQ_B(Q_BA'VAQ_B)^{-1}Q_BA' = A(A'VA)^{-1}C[C'(A'VA)^{-1}C]^{-1}C'(A'VA)^{-1}A'.
\]

(b) \[
    V^{-1} - Q_B(Q_BVQ_B)^{-1}Q_B = V^{-1}B(B'V^{-1}B)^{-1}B'V^{-1}.
\]

\(Q_B\) can be replaced by a matrix with the same range. The above results are used in the theory of singular linear regression models.

Definition 7.2. Given \(A\) and \(B\) both \(m \times n\) matrices, then \(A(A + B)^-B\) is called the parallel sum of \(A\) and \(B\). Some authors call \((A^+ + B^+)\) the parallel sum and, under certain conditions, the two definitions are equivalent. For properties relating to both definitions and their equivalence, see Rao and Mitra [1971: 186–192]. They also define a parallel difference.

7.20. For conformable matrices

(a) \[
    AA'(AA' + BB')^{-1}BB' = BB'(AA' + BB')^{-1}AA'.
\]

(b) \[
    [AA'(AA' + BB')^{-1}BB']^{-1} = (AA')^{-1} + (BB')^{-1}.
\]

Proofs. Section 7.2.3.

7.18. Harville [1997: 421]. We obtain (2) by multiplying out (1) to get \(A(A + B)^-A = A, B(A + B)^-B = B, A(A + B)^-B,\) and \(B(A + B)^-A\).


7.2.4 Real Symmetric Matrices

Let \(A\) be a real symmetric matrix.

7.21. By (16.44) there exists orthogonal \(T\) such that

\[
    T'AT = \begin{pmatrix}
        \Lambda_r & 0 \\
        0 & 0
    \end{pmatrix},
\]

where \(\Lambda_r\) is a nonsingular \(r \times r\) diagonal matrix consisting of the nonzero eigenvalues of \(A\). Then

\[
    A^- = T \begin{pmatrix}
        \Lambda_r^{-1} & X \\
        Y & Z
    \end{pmatrix} T',
\]
where $X$, $Y$, and $Z$ are arbitrary. Note that $A^-$ need not be symmetric. (When $A$ is Hermitian, then $T$ is unitary and $T'$ is replaced by $T^*$.)

7.22. Suppose $A$ is $n \times n$, $P$ is symmetric and idempotent, $A + cP$ is nonsingular, and $PA = 0$.

(a) $(A + cP)^{-1}$ is a weak inverse of both $A$ and $P$.

(b) In particular, if $A1_n = 0$, $J_n = 1_n1'_n$ ($= nP$), and $A + dJ_n$ is nonsingular, then $(A + dJ_n)^{-1}$ is a weak inverse of $A$. Furthermore,

$$A^+ = (A + dJ_n)^{-1} - (dn^2)^{-1}J_n.$$ 

These results are useful in experimental designs (e.g., John and Williams [1995: 23]).

7.23. Suppose that $1 + 1 \neq 0$ in the underlying field $\mathcal{F}$. Since $(A^-)'$ is a weak inverse of $A'$, a symmetric weak inverse of a symmetric matrix $A$ always exists, namely $B = \frac{1}{2}[A^- + (A^-)']$.

7.24. From the definition of a weak inverse, if $A$ and $A^-A$ are symmetric, then $(A^-)^2$ is a weak inverse of $A^2$.

Proofs. Section 7.2.4.


7.23. Since $A^- = A'^- = A^-$, we have $AA^-A = A$ and $B = A^-.$

7.2.5 Decomposition Methods

7.25. (Diagonalizable Matrices) If $A$ is diagonalizable of rank $r$, we have from (16.17) the spectral decomposition $A = \sum_{i=1}^{n} \lambda_i F_i = \sum_{i=1}^{r} \lambda_i F_i$, where $\lambda_{r+1} = \cdots = \lambda_n = 0$. Then:

(a) $\sum_{i=1}^{r} \lambda_i^{-1} F_i$ is a weak inverse of $A$.

(b) $(A + \sum_{i=r+1}^{n} a_i F_i)^{-1}$ is a weak inverse of $A$ for all nonzero real $a_{r+1}, \ldots, a_n$.

7.26. There exist permutation matrices $\Pi_1$ and $\Pi_2$ such that

$$\Pi_1 A \Pi_2 = B = \begin{pmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{pmatrix},$$

where $B_{11}$ is a nonsingular $r \times r$ matrix and $r = \text{rank } A$. Then $A = \Pi_1 B \Pi_2$ and

$$B^- = \begin{pmatrix} B_{11}^{-1} & 0 \\ 0 & 0 \end{pmatrix}$$

is a weak inverse of $B$. Also $\Pi_2 B^- \Pi_1$ is a weak inverse of $A$.

Proofs. Section 7.2.5.


7.3 OTHER INVERSES

In this section we assume real matrices. However, many of the results hold for complex matrices by simply replacing $'$ by $*$.

7.3.1 Reflexive ($g_{12}$) Inverse

Let $A$ be an $m \times n$ matrix and $G$ an $n \times m$ matrix. As noted at the beginning of this chapter, $G = A_{12}$ is a $g_{12}$-inverse of $A$ if $AGA = A$ and $GAG = G$, i.e., if $G$ is a weak inverse of $A$ and $A$ is a weak inverse of $G$. Such an inverse is usually referred to as a reflexive generalized inverse or reflexive $g$-inverse.

7.27. If $A$ is $m \times n$, we have from (3.5) the full-rank factorization $A = C_{m \times r}R_{r \times n}$, where $C$ and $R$ have rank $r$. Let $D$ and $S$ be the left and right inverses of $C$ and $R$, respectively, so that $DC = I_r$ and $RS = I_r$. Then $SD$ is a reflexive $g$-inverse of $A$.

7.28. If $A^{-1}$ and $A_2^{-1}$ are any (possibly different) weak inverses of $A$, then $A_1^{-1}AA_2^{-1}$ is a $g_{12}$-inverse of $A$.

7.29. Every reflexive $g$-inverse of a matrix $A$ can be expressed in the form of $A^{-1}AA^{-1}$ for some weak inverse $A^{-1}$ of $A$.

7.30. A weak inverse $G$ of $A$ is a $g_{12}$-inverse if and only if $\text{rank } G = \text{rank } A$.

7.31. If $G$ is a $g_{12}$-inverse of $A$, then $G'$ is a $g_{12}$-inverse of $A'$.

7.32. (Invariance) If $A$, $B$, and $C$ are nonzero conformable matrices, then $AB_{12}C$ is invariant with respect to $B_{12}$ if and only if $C(A') \subseteq C(B')$ and $C(C) \subseteq C(B)$.

Proofs. Section 7.3.1.

7.28. Harville [1997: 496, lemma 20.3.2].
7.31. Harville [1997: 497].
7.32. Tian [2006a: 100] proved this using his extremal rank technique. He also gave necessary and sufficient conditions for the rank to be invariant.

7.3.2 Minimum Norm ($g_{14}$) Inverse

The matrix $G$ is a $g_{14}$-inverse of $A$ if $AGA = A$ and $GA$ is symmetric (or Hermitian if $A$ is complex). It is usually referred to as a minimum norm $g$-inverse.

7.33. The following conditions are equivalent.

(1) $G$ is a $g_{14}$-inverse of $A$. 

(2) \( \text{GAA}' = \text{A}' \).

(3) \( \text{AA}'G = A \).

(4) \( \text{GA} = \text{P}_{\mathcal{C}(\text{A}')} \), where \( \text{P}_{\mathcal{C}(\text{A}')} \), being symmetric and idempotent, represents the orthogonal projection onto \( \mathcal{C}(\text{A}') \). (In this case \( \text{GA} \) is invariant to the choice of \( \text{G} \).)

In the complex case we replace ’ by *.

7.34. If \( \text{G} \) is a \( g_{14} \)-inverse, then \( x = \text{Gy} \) minimizes \( \|x\|_2 \) subject to \( Ax = y \).

7.35. \( A\{14\} = \{G : G = \text{A}_{14}^{-1} + Z(I_n - \text{AA}_{14}^{-1})\} \), where \( Z \) is an arbitrary \( n \times m \) matrix.

7.36. (Product Invariance) If \( A, B, \) and \( C \) are nonzero conformable matrices, then \( AB_{14}C \) is invariant with respect to \( B_{14} \) if and only if \( C(C) \subseteq C(B) \).

Proofs. Section 7.3.2.


7.35. Ben-Israel and Greville [2003: 55].

7.36. Tian [2000a: 105].

7.3.3 Minimum Norm Reflexive (\( g_{124} \)) Inverse

Let \( A \) be an \( m \times n \) matrix and \( G \) an \( n \times m \) matrix. As noted at the beginning of this chapter, \( G \) is a \( g_{124} \)-inverse of \( A \) if \( AGA = A, GAG = G \) and \( GA \) is symmetric. Since it combines a \( g_{12} \) and a \( g_{14} \) inverse, it is referred to as a minimum norm reflexive \( g \)-inverse.

7.37. A matrix \( G \) is a \( g_{124} \)-inverse of \( A \) if and only if \( G = A'(\text{AA}')^{-} \) for some weak inverse \( (\text{AA}')^{-} \) of \( \text{AA}' \).

7.38. If \( G \) is a \( g_{124} \)-inverse of \( A \), then \( \mathcal{C}(G) = \mathcal{C}(A') \).

7.39. \( A\{124\} = \{G : G = \text{A}_{124}^{-1} + \text{A}_{124}^{-}Z(I_n - \text{AA}_{124}^{-})\} \), where \( Z \) is an arbitrary \( n \times m \) matrix.

Proofs. Section 7.3.3.


7.39. Quoted by Ben-Israel and Greville [2003: 56].
7.3.4 Least Squares ($g_{13}$) Inverse

Let $A$ be an $m \times n$ matrix and $G$ an $n \times m$ matrix. As noted at the beginning of this chapter, $G$ is a $g_{13}$-inverse of $A$ if $AGA = A$ and $AG$ is symmetric. It is usually referred to as a least squares $g$-inverse and is denoted by $A_{13}^{-}$. In what follows, we can replace $'$ by $^*$ in the complex case.

7.40. A $p \times n$ matrix $G$ is a $g_{13}$-inverse of the $n \times p$ matrix $X$ if and only if $(y - Xb)'(y - Xb)$ is minimized at $b = Gy$.

7.41. The following statements are equivalent.

1. A matrix $G$ is a $g_{13}$-inverse of $A$.
2. $A'AG = A'$ or, equivalently, $G'A'A = A$.
3. $AG = P_{C(A)}$, where $P_{C(A)} = A(A'A)^{-}A'$ represents the orthogonal projection onto $C(A)$.

7.42. Let $G$ be a $g_{13}$-inverse of $A$. Then:

(a) $AG$ is invariant to the choice of $G$.
(b) $C(G'A') = C(A)$.

7.43. $(A'A)^{-}A'$ is a $g_{13}$-inverse of $A$ for any weak inverse, $(A'A)^{-}$, of $A'A$.

7.44. $A\{13\} = \{G : G = A_{13}^{-} + (I_n - A_{13}^{-}A)Z\}$, where $Z$ is an arbitrary $n \times m$ matrix.

7.45. (Product Invariance) If $A$, $B$, and $C$ are nonzero conformable matrices, then $AB_{13}C$ is invariant with respect to $B_{13}$ if and only if $C(A') \subseteq C(B')$.

Proofs. Section 7.3.4.

7.42. Harville [1997: 501, corollary 20.3.15].
7.44. Quoted by Ben-Israel and Greville [2003: 55].
7.45. This result is proved by Tian [2006a] using his extremal rank method. The same condition also applies for rank invariance.
7.3.5 Least Squares Reflexive (g123) Inverse

Let $A$ be an $m \times n$ matrix and $G$ an $n \times m$ matrix. As noted at the beginning of this chapter, $G$ is a $g_{123}$-inverse of $A$ if $AGA = A$, $GAG = G$, and $AG$ is symmetric. Such an inverse is also called a least squares reflexive $g$-inverse.

7.46. If $G$ is a $g_{123}$-inverse of $A$, then $C(G') = C(A)$ and $N(G) = [C(A)]^\perp = N(A')$.

7.47. $G$ is a $g_{123}$ inverse of $A$ if and only if $G = (A'A)^{-1}A'$ for some weak inverse $(A'A)^{-}$ of $A'A$.

7.48. $A\{123\} = \{G : G = A_{123}^{-} + (I_n - A_{123}^{-}A)ZA_{123}^{-}\}$, where $Z$ is an arbitrary $n \times m$ matrix.

Proofs. Section 7.3.4.

7.46. Harville [1997: 501, lemma 20.3.16].


7.48. Quoted by Ben-Israel and Greville [2003: 56].

7.4 MOORE–PENROSE ($G_{1234}$) INVERSE

7.4.1 General Properties

Let $A$ be an $m \times n$ matrix and $G$ an $n \times m$ matrix. If $G$ satisfies all four conditions mentioned at the beginning of this chapter, then it is called the Moore–Penrose inverse of $A$ and is denoted by $A^+$. This definition was given by Penrose [1955]. For convenience, we list the four conditions for the complex case, namely: (1) $AGA = A$, (2) $GAG = G$, (3) $AG = (AG)^*$, and (4) $GA = (GA)^*$.

The Moore–Penrose inverse of a general matrix $A$ can be obtained using a QR decomposition (16.42) or the singular value decomposition given below (cf. 7.50). For diagonalizable matrices, which includes symmetric matrices, see (16.17c). Moore–Penrose inverses are particularly useful in experimental design. John and Williams [1995] discuss the Moore–Penrose inverse of the so-called information matrix of a design for a wide range of designs including the incomplete block, the connected, and the cyclic designs.

There are a number of references referring to the real case, namely Abadir and Magnus [2005: section 10.3], Graybill [1983: chapter 6, with $A^{-} \rightarrow A^+$], Harville [1997: chapter 20], Magnus and Neudecker [1999: 33, 34, 38], and Schott [2005: section 5.2]. For the complex case see Ben-Israel and Greville [2003], Campbell and Meyer [1979: chapter 1], and Rao and Mitra [1971: section 3.3 and, for some miscellaneous expansions of $A^+$, section 3.5].

7.49. (Representation) If $A$ is a complex matrix of rank $r$, then we have the singular value decomposition of $A$, namely $A = P_r\Delta_rQ_r^*$ (cf. Section 16.3), where $P_r$ is $m \times r$ with orthonormal columns, $Q_r$ is $n \times r$ with orthonormal columns, and $\Delta_r$ is an $r \times r$ diagonal matrix with positive diagonal elements. Then

$$A^+ = Q_r\Delta_r^{-1}P_r^*.$$
7.50. \(A^+\) is unique.

7.51. Let \(A\) be an \(m \times n\) real matrix of rank \(r\). Then \(A^+\) can be computed by the following steps.

1. Compute \(B = A'A\).
2. Let \(C_1 = I_n\).
3. Compute \(C_{j+1} = I_n (1/j) \text{trace}(C_j B) - C_j B\), for \(j = 1, 2, \ldots, r - 1\).
4. Compute \(A^+ = r C_r A' / \text{trace}(C_r B)\).

Also \(C_{r+1} B = 0\) and \(\text{trace}(C_r B) \neq 0\). Since \(C_{r+1} B = 0\), \(r\) does not need to be known in advance. This result is mainly of historical interest, but it does give a method for small matrices. Numerically stable methods for computing \(A^+\) are given by Golub and Van Loan [1996].

7.52. Below we give some basic properties of the Moore–Penrose inverse of a single matrix or vector. We assume matrices and vectors are complex, unless otherwise stated. Most of the following are readily proved by showing that the four conditions are satisfied and also invoking the uniqueness of the Moore–Penrose inverse.

(a) From (7.49) and (7.50), \(A^+\) always exists and is unique.

(b) \(A^+\) is the minimum norm least-squares \(g\)-inverse of \(A\), i.e., for every \(b\) that minimizes \((y - Ab)^*(y - Ab)\), \(b^*b\) is minimized when \(b = A^+ y\).

(c) \(a^+ = (a^* a)^{-1} a^*\) and \((ab^*)^+ = (a^* a)^{-1} (b^* b)^{-1} (b a^*)\).

(d) If \(c \neq 0\), then \((cA)^+ = (1/c) A^+\).

(e) If \(D = \text{diag}(d_1, d_2, \ldots, d_n)\), then \(D^+ = \text{diag}(d_1^+, d_2^+, \ldots, d_n^+)\), where (for \(i = 1, 2, \ldots, n\))

\[
d_i^+ = \begin{cases} 
1/d_i, & \text{if } d_i \neq 0, \\
0, & \text{if } d_i = 0.
\end{cases}
\]

(f) \(A^+ = A^{-1}\) for nonsingular \(A\).

(g) \(A^+ = A^\star\) if the columns of \(A\) are orthogonal with respect to the inner product \(\langle x, y \rangle = y^* x\).

(h) \((A^+)^+ = A\).

(i) \((A')^+ = (A^+)'\), \((A) = (A^+)\), and \((A^*)^+ = (A^+)^\star\).

(j) \(AA^+ = A^+ A\) if and only if \(C(A) = C(A^*)\), i.e., it holds when \(A\) is Hermitian.

(k) \(\text{rank } A = \text{rank } A^+ = \text{rank } (AA^+) = \text{rank } (A^+ A)\).

(l) For any \(m \times n\) complex matrix \(A\):

(i) \(C(A) = C(AB^+) = C(AB^*)\).

(ii) \(C(A^+) = C(A^*) = C(A^+ A) = C(A^* A)\).

(iii) \(C(I_m - AA^+) = N(AB^+) = N(A^*) = N(A^+)\).
(iv) $C(I_n - A^+A) = N(A^+A) = N(A)$.

(m) $A^+$ need not be a continuous function of the elements of $A$. Not only can $A^+(t)$ be discontinuous in the sense that $\lim_{t \to 0} A^+(t) \neq A^+(0)$, but as $A(t)$ moves closer to $A(0)$, $A^+(t)$ can move further away from $A^+(0)$. However, $A^+(t)$ is continuous on $[a, b]$ if and only if rank $[A(t)]$ is constant on $[a, b]$.

7.53. Let $A$ be an $n \times n$ real symmetric matrix with $r$ nonzero eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_r$, and let $A_r = \text{diag}(\lambda_1, \lambda_2, \ldots, \lambda_r)$. Then:

(a) From (16.44) there exists an orthogonal matrix $Q$ such that

$$A = Q \text{diag}(\lambda_1, \ldots, \lambda_r, 0, \ldots, 0)Q'.$$

Then

$$A^+ = Q \begin{pmatrix} \lambda_r^{-1} & 0 \\ 0 & 0 \end{pmatrix} Q' = \sum_{i=1}^{r} \lambda_i^{-1} q_i q_i'.$$

(b) From (a) we have

$$\text{trace } A^+ = \sum_{i=1}^{r} \lambda_i^{-1}.$$

7.54. For any real matrix $A$:

(a) $A^+A$ and $AA^+$ are symmetric and idempotent, and they are equal if $A$ is symmetric.

(b) Since $A^+A$ and $AA^+$ are symmetric:

(i) $A'AA^+ = A' = A^+AA'$.

(ii) $A' A^+ A' = A^+ = A^+ A' A'$.

(c) $(A'A)^+ = A^+ A'^+$ and $(AA')^+ = A'^+A^+$.

(d) $A^+ = (A'A)^+ A' = A'(AA')^+$.

Also:

(i) If $A$ has full column rank, then $A^+ = (A'A)^{-1} A'$ and $A^+ A = I_n$.

(ii) If $A$ has full row rank, then $A^+ = A'(AA')^{-1}$ and $AA^+ = I_m$.

(e) $(AA^+)^+ = AA^+$ and $(A^+ A)^+ = A^+ A$.

(f) $A(A'A)^+ A' = A = AA'(AA')^+ A$.

(g) If $V$ is positive definite, then $(X'V^{-1}X)(X'V^{-1}X)^+X' = X'$.

(h) For any weak inverse $A^{-}$, $A^+ = A'(AA')^{-}A(A'A)A^{-}A'$.

(i) If $A^{-} A$ is real symmetric, then it is unique and equals $A^+A$.

(j) If rank $A = 1$, then $A^+ = [\text{trace}(AA')^{-1}] A'$.

The above results also hold for $A$ complex if we replace ' by * and symmetric by Hermitian.
7.55. Any weak inverse of $A$ can be expressed as

$$A^+ = A^+ + H - A^+ AHH^+,$$

for any $H$ of appropriate size. This follows from (7.6a).

7.56. Let $A$ be a real matrix. The following conditions are equivalent.

1. A matrix $G$ is the Moore–Penrose inverse of $A$.
3. $AG = P_A$ and $GA = P_G$,

where $P_A$ and $P_G$ represent orthogonal projections onto $C(A)$ and $C(G)$, respectively. (This was the original definition of the Moore–Penrose inverse given by Moore [1935]. The equivalence of the two definitions is proved by Campbell and Meyer [1979: 91 and Schott [2005: 181–182, real case].)

7.57. If $A$ is a real normal matrix (i.e., $A'A = AA'$) with Moore–Penrose inverse $A^+$, then:

(a) $A^+A = AA^+$.
(b) $(A^k)^+ = (A^+)^k$ for any positive integer $k$.
(c) If $A$ is symmetric, it is normal and $AA^+ = A^+A$.

7.58. Let $A$ be a real $m \times n$ matrix, and suppose that certain rows are identical (respectively zero). Then the same rows in $A'^+$ and also in $AA^-$ are identical (respectively zero).

7.59. (Expressed as a Limit) If $A$ is an $m \times n$ matrix then

$$A^+ = \lim_{\delta \to 0} (A'A + \delta^2I_n)^{-1} A' = \lim_{\delta \to 0} A'(AA' + \delta^2I_m)^{-1}A'.$$

7.60. (Continuity) Let $A$ be an $m \times n$ matrix and $A_1, A_2, \ldots, \ldots$ be a sequence $m \times n$ matrices such that $A_k \to A$ as $k \to \infty$ (cf. Definition 19.3), then

$$A_k^+ \to A^+ \text{ as } k \to \infty$$

if and only if an integer $N$ exists such that

$$\text{rank } A_k = \text{rank } A \quad \text{for all } k > N.$$

7.61. Given a real matrix $A$, let $F_{13}$ be any $g_{13}$-inverse of $AA'$, and let $H_{14}$ be any $g_{14}$-inverse of $A'A$. Then

$$A^+ = A'F_{13} = H_{14}A'.$$

7.62. (Idempotent matrices) Let $A$ be a real matrix.

(a) If $A$ is symmetric and idempotent, then $A^+ = A$.
(b) $A'A$ is idempotent if and only if $A^+ = A'$. 
7.63. (Non-negative Definite Matrices)

(a) Suppose $A$ is an $n \times n$ (real) non-negative definite matrix of rank $r$. We can write $A = R'R$, where $R$ is $r \times n$ of rank $r$ (cf. 10.10)). Then, since $(RAR')^{-1} = (RR')^{-2}$ and, using (7.65a) and (7.54d), we have

$$A^+ = R'(RAR')^{-1}R = R'(RR')^{-2}R = R^+(R^+)'.$$

The last result also follows directly from (7.54c).

(b) It follows from (a) that if $A$ is non-negative definite (respectively positive definite), then $A^+$ is also non-negative definite (respectively positive definite).

7.64. (Non-negative Definite Difference) Suppose that $A$, $B$, and $A - B$ are non-negative definite matrices, then $B^+ - A^+$ is non-negative definite if and only if rank $A =$ rank $B$.

7.65. (Full-Rank Factorization) If $A = CR$ is a full rank decomposition of an $n \times n$ complex matrix of rank $r$, where $C$ is $m \times r$ of rank $r$ and $R$ is $r \times n$ of rank $r$, (cf. 3.5), then:

(a) $A^+ = R^*(C^*AR^*)^{-1}C^* = R^*(RR^*)^{-1}(C^*C)^{-1}C^*$.

(b) $A^+ = R^+C^+.$

We note that (7.63) is a special case of the above results.

7.66. Let $A$ be an $m \times n$ matrix, and let $B$ be an $n \times m$ matrix. Then $B$ is the Moore–Penrose inverse of $A$ if and only if $B$ is a least squares $(g_{13})$ inverse of $A$ and $A$ is a least squares inverse of $B$.

Proofs. Section 7.4.1.


7.50. Schott [2005: 181].

7.51. This is quoted by Graybill [1983: 128] and proved by Penrose [1956].


7.52c–h. Simply check that the four conditions are satisfied.

7.52i. Take the conjugate transpose of the four conditions.

7.52j. Abadir and Magnus [2005: 290, real case].


7.52l. Campbell and Meyer [1979: 12].

7.54a. Follows from the definition of $A^+$.
7.54f. Abadir and Magnus [2005: 287]. Follows from the fact that $A(A'A)^+A$ is the orthogonal projection onto $C(A)$.
7.54g. Abadir and Magnus [2005: 287].
7.54h. Searle [1982: 216].
7.54i. Both are equal to the orthogonal projection matrix, which is unique.
7.54j. Abadir and Magnus [2005: 288].
7.57a. From (2.35b), $C(A) = C(AA') = C(A'A) = C(A')$; we then apply (7.52p(i)).
7.57b. Proof can be demonstrated for $k = 2$. Using (a), $A^2(A^+)^2A^2 = AAA^+A^+AA = AA^+AAA^+A = A^2$; then use induction.
7.59. Harville [1997: 508-510]. This result holds for complex matrices if we replace $'$ by $*$, as quoted by Rao and Mitra [1971: 64].
7.64. Quoted by Schott [2005: 215, exercise 5.19].
7.65b. Follows from (a) and (7.54d(i)-(ii)); see also Schott [2005: 189, real case]. For some general conditions for $(CR)^+ = R^+C^+$ to hold when ranks are not specified see Ben-Israel and Greville [2003: 160-161].
7.66. Quoted by Schott [2005: 219, exercise 5.47].
7.4.2 Sums of Matrices

7.67. Let $U$ and $V$ be real $m \times n$ matrices. Define

$$C = (I_m - UU^+)V,$$
$$M = \{I_n + (I_n - C^+)C(V'U'U^+V(I_n - C^-C))^{-1}, \text{ and}
W = (I_n - C^+)MV'U^+U(I_m - VC^+).

(a) If $UV' = 0$, then

$$(U + V)^+ = U^+ + (I_n - U^+V)(C^+ + W).$$

(b) If $UV' = 0$ and $U'V = 0$, then

$$(U + V)^+ = U^+ + V^+.$$

7.68. (Orthogonal Sum) Let $A = \sum_{i=1}^{k} A_i$, where the $A_i$ are all real $m \times n$ matrices. If $A_iA_j' = 0$ and $A_i'A_j = 0$ for all $i, j = 1, 2, \ldots, k, i \neq j$, then from (7.67b) we have

$$A^+ = \sum_{i=1}^{k} A_i^+.$$

Proofs. Section 7.4.2.

7.67a. Boullion and Odell [1971].

7.67a–b. Schott [2005: 197].

7.4.3 Products of Matrices

7.69. Suppose $A$ is any $n \times n$ complex matrix.

(a) Let $P$ be any $r \times n$ ($r \geq n$) matrix with orthonormal columns (i.e., $P^*P = I_n$) and $Q$ be any $s \times n$ ($s \geq n$) matrix with orthonormal columns (i.e., $Q^*Q = I_n$), then

$$(PAQ^*)^+ = QA^+P^*.$$

(b) If $B = U^*AU$ for some unitary matrix $U$, then $B^+ = U^*A^+U$.

7.70. Let $A$ be a real $m \times n$ matrix and $B$ be a real $n \times p$ matrix. The following conditions are equivalent.

1. $(AB)^+ = B^+A^+$.
3. $A^+ABB'$ and $A'ABB^+$ are symmetric matrices.
5. $A^+AB = B(AB)^+AB$ and $BB^+A' = A'AB(AB)^+$. 
Let $A$ be an $m \times p$ real matrix, and let $B$ be a $p \times n$ real matrix. If $B_1 = A^+AB$ and $A_1 = AB_1B_1^+$, then $AB = A_1B_1$ and $(AB)^+ = B_1^+A_1^+$.

Let $A$ be any $m \times n$ matrix, and let $K$ be an $n \times n$ nonsingular matrix. If $B = AK$, then $BB^+ = AA^+$. It may not be true that $B^+B = A^+A$.

If $A$ and $B$ are conformable complex matrices, then

$$ (AB)^+ = (A^+AB)^+(ABB^+)^+ = (P_C(A^+)B)^+(AP_C(B))^+ , $$

where $P_C(B)$ is the orthogonal projection onto $C(B)$, and so on (cf. 7.54a).

The following hold:

(a) $A = 0$ if and only if $A^+ = 0$.

(b) $AB = 0$ if and only if $B^+A^+ = 0$.

(c) $A^+B = 0$ if and only if $A'B = 0$.

(d) If $Ax = 0$ for some vector $x$, then $A^+x = 0$ also.

Suppose we have real conformable matrices.

(a) $A'AB = A'C$ if and only if $AB = AA^+C$.

(b) If $B$ has full row rank so that $\det(BB') \neq 0$, then $(AB)(AB)^+ = AA^+$.

Let $A$ be a real $m \times n$ matrix with $n \leq m$, and let $B$ be any real $n \times n$ matrix satisfying $(A'A)^2B = A'A$. Then $A^+ = B'A'$.

Suppose $A$ is a real symmetric matrix.

(a) $A^+ = B'AB$, where $B$ is any solution of $A^2B = A$.

(b) $A^+ = (AK)^2A$, where $K$ is any solution of $A^2KA^2 = A^2$.

Proofs. Section 7.4.3.

7.69a. Harville [1997: 506, real case]).

7.69b. Quoted by Ben-Israel and Greville [2003: 49].

7.70. Schott [2005: 190]. For many other equivalent but more complex conditions involving the Moore–Penrose inverse of products, see Tian [2006c] and references therein. For a related paper see also Tian [2005a].


7.73. Campbell and Meyer [1979: 20].

7.74. Abadir and Magnus [2005: 288].


7.5 GROUP INVERSE

We recall from Definition 7.1 that $A^#$ is the group inverse of a square real or complex matrix $A$ if it satisfies the three conditions

$$AA^#A = A, \quad A^#AA^# = A^#, \quad AA^# = A^#A.$$ 

Such an inverse is a special case of the so-called Drazin inverse, discussed by Ben-Israel and Greville [2003: chapter 4, section 4] and Campbell and Meyer [1979: chapters 7-9]. Group inverses are particularly useful in the theory of finite Markov chains (cf. Meyer [1975] and Noumann and Xu [2005]).

7.78. An $n \times n$ matrix $A$ has a group inverse if and only if $\mathcal{C}(A) \oplus \mathcal{N}(A) = \mathbb{C}^n$. When the group inverse exists, it is unique.

7.79. A square matrix $A$ has a group inverse if and only if $\text{rank} A = \text{rank}(A^2)$.

7.80. Let a square matrix $A$ have a full-rank factorization $A = FG$ (cf. 3.5). Then $A$ has a group inverse if and only if $GF$ is nonsingular, in which case

$$A^# = F(GF)^{-2}G.$$ 

7.81. (General Properties) From the definition we have the following:

(a) If $A$ is nonsingular, then $A^# = A^{-1}$.

(b) $(A^#)^# = A$.

(c) $(A^*)^# = (A^#)^*$.

(d) $(A^')^# = (A^#)'$.

(e) $(A^k)^# = (A^#)^k$ for every positive integer $k$.

(f) $A^# = A(A^3)^{-A}$.

Proofs. Section 7.5.


7.6 SOME GENERAL PROPERTIES OF INVERSES

7.82. (Representations) The following is a useful summary from Rao and Rao [1998: 295–296]) giving representations for all the inverses of an $m \times n$ real (respectively complex) matrix $A$ of rank $r$. We begin with the singular value decomposition of $A$, namely

$$A_{m \times n} = P_{m \times m} \begin{pmatrix} \Delta_r & 0 \\ 0 & 0 \end{pmatrix} Q_{n \times n}^t,$$

where $P$ is an $m \times m$ orthogonal (respectively unitary) matrix, $Q$ is an $n \times n$ orthogonal (respectively unitary) matrix and $\Delta_r = \text{diag}(\delta_1, \delta_2, \ldots, \delta_r)$ is an $m \times n$ matrix with $\delta_1 \geq \delta_2 \geq \cdots \geq \delta_r > 0$. For complex matrices we replace $'$ by *. We shall use the notation $G_{1,\ldots}$ to denote the $n \times m$ $g_{1,\ldots}$-inverse of $A$. 
7.83. (Matrix Bounds) If $A$ is $m \times n$, then using the Löwner ordering (cf. Definition 10.1):

(a) \[ (I_m - AG_1)'(I_m - AG_1) \succeq (I_m - AG_{13})'(I_m - AG_{13}). \]

(b) \[ (I_m - AG_1)'(I_m - AG_1) \succeq (I_m - AG_{14})'(I_m - AG_{14}). \]

(c) \[
(I_m - AG_1)'(I_m - AG_1) \succeq (I_m - AG_{123})'(I_m - AG_{123}) \\
(I_m - AG_1)(I_m - AG_1)' \succeq (I_m - AG_{123})(I_m - AG_{123})'.
\]

(d) \[
(I_n - G_1 A)'(I_n - G_1 A) \succeq (I_n - G_{124} A)'(I_n - G_{124} A) \\
(I_n - G_1 A)(I_n - G_1 A)' \succeq (I_n - G_{124} A)(I_n - G_{124} A)'.
\]

(e) \[
(I_m - AG_1)'(I_m - AG_1) \succeq (I_m - AA^+)'(I_m - AA^+) \\
(I_m - AG_1)(I_m - AG_1)' \succeq (I_m - AA^+)(I_m - AA^+)'. \\
(I_n - G_1 A)'(I_n - G_1 A) \succeq (I_n - A^+ A)'(I_n - A^+ A) \\
(I_n - G_1 A)(I_n - G_1 A)' \succeq (I_n - A^+ A)(I_n - A^+ A)'.
\]

(f) From (a) and (b), the first results of (c) and (d), and the first and third results of (e) we can obtain lower bounds, as in the following example. For any unitarily invariant norm $\| \cdot \|_{ui}$ on the space of all $m \times m$ matrices,

\[
\min_G \|I_m - AG\|_{ui} = \|I_m - AG_{13}\|_{ui},
\]

where the minimum is taken over all weak inverses $G_1$.

Proofs. Section 7.6.

SOME SPECIAL MATRICES

In this chapter we put collect together a number of matrices that have a special structure or properties. Other more general types of matrix occur elsewhere in this book such as Hermitian, symmetric, and normal matrices in Chapter 5, various non-negative matrices in Chapter 9, and non-negative definite matrices in Chapter 10.

8.1 ORTHOGONAL AND UNITARY MATRICES

Definition 8.1. An \( n \times n \) matrix \( T \) is orthogonal if \( T'T = I_n \). It immediately follows by taking determinants that \( T \) is nonsingular, \( T' = T^{-1} \) and \( TT' = I_n \). An \( n \times n \) complex matrix is unitary if \( U^*U = I \), and then \( U^{-1} = U^* \). Although an orthogonal matrix can be real or complex, we shall focus on real orthogonal matrices rather than complex orthogonal matrices in this chapter, unless otherwise stated.

8.2. An \( n \times n \) complex matrix \( A \) is unitary if and only if \( \|Ax\|_2 = \|x\|_2 \) for all \( x \in \mathbb{C}^n \).
8.3. Let $U$ be a unitary matrix partitioned as

$$U = \begin{pmatrix} A & B \\ C & D \end{pmatrix},$$

where $A$ is $m \times m$ and $D$ is $n \times n$.

(a) If $m = n$, then $A$ and $D$ have the same singular values.

(b) If $m < n$ and the singular values of $A$ are $\sigma_1, \sigma_2, \ldots, \sigma_m$, then the singular values of $D$ are also $\sigma_1, \sigma_2, \ldots, \sigma_m$ together with $n - m$ values equal to 1.

(c) $\det A = \det D$.

8.4. (Symmetric Unitary Matrix) Let $U$ be a symmetric unitary matrix, that is, $U' = U$. Then there exists a complex matrix $S$ with the following properties.

(a) $S^2 = U$.

(b) $S$ is unitary.

(c) $S$ is symmetric.

(d) $S$ commutes with every matrix that commutes with $U$.

8.5. A unitary matrix is an isometry, that is, a linear transformation that preserves Euclidean length.

8.6. Let $T$ be a real $n \times n$ orthogonal matrix and $U$ a unitary matrix.

(a) Given $(x, y) = x'y$, the columns (rows) of $T$ form an orthonormal set. The same holds for $U$ if we define $(x, y) = x*y$.

(b) $\det T = \pm 1$. If $\det = 1$ then $T$ represents a rotation.

(c) $|\det U| = 1$, where $|\cdot|$ is the complex modulus.

(d) (i) If $\lambda$ is an eigenvalue of $T$ then so is $\lambda^{-1}$.

(ii) The eigenvalues of $T$ are $\pm 1$ or occur in conjugate pairs $e^{i\theta}$ and $e^{-i\theta}$ ($\theta$ real) on the unit circle, so that all the eigenvalues have unit modulus (cf. 16.46b).

(iii) It follows from (ii) that if $n$ is odd, then at least one eigenvalue is $+1$ or $-1$.

(e) The eigenvalues of $U$ are $\lambda_i = e^{i\theta}$ ($\theta$ real) for all $i$, so that $|\lambda| = 1$.

8.7. If the $n \times n$ matrix $A$ has all its eigenvalues equal to 1 in absolute value, then $A$ is unitary if $\|Ax\|_2 \leq \|x\|_2$ for all $x \in \mathbb{C}^n$.

8.8. Suppose $C$ is an $n \times n$ real skew-symmetric matrix, that is, $C' = -C$ (cf. (5.19) for real matrices). Then:

(a) $I_n + C$ is nonsingular.

(b) $A = (I_n - C)(I_n + C)^{-1}$ is orthogonal with $\det A = 1$. 
(c) \( A = e^{\mathbf{C}} \) is orthogonal with \( \det A = 1 \).

8.9. (Rotation Matrix in the Plane) The matrix

\[
\mathbf{T}_\theta = \begin{pmatrix}
\cos \theta & -\sin \theta \\
\sin \theta & \cos \theta
\end{pmatrix}
\]

represents a rotation in two dimensions in a counter clockwise direction through an angle \( \theta \). We note that \( \mathbf{T}_\theta \mathbf{T}_\phi = \mathbf{T}_{\theta+\phi} \) and \( \mathbf{T}_{-\theta} = \mathbf{T}_\theta^{-1} \). Every \( 2 \times 2 \) orthogonal matrix with determinant equal to +1 can be expressed in the form of \( \mathbf{T}_\theta \) for some \( \theta \).

The following matrix

\[
\mathbf{S}_\theta = \begin{pmatrix}
1 & 0 \\
0 & -1
\end{pmatrix}
\begin{pmatrix}
\cos \theta & -\sin \theta \\
\sin \theta & \cos \theta
\end{pmatrix} = \begin{pmatrix}
\cos \theta & -\sin \theta \\
-\sin \theta & -\cos \theta
\end{pmatrix}
\]

represents a rotation combined with a reflection in the x-axis.

A reflection matrix is symmetric; for example,

\[
\mathbf{V}_\theta = \begin{pmatrix}
\cos \theta & \sin \theta \\
\sin \theta & -\cos \theta
\end{pmatrix}
\]

represents a reflection across a line at an angle of \( \theta/2 \) and has a determinant of -1.

8.10. (Helmert Matrix) We have the following orthogonal matrix \( \mathbf{T} \):

\[
\begin{pmatrix}
\frac{1}{\sqrt{n}} & \frac{1}{\sqrt{n}} & \frac{1}{\sqrt{n}} & \frac{1}{\sqrt{n}} & \cdots & \frac{1}{\sqrt{n}} & \frac{1}{\sqrt{n}} \\
\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 & 0 & \cdots & 0 & 0 \\
\frac{1}{\sqrt{6}} & \frac{1}{\sqrt{6}} & \frac{1}{\sqrt{6}} & -\frac{2}{\sqrt{6}} & \cdots & 0 & 0 \\
\frac{1}{\sqrt{12}} & \frac{1}{\sqrt{12}} & \frac{1}{\sqrt{12}} & \frac{1}{\sqrt{12}} & \cdots & 0 & 0 \\
\frac{1}{\sqrt{n(n-1)}} & \frac{1}{\sqrt{n(n-1)}} & \frac{1}{\sqrt{n(n-1)}} & \frac{1}{\sqrt{n(n-1)}} & \cdots & \frac{1}{\sqrt{n(n-1)}} & \frac{1}{\sqrt{n(n-1)}}
\end{pmatrix}
\]

This matrix has been used for proving the the statistical independence of a number of statistics.

8.11. (Householder Transformation) This \( n \times n \) orthogonal matrix is defined to be \( \mathbf{H}_n = \mathbf{I}_n - 2\mathbf{h}\mathbf{h}^\prime \), where \( \mathbf{h}'\mathbf{h} = 1 \). Since, from (4.33), \( \det \mathbf{H}_n = (1 - 2\mathbf{h}'\mathbf{h}) = -1 \), \( \mathbf{H}_n \) represents a reflection.

Given \( \mathbf{x} = (x_1, x_2, \ldots, x_n)' \) with \( x_1 \neq 0 \), let \( y_1 = -(\text{sign} \; x_1)\sqrt{x'x} \), and define \( h_1 = (1 - x_1/y_1)^{1/2} \) and \( h_i = -x_i/(2h_1y_1) \) for \( i = 2, 3, \ldots, n \). Then \( \mathbf{H}_n \mathbf{x} = (y_1, 0, \ldots, 0)' \). Similarly we can define

\[
\mathbf{H} = \begin{pmatrix}
1 & 0' \\
0 & \mathbf{H}_{n-1}
\end{pmatrix}
\]

so that \( \mathbf{H} \mathbf{x} = (y_1, y_2, 0, \ldots, 0)' \), where \( y_1 = x_1 \) and \( \mathbf{H} \) is orthogonal. By using a succession of such transformations, a matrix can be transformed to an upper-triangular matrix. For further details see Golub and Van Loan [1996: chapter 5] and Seber and Lee [2003: 343-347].
8.12. (Givens Transformation) This orthogonal matrix \( G = (g_{ij}) \) takes the form of an identity matrix except for four elements: \( g_{rr} = g_{ss} = \cos \theta \) and, for \( r > s \), 
\( -g_{rs} = g_{sr} = \sin \theta \). Premultiplying by \( G \) rotates the \( r \)-th and \( s \)-th rows in a clockwise direction through angle \( \theta \). An example of a \( 4 \times 4 \) Givens matrix is

\[
G = \begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & \cos \theta & 0 & \sin \theta \\
0 & 0 & 1 & 0 \\
0 & -\sin \theta & 0 & \cos \theta
\end{pmatrix}.
\]

Products of such matrices can be used to transform a matrix to upper-triangular form. For further details see Golub and Van Loan [1996: 215–221] and Seber and Lee [2003: 348–352].

8.13. If \( B \) is a real nonsingular matrix, then \( B(B'B)^{-1/2} \) is orthogonal (cf. 10.32).

Proofs. Section 8.1.

8.1. \( \bar{U}'U = U'\bar{U} = (U^*U)' = I_n \).

8.2. \( x^*A^*Ax = x^*x \) for all \( x \) implies \( A^*A = I_n \).


8.5. \( \|Ux\| = x^*U^*Ux = \|x\| \).

8.6b. Follows from \( (\det T)^2 = \det(T'T) = 1 \).

8.6c. Rao and Bhimasankaram [2000: 314] and Zhang [1999: 132]. Follows from \( 1 = \det(UU^*) = \det U \cdot \det \bar{U} = (a + ib)(a - ib) = a^2 + b^2 = |U|^2 \).

8.6d. For (i), \( Tx = \lambda x \) implies \( \lambda^{-1}x = T'x \) and \( \det(T - \lambda I_n) = \det(T - \lambda I_n) = 0 \) (i.e., \( T \) and \( T' \) have the same eigenvalues).

8.6e. Zhang [1999: 132].


8.9. \( T^\theta T_\theta = I_2 \).

8.10. \( T'T = I_n \).

8.11. \( H_n' H_n = I_n \).

8.2 PERMUTATION MATRICES

Definition 8.2. Let $\Pi_{ij}$ be the identity matrix $I_n = (e_1, e_2, \ldots, e_n)$ with its $i$th and $j$th rows interchanged. Then $\Pi_{ij}^2 = I_n$, so that $\Pi_{ij}$ is a symmetric and orthogonal matrix. Premultiplying any matrix by $\Pi_{ij}$ will interchange its $i$th and $j$th rows so that $\Pi_{ij}$ is an (elementary) permutation matrix. Postmultiplying a matrix by an elementary permutation matrix will interchange two columns.

Any reordering of the rows of a matrix can be done using a sequence of elementary permutations $\Pi = \Pi_{i_Kj_K} \cdots \Pi_{i_1j_1}$, where

$$\Pi \Pi' = \Pi_{i_Kj_K} \cdots \Pi_{i_1j_1} \cdots \Pi_{i_Kj_K} = I_n.$$

The orthogonal matrix $\Pi$ is called a permutation matrix.

The permutation matrix $\Pi_0 = (e_n, e_1, e_2, \ldots, e_{n-1})$, which has been called the forward shift permutation matrix (and also primary permutation matrix), is useful in the theory of circulants.

For a helpful discussion of permutations and cyclic permutations see Davis [1979] and Rao and Bhimasankaram [2000: section 6.2].

8.14. $\Pi_0$ has the following properties.

(a) $\Pi_0 A \Pi_0 = (a_{i+1,j+1})$ with $n + 1 \equiv 1$ (i.e., subscripts are taken mod $n$).

(b) $\Pi_0^2 = (e_{n-1}, e_n, e_1, \ldots, e_{n-2})$.

(c) $\Pi_0^3 = I_n$.

(d) $\Pi_0 = F^* \Gamma F$, where $\Gamma = \text{diag}(1, \omega, \omega^2, \ldots, \omega^{n-1})$, the $\omega^i$ are the $n$th roots of 1, and $F$ is an $n \times n$ Fourier matrix (cf. Section 8.12.2).

8.15. An $n \times n$ permutation matrix $\Pi_n$ has exactly one entry in each row and column equal to 1, and zeros elsewhere. For example

$$\Pi_3 = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} = (e_2, e_1, e_3), \text{ say}.$$

Thus $\Pi_n$ consists of $I_n$ with its rows resequenced. It is also $I_n$ with its columns resequenced, but not necessarily in the same sequence; that is, $\Pi_n$ is not necessarily symmetric. Left multiplying an $m \times n$ matrix $A$ by $\Pi_n$ produces the same resequences of the rows of $A$ as $\Pi_n$, while right multiplying by $\Pi_n$ does the same for the columns.

8.16. If $\Pi_n$ is a permutation matrix, then so is $\Pi_n^k$, where $k$ is any positive integer.

8.17. If $A$ is $n \times n$, then the diagonal elements of $\Pi_n^t A \Pi_n$ are the same elements (rearranged) as the diagonal elements of $A$.

Definition 8.3. If $A$ is $n \times n$ and $\Pi$ is a permutation matrix, then the matrix $\Pi A \Pi = \Pi^{-1} A \Pi$ is said to be permutation similar to $A$. This concept is linked to irreducibility in (8.101).

Proofs. Section 8.2.


8.3 CIRCULANT, TOEPLITZ, AND RELATED MATRICES

8.3.1 Regular Circulant

Definition 8.4. An $n \times n$ real or complex matrix $A$ is a (regular) circulant if it has the form

$$A = \begin{pmatrix}
a_0 & a_1 & a_2 & \cdots & a_{n-1} \\
a_{n-1} & a_0 & a_1 & \cdots & a_{n-2} \\
a_{n-2} & a_{n-1} & a_0 & \cdots & a_{n-3} \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
a_1 & a_2 & a_3 & \cdots & a_0
\end{pmatrix},$$

that is, all the elements are equal on the main diagonal and on each of the diagonals parallel to the main diagonal. Note that $A$ is counter symmetric as it is symmetric about its main counter (opposite) diagonal. Most authors omit the word "regular" from the definition, but we follow Graybill [1983] and include it so as to be able to distinguish between two types of symmetric circulant below. Thus, if we define $(j - i) \mod n$ as

$$(j - i) \mod n = \begin{cases} 
n + j - i, & \text{when } i > j, \\
j - i, & \text{when } i \leq j, \end{cases}$$

then $A$ is a regular circulant if and only if $(j - i) \mod n = (s - r) \mod n$ implies that $a_{ij} = a_{rs}$. Alternatively, $A$ is a regular circulant if and only if $a_{ij} = a_{(j - i) \mod n}$. Another way of defining a regular circulant is $a_{ij} = a_{1m}$, where

$$m = \begin{cases} 
j + i - 1, & j \geq i, \\
n - (j - i + 1), & j < i.
\end{cases}$$

We can also use the notation $A = \text{circ}(a_0, a_1, \ldots, a_{n-1})$. In applications the circulants are generally real.

Regular circulants can arise as incident matrices of experimental designs such as the balanced incomplete block design (BIBD) and cyclic designs (e.g., Rao and Rao [1998: 513]). There are other types of circulant such as skew circulants (Davis [1979: 83]) and alternating circulants (Tee [2005: 136]).

Definition 8.5. The polynomial $p(z) = a_0 + a_1 z + \cdots + a_{n-1} z^{n-1}$ is sometimes called the representer of the circulant and it occurs, for example, in signal processing.

8.18. The forward shift permutation matrix $\Pi_0$ of (8.14) can be expressed as $\Pi_0 = \text{circ}(0, 1, \ldots, 0)$.

8.19. $\text{circ}(a_0, a_1, \ldots, a_{n-1}) = p(\Pi_0) = a_0 + a_1 \Pi_0 + a_2 \Pi_0^2 + \cdots + a_{n-1} \Pi_0^{n-1}$.

8.20. The following conditions are equivalent.

1. $A$ is an $n \times n$ regular circulant.

2. $\Pi_0 A \Pi_0 = A$.

3. $A^* \Pi_0 = A$.

8.21. If $A$ is a real regular circulant, then so is the Moore–Penrose inverse $A^+$. 

8.22. Let \( A \) be a regular circulant. Then:

(a) \( A^{*} \) is a regular circulant.

(b) \( A^{k} \) is a regular circulant, where \( k \) is a positive integer.

(c) \( A^{-1} \) is also a regular circulant, if \( A \) is nonsingular. In this case, to compute \( A^{-1} \) we only need to find its first row.

8.23. If \( A \) is a regular circulant with first row \((a_0, a_1, a_2, \ldots, a_{n-1})\), and if

\[ |a_q| > \sum_{i=0; i \neq q}^{n-1} |a_i| \]

for some \( q \), then \( A \) is nonsingular.

8.24. If \( A \) and \( B \) are any \( n \times n \) regular circulants, then \( AB \) is a regular circulant and \( AB = BA \).

8.25. If \( A \) is a regular circulant, then so is \( A^{*} \) (by 8.22a) and \( A^{*}A \) (by 8.24), with \( A^{*}A = AA^{*} \). Thus a regular circulant is a normal matrix.

8.26. Let \( A \) and \( C \) be \( n \times n \) regular circulants, and suppose there exists a matrix \( X \) such that \( AX = C \). Then there exists a regular circulant \( B \) such that \( AB = C \).

**Definition 8.6.** The \( n \times n \) matrix \( C_{h} \) \((h = 1, 2, \ldots, n-1)\) that has \( a_{h} = 1 \) and the other \( a_{i} = 0 \) is sometimes referred to as a basic circulant matrix. For example, if \( n = 3 \),

\[
A = \begin{pmatrix}
a_0 & a_1 & a_2 \\
a_2 & a_0 & a_1 \\
a_1 & a_2 & a_0
\end{pmatrix}
\]

and

\[
C_1 = \begin{pmatrix}
0 & 1 & 0 \\
0 & 0 & 1 \\
1 & 0 & 0
\end{pmatrix}.
\]

Here \( C_1 = \text{circ}(0, 1, 0) \). Note that, in general, \( C_1 \) is the same as \( II_0 \) of Definition 8.2.

8.27. If \( C_0 = I_n \), then:

(a) \( A = \sum_{h=0}^{n-1} a_h C_h \).

(b) \( C_h = C_1^h \) \((h = 1, 2, \ldots, n-1)\) and \( C_n = I_n \) (by 8.14c).

8.28. (Eigenvalues and Eigenvectors) Referring to (8.14d), we have the following results.

(a) The eigenvectors of \( C_1 \) are given by

\[
\gamma_j = n^{-1/2}(1, \omega^j, \omega^{2j}, \ldots, \omega^{(n-1)j})',
\]

with corresponding eigenvalues \( \lambda_{1j} = \omega^j \), for \( j = 0, 1, \ldots, n-1 \), where \( \omega = \exp(2\pi i / n) = \cos(2\pi / n) + i \sin(2\pi / n) \) and \( i = \sqrt{-1} \). (Note that the \( \lambda_{1j} \) are the \( n \) roots of unity.)

(b) Since \( C_h x = C_1^h x = \lambda_h^j x \), the eigenvectors of \( C_h \) are still the \( \gamma_j \) with eigenvalues \( \lambda_{hj} = \omega^{jh} \) \((h, j = 0, 1, \ldots, n-1)\).
(c) We now turn our attention to \( A \) of (8.27).

(i) \( A \) has eigenvectors \( \gamma_j \) with (not necessarily distinct) eigenvalues

\[
\lambda_j = \sum_{h=0}^{n-1} a_h \omega^h = p(\omega_j) = \sum_{h=0}^{n-1} a_h \omega_j^h, \quad j = 0, 1, \ldots, n - 1,
\]

where \( \omega_j = \omega^j \), and \( p(z) \) is given in Definition 8.5 (above 8.18). Note that the \( \gamma_j \) are the same for all regular circulants.

(ii) Setting \( j = 0 \) in (i), \( \lambda_0 = a_0 + a_1 + \ldots + a_{n-1} \) is always an eigenvalue.

(iii) The eigenvectors are mutually orthogonal, that is, \( \gamma_j^* \gamma_k = \delta_{jk} \).

(iv) If \( F \) is an \( n \times n \) Fourier matrix (cf. Section 8.12.2), then it is unitary and \( FAF^* = A \), that is, \( AF^* = F^*A \), where \( A = \text{diag}(\lambda_1, \lambda_2, \ldots, \lambda_n) \). Thus the columns of \( F^* \) are a universal set of right eigenvectors for all regular circulants. Also \( A = F^*\Lambda F \).

(v) A spectral decomposition of \( A \) is given by

\[
A = \sum_{j=0}^{n-1} \lambda_j \gamma_j \gamma_j^*.
\]

Here \( \gamma_j^* \) is the complex conjugate of \( \gamma_j \) obtained by replacing \( \omega_j \) in \( \gamma_j \) by its complex conjugate

\[
\bar{\omega} = \exp(-2\pi i/n) = \cos(2\pi/n) - i \sin(2\pi/n).
\]

(vi) The matrix \( \gamma_j \gamma_j^* \) is a regular circulant that can be written in the form

\[
\gamma_j \gamma_j^* = \sum_{h=0}^{n-1} \omega^{-hj} C_h.
\]

(g) The Moore–Penrose inverse of \( A \), which is also a regular circulant, is given by

\[
A^+ = \sum \lambda_j^{-1} \gamma_j \gamma_j^*,
\]

where the summation is over all \( r \) nonzero eigenvalues of \( A \), with \( r = \text{rank} A \).

If \( r = n \) then \( A^+ = A^{-1} = F^*\Lambda^{-1}F \).

(h) \( A^+ = \sum_{h=0}^{n-1} \psi_h C_h \), where \( \psi_h = n^{-1} \sum_j \lambda_j^{-1} \omega^{-hj} \).

8.29. Let \( A = \text{circ}(c_1, c_2, \ldots, c_n) \) be a real \( n \times n \) regular circulant.

(a) If \( n \) is odd and \( \lambda_0 = \sum_{i=1}^{n} c_i \geq 0 \) (cf. 8.28f(ii)), then \( \det A \geq 0 \).

(b) If \( n \) is even, \( n = 2r + 2 \), \( \lambda_0 > 0 \), and

\[
| \sum_{j=1}^{r+1} c_{2j-1} | \geq | \sum_{j=1}^{r+1} c_{2j} |,
\]

then \( \det A \geq 0 \).
Proofs. Section 8.3.1.


8.20. Schott [2005: 329]. The second result follows by multiplying on the left
by $\Pi_0'$ and on the right by $\Pi_0$.


8.27. We simply multiply out the expressions.

8.28. John and Williams [1995: Appendix A7]. For (c)(iv) see Davis [1979:
72], Schott [2005: 332], and Zhang [1999: 107].

8.29. Davis [1979: 76–77].

8.3.2 Symmetric Regular Circulant

To obtain a symmetric regular circulant one writes down a regular circulant and
then determines which elements are equal to achieve symmetry; for example, we
have the following matrix

$$A = \begin{pmatrix}
a_0 & a_1 & a_2 & a_1 \\
a_1 & a_0 & a_1 & a_2 \\
a_2 & a_1 & a_0 & a_1 \\
a_1 & a_2 & a_1 & a_0
\end{pmatrix}. $$

Note that this matrix is symmetric about its main diagonal and about its counter
(opposite) diagonal, so it is doubly symmetric. Trivial examples are $I_n$ and $J_n =
1_n 1_n^*$. Although our focus is on real symmetric matrices, the eigenvalue theory
below applies generally to real and complex matrices.

Symmetric regular circulants arise in cyclic designs as the product of the in-
cidence matrix and its transpose (the concurrence matrix of John and Williams
[1995: 51]). The eigenvalues are related to the so-called canonical efficiency factors.
Symmetric regular circulants also arise with variance matrices, and Khattree [1996]
gives seven applications.

8.30. (Some General Properties) Let $A$ be an $n \times n$ symmetric regular circulant.
Then:

(a) $A$ has at most $\lfloor n/2 \rfloor + 1$ distinct elements, where $\lfloor a \rfloor$ is the integral part of $a$.

(b) $A'$ is a symmetric regular circulant.

(c) If $A$ is nonsingular, then $A^{-1}$ is a symmetric regular circulant.
8.31. Let $A$ and $B$ be $n \times n$ symmetric regular circulants, then

(a) $AB = BA$.

(b) $AB$ is a symmetric regular circulant.

(c) $aA + bB$, where $a$ and $b$ are any real numbers, is a symmetric regular circulant. Hence $aI_n + bJ_n$, where $J_n = 1_n 1'_n$, is a symmetric regular circulant.

8.32. (Eigenvalues and Eigenvectors) If $A$ is a symmetric regular circulant, then we have the following results.

(a) $a_h = a_{n-h}$ ($h = 1, 2, \ldots, m$), where

$$
m = \begin{cases} 
n/2, & n \text{ even}, \\
(n-1)/2, & n \text{ odd}.
\end{cases}
$$

(b) The eigenvectors are $\gamma_j$ ($j = 0, 1, \ldots, n-1$) of (8.28a).

(c) The eigenvalues of $A$ are

$$\lambda_j = \sum_{h=0}^{n-1} a_h \cos(2\pi jh/n), \quad j = 0, 1, \ldots, n-1.$$

(d) $\lambda_j = \lambda_{n-j}$.

(e) If $n = 2m$, then $\lambda_0 = a_0 + 2(a_1 + a_2 + \cdots + a_{m-1}) + a_m$.
If $n = 2m + 1$, then $\lambda_0 = a_0 + 2(a_1 + a_2 + \cdots + a_m)$.

(f) $A^\dagger = \sum_{h=0}^{n-1} \psi_h C_h$, where $\psi_h = n^{-1} \sum_j \lambda_j^{-1} \cos(2\pi jh/n)$. Here we have used (d) so that the sum is over all nonzero eigenvalues, but only choosing one of $\lambda_j$ and $\lambda_{n-j}$.

Proofs. Section 8.3.2.


8.32. John and Williams [1995: appendix A7].

8.3.3 Symmetric Circulant

Definition 8.7. A matrix is a symmetric circulant if $a_{ij} = a_{(i+j-2)n}$. An example of an $n \times n$ symmetric circulant is

$$A = \begin{pmatrix}
a_0 & a_1 & a_2 & \cdots & a_{n-1} \\
a_1 & a_2 & a_3 & \cdots & a_0 \\
a_2 & a_3 & a_4 & \cdots & a_1 \\
& \cdots & \cdots & \cdots & \cdots \\
a_{n-1} & a_0 & a_1 & \cdots & a_{n-2}
\end{pmatrix}.$$

Note that the elements on each of the counterdiagonals are equal.
8.33. The Moore-Penrose inverse $A^+$ of a symmetric circulant is a symmetric circulant.

8.34. If $A$ is a symmetric circulant and is nonsingular, then $A^{-1}$ is a symmetric circulant.

8.35. Let $A$ be an $n \times n$ symmetric circulant with first row elements $a_0, a_1, \ldots, a_{n-1}$ and eigenvalues $\lambda_0, \lambda_1, \ldots, \lambda_{n-1}$. If $\omega_j = \omega^j$ ($j = 0, 1, \ldots, n - 1; \omega^0 = 1$) are the $n$ roots of unity, then

$$\lambda_i^2 = \omega_i^0 \sum_{j=0}^{n-1} a_j^2 + \omega_i \sum_{j=0}^{n-1} a_j a_{(j+1)|n} + \omega_i^2 \sum_{j=0}^{n-1} a_j a_{(j+2)|n}$$

$$+ \cdots + \omega_i^{n-1} \sum_{j=0}^{n-1} a_j a_{(j+n-1)|n}.$$ 

Also $\lambda_0 = a_0 + a_1 + \cdots + a_{n-1}$.

8.36. If $A$ and $B$ are $n \times n$ symmetric circulants, then $AB$ is a regular circulant, but, in general, $AB \neq BA$.

8.37. If $B$ is a regular circulant and $C$ is a symmetric circulant, then $BC$ and $CB$ are symmetric circulants and, in general, $BC \neq CB$.

8.38. Combining the above two results, we have that the product of an even number of symmetric circulants is a regular circulant, and the product of an odd number of symmetric circulants is a symmetric circulant.

8.39. Let $A$ be an $n \times n$ regular circulant, $C$ be an $n \times n$ symmetric circulant, and suppose there is a solution $X$ to the matrix equation $AX = C$. Then there exists an $n \times n$ symmetric circulant $B$ such that $AB = C$.

8.40. Let $A$ be a regular circulant, and let $B$ be a symmetric circulant with the same first row $a_0, a_1, \ldots, a_{n-1}$. If the matrices are both $n \times n$, then

$$\det A = (-1)^{[(n-1)/2]} \det B,$$

where $[(n-1)/2]$ is the integral part of $(n - 1)/2$.

8.41. Let $A$ be an $n \times n$ matrix that is both a symmetric circulant and a symmetric regular circulant. If $n$ is odd, then $A$ takes the form $a_{ij} = a$ for all $i, j$. If $n$ is even, then $A$ takes the form $a_{ij} = a_0$ if $i + j$ is even and $a_{ij} = a_1$ if $i + j$ is odd.

Proofs. Section 8.3.3.

8.33. Graybill [1983: 249, his $A^-$ is our $A^+$].

8.34. Graybill [1983: 243].


8.3.4 Toeplitz Matrix

**Definition 8.8.** An $n \times n$ matrix $A$ is a Toeplitz matrix if all the elements on the main diagonal are equal, all the elements on each superdiagonal are equal, and all elements on each subdiagonal are equal, that is, $a_{ij} = a_{i+s,j+s}$ for all $i, j, s$. For example,

$$A_1 = \begin{pmatrix} a_0 & a_1 & a_2 & a_3 & \cdots & a_{n-1} \\ a_{-1} & a_0 & a_1 & a_2 & \cdots & a_{n-2} \\ a_{-2} & a_{-1} & a_0 & a_1 & \cdots & a_{n-3} \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ a_{-(n-1)} & a_{-(n-2)} & a_{-(n-3)} & a_{-(n-4)} & \cdots & a_0 \end{pmatrix}$$

is a Toeplitz matrix. The general term is $a_{ij} = a_{j-i}$ for some sequence $a_{-(n-1)}, a_{-(n-2)}, \ldots, a_{-1}, a_0, a_1, a_2, \ldots, a_{n-2}, a_{n-1} \in \mathbb{C}$.

For general references see Grenander and Szegö [1958], Böttcher and Silbermann [1999], and Widom [1965].

A symmetric Toeplitz matrix has $a_{ij} = a_{ji}$, and there are at the most $n$ “free” elements in the matrix. In the above example these would be the first row of elements. An example of a symmetric Toeplitz matrix arises in the study of a stationary process consisting of a set of random variables $\{u_t | t = 1, 2, \ldots, n\}$ with $\text{cov}(u_t + \tau, u_t) = \kappa(|\tau|)$. Then the variance matrix of $\mathbf{u} = (u_1, u_2, \ldots, u_n)'$ is the positive definite Toeplitz matrix

$$\text{var}(\mathbf{u}) = \begin{pmatrix} \kappa(0) & \kappa(1) & \kappa(2) & \cdots & \kappa(n-1) \\ \kappa(1) & \kappa(0) & \kappa(1) & \cdots & \kappa(n-2) \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \kappa(n-1) & \kappa(n-2) & \kappa(n-3) & \cdots & \kappa(0) \end{pmatrix}.$$ 

When $\kappa(0) = 1, n = p$, and $\kappa(i) = \rho_i$ for each $i$, the above matrix comes from the so-called Yule-Walker equations that arise in the study of a pth-order autoregressive (AR(p)) time series. Algorithms for solving these and similar equations, and for inverting a symmetric positive definite Toeplitz matrix, are given by Golub and Van Loan [1996: section 4.7].

8.42. Let

$$B = \begin{pmatrix} 0 & 1 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 1 & 0 & \cdots & 0 \\ 0 & 0 & 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & 1 \\ 0 & 0 & 0 & 0 & \cdots & 0 \end{pmatrix} \quad \text{and} \quad F = \begin{pmatrix} 0 & 0 & \cdots & 0 & 0 & 0 \\ 1 & 0 & \cdots & 0 & 0 & 0 \\ 0 & 1 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & \cdots & 1 & 0 & 0 \\ 0 & 0 & \cdots & 0 & 1 & 0 \end{pmatrix}.$$ 

Then $B$ and $F$ are Toeplitz matrices, and are sometimes referred to as backward shift and forward shift matrices because of their effect on the elements of the columns of $\mathbf{I}_n = (\mathbf{e}_1, \mathbf{e}_2, \ldots, \mathbf{e}_n)$. Then $A$, defined in the above definition 8.8, satisfies

$$A = \sum_{i=0}^{n-1} a_i F^i + \sum_{i=0}^{n-1} a_i B^i.$$
8.43. A regular circulant is a Toeplitz matrix, but a Toeplitz matrix is not necessarily a regular circulant, though it is sometimes approximated by a regular circulant (cf. Brillinger [1975: 73-74] and the references therein). Any symmetric regular circulant is a symmetric Toeplitz matrix.

8.44. Let \( A \) be a Toeplitz matrix.

(a) \( A' \) is also a Toeplitz matrix.

(b) Any symmetric Toeplitz is also doubly symmetric.

(c) If \( a_{ij} \) is defined by \( a_{ij} = a_{|i-j|} \), then \( A \) is a symmetric Toeplitz matrix.

The case when \( A \) is tridiagonal is considered in (8.110).

**Proofs.** Section 8.3.4.


### 8.3.5 Persymmetric Matrix

**Definition 8.9.** An \( n \times n \) matrix \( B = (b_{ij}) \) is called persymmetric (countersymmetric) if \( b_{ij} = b_{n-j+1,n-i+1} \) for all \( i,j \). Such a matrix is symmetric around the counter diagonal. An example is

\[
B = \begin{pmatrix}
a & b & c \\
d & e & b \\
f & d & a
\end{pmatrix}.
\]

8.45. Let

\[
E_n = (e_n, e_{n-1}, \ldots, e_1) = \begin{pmatrix}
0 & 0 & \cdots & 0 & 1 \\
0 & 0 & \cdots & 1 & 0 \\
\vdots & \vdots & \ddots & \vdots & \vdots \\
1 & 0 & \cdots & 0 & 0
\end{pmatrix},
\]

the so-called exchange permutation matrix. Then, if \( B \) is \( n \times n \), it is easy to show the following.

(a) If \( x' = (x_1, x_2, \ldots, x_n) \), then \((E_n x)' = (x_n, x_{n-1}, \ldots, x_1)\).

(b) \( E_n^{-1} = E_n \).

(b) \( B \) is persymmetric if and only if \( B = E_n B' E_n \).

(c) If \( B \) is persymmetric and nonsingular, then \( B^{-1} \) is persymmetric.

(d) If \( T \) is an \( n \times n \) Toeplitz matrix, then \( T \) is persymmetric. The converse is not necessarily true.
8.3.6 Cross-Symmetric (Centrosymmetric) Matrix

**Definition 8.10.** An \(m \times n\) matrix \(A = (a_{ij})\) is said to be cross-symmetric (centrosymmetric) if \(a_{ij} = a_{m+1-i,n+1-j}\) for all \(i, j\) and, we call it a C-matrix. For a list of examples of such matrices in statistics and time series see Dagum and Lopati [2004]. They also consider a useful transformation and its properties, called a \(t\)-transformation, which takes \(a_{ij} \rightarrow a_{m+1-i,n+1-j}\).

Note that when \(m = n:\)

1. The elements of the first column read downwards are the same as the elements read upwards in the \(n\)th column; the elements in the second column read downwards are the same as the elements read upwards in the \((n-1)\)th columns; and so forth.

2. The elements read from left to right in the first row are the same as the elements read from right to left in the \(n\)th row; the elements in the second row read from left to right are the same as the elements read from right to left in the \((n-1)\)th row; and so forth.

3. If \(n\) is odd, then the middle row (and column) are symmetric about the diagonal element.

An example is

\[
\begin{pmatrix}
a & b & c \\
c & d & c \\
e & b & a \\
\end{pmatrix}
\]

8.3.7 Block Circulant

**Definition 8.11.** Given an \(n \times n\) regular circulant matrix with first row elements \(a_0, a_2, \ldots, a_{n-1}\), we can construct an \(nk \times nk\) block circulant matrix \(A\) by replacing \(a_j\) by a \(k \times k\) matrix \(A_j\) \((j = 0, 1, \ldots, n - 1)\). Thus

\[
A = \begin{pmatrix}
A_0 & A_1 & A_2 & \cdots & A_{n-1} \\
A_{n-1} & A_0 & A_1 & \cdots & A_{n-2} \\
A_{n-2} & A_{n-1} & A_0 & \cdots & A_{n-3} \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
A_1 & A_2 & A_3 & \cdots & A_0
\end{pmatrix}
\]

Note that \(A\) is not necessarily a regular circulant. Typically each \(A_j\) is also a regular circulant or Toeplitz matrix, or it may even be a block circulant with components which are also regular circulants or Toeplitz matrices. For example, in experimental designs we might encounter the symmetric block matrix \((n = 2, k = 3)\)

\[
A = \begin{pmatrix}
4 & 0 & 0 & | & 0 & 2 & 2 \\
0 & 4 & 0 & | & 2 & 0 & 2 \\
0 & 0 & 4 & | & 2 & 2 & 0 \\
0 & 2 & 2 & | & 4 & 0 & 0 \\
2 & 0 & 2 & | & 0 & 4 & 0 \\
2 & 2 & 0 & | & 0 & 0 & 4
\end{pmatrix} = \begin{pmatrix}
A_0 & A_1 \\
A_1 & A_0
\end{pmatrix}
\]
Block circulants are used, for example, in n-cyclic designs (cf. John and Williams [1995: 57–58]), while block Toeplitz matrices occur in vector-valued time series.

8.46. A regular circulant of (composite) order \( n = pq \), where \( p \) and \( q \) are integers, is automatically a block circulant in which each block is Toeplitz. The blocks are of order \( q \), and the arrangement of blocks is \( p \times p \) (cf. Davis [1979: 70–71]). The family of such circulants we denote by \( B_{p,q} \).

8.47. If \( A \in B_{p,q} \), then we have the sum of Kronecker products

\[
A = I_p \otimes A_0 + \Pi_0 \otimes A_1 + \Pi_0^2 \otimes A_2 + \cdots + \Pi_0^{p-1} \otimes A_{p-1},
\]

where \( \Pi_0 \) is the forward shift permutation matrix of order \( p \) (cf. Definition 8.2 in Section 8.2), and the \( A_j \) are Toeplitz of order \( q \).

8.48. If \( A, B \in B_{p,q} \) and the \( \alpha_i \) are scalars, then \( A, A^*, \alpha_1 A + \alpha_2 B, AB, p(A) = \sum_{i=1}^{r} \alpha_i A^i, A^+ \) and \( A^{-1} \) (if it exists) all belong to \( B_{p,q} \). We can use the relationship (8.47) so that \( AB = BA \) if \( \alpha_j B_k = B_k A_j \) for all \( j, k \).

8.49. Let \( C_{h_k} \) be a basic circulant of order \( n_k \) (cf. Definition 8.6 below (8.26)), and define the \( n \times n \) Kronecker product matrix

\[
C_h = C_{h_1} \otimes C_{h_2} \otimes \cdots \otimes C_{h_m},
\]

where \( n = n_1 n_2 \cdots n_m \). Then a block circulant matrix \( A \) of order \( n \) can be defined by

\[
A = \sum_{h_1=0}^{n_1-1} \sum_{h_2=0}^{n_2-1} \cdots \sum_{h_m=0}^{n_m-1} a_{h_1 h_2 \cdots h_m} C_h.
\]

The eigenvalues and eigenvectors of \( A \) can then be readily found (cf. John and Williams [1995: 232] and Tee [2005]).

Proofs. Section 8.3.7.

8.47. Davis [1979: 178].

8.48. Davis [1979: 181].

8.3.8 Hankel Matrix

Definition 8.12. A Hankel matrix \( A = (a_{ij}) \) has the following structure:

\[
A = \begin{pmatrix}
    a_0 & a_1 & a_2 & \cdots & a_{K-1} \\
    a_1 & a_2 & a_3 & \cdots & a_K \\
    a_2 & a_3 & a_4 & \cdots & a_{K+1} \\
    \vdots & \vdots & \vdots & \ddots & \vdots \\
    a_{L-1} & a_L & a_{L+1} & \cdots & a_{K+L-2}
\end{pmatrix},
\]

where \( a_{ij} = a_{i+j-2} \), so that the elements are equal on each of the counterdiagonals \( i + j = \text{const} \). This matrix arises, for example, from a real time series \( X = (a_0, a_1, \ldots, a_{N-1}) \) of length \( N \) with \( L \) the window length \( (1 < L < N) \) and
$K = N - L + 1$; it is called the \textit{trajectory matrix} of $X$. If $N$ and $L$ are fixed, then there is a one-to-one relationship between $A$ and $X$ (cf. Golyandina et al. [2001: 16]).

If $L = K = n$, so that $A$ is $n \times n$, then the general term is given by $a_{ij} = a_{i+j-2}$ for some given sequence $a_0, a_1, \ldots, a_{2n-3}, a_{2n-2}$. In this case $A$ is symmetric.

For further details about Hankel matrices and structured matrices in general see Bini et al. [2001].

\textbf{8.50.} Let $\Pi = (e_n, e_{n-1}, \ldots, e_1)$ be the \textit{backward identity} permutation matrix. Then:

(a) $\Pi T$ is a Hankel matrix for any Toeplitz matrix $T$.

(b) $\Pi H$ is Toeplitz matrix for any square Hankel matrix $H$.

(c) Since $\Pi = \Pi' = \Pi^{-1}$ and square Hankel matrices are symmetric, any Toeplitz matrix is product of two symmetric matrices ($\Pi$ and a Hankel matrix).

\textbf{Proofs.} Section 8.3.8.

8.50. Quoted by Horn and Johnson [1985: 28].

\section*{8.4 DIAGONALLY DOMINANT MATRICES}

\textbf{Definition 8.13.} Let $A = (a_{ij})$ be a real or complex $n \times n$ matrix ($n \geq 2$), and define

$$R_p = \sum_{j=1: j \neq p}^n |a_{pj}| \quad \text{and} \quad C_q = \sum_{i=1: i \neq q}^n |a_{iq}|$$

to be, respectively, the sum of the absolute values of the off-diagonal elements of the $p$th row of $A$, and the sum of the absolute values of the off-diagonal elements of the $q$th column of $A$. (In the above, $|x|$ denotes the modulus of $x$ if $x$ is not real.)

Considering first the rows, if $|a_{pp}| > R_p$, then the $p$th row is said to have a strictly dominant diagonal. If $|a_{pp}| \geq R_p$ for $p = 1, 2, \ldots, n$, then $A$ is said to be \textit{(row) diagonally dominant}, while if $|a_{pp}| > R_p$ for $p = 1, 2, \ldots, n$, then $A$ is said to be \textit{strictly (row) diagonally dominant}; we denote this by r.d.d. Some authors omit the word "row" and then do not refer to columns. However, there is a corresponding set of definitions for columns. For example, if $|a_{qq}| > C_q$, then the $q$th column of $A$ is said to have a dominant diagonal, while if $|a_{qq}| > C_q$ for $q = 1, 2, \ldots, n$, then $A$ is said to be \textit{strictly column diagonally dominant} and we write c.d.d. If $A$ is either r.r.d. or c.d.d., we say that $A$ is d.d.

\textbf{8.51.} Let $A$ be any $n \times n$ matrix (real or complex).

(a) If $\Pi$ is any $n \times n$ permutation matrix and $A$ is r.d.d. (respectively c.d.d.), then $\Pi' A \Pi$ is r.d.d. (respectively c.d.d.).

(b) If $D$ is any $n \times n$ nonsingular diagonal matrix and $A$ is r.d.d. (respectively c.d.d.), then $DA$ (respectively $AD$) is r.d.d. (respectively c.d.d.).

(c) If any diagonal element of $A$ is zero, then $A$ is neither r.d.d. nor c.d.d.
(d) If \( \lambda \) is any eigenvalue of \( A \), then \( A - \lambda I_n \) is neither r.d.d. nor c.d.d.

(e) If \( A \) is r.d.d. (respectively c.d.d.), then at least one column (respectively row) must have a dominant diagonal.

(f) If \( A \) is a regular circulant with first row elements \( a_0, a_1, \ldots, a_{n-1} \) such that

\[
|a_j| > \sum_{i=0, i \neq j}^{n-1} |a_i|
\]

for some \( j \), then \( A \) is nonsingular.

**Definition 8.14.** Let \( A \) a matrix such that

\[
|a_{ij}| > \sum_{h=1, h \neq i}^{n} |a_{hj}|.
\]

Then the \( j \)th column is said to have a dominant element, and it is in the \( i \)th row.

8.52. (Conditions for Nonsingularity) Let \( A \) be \( n \times n \).

(a) (Levy–Desplanques) If \( A \) is d.d., then \( A \) is nonsingular. Conversely, if \( A \) is singular, then \( A \) is neither r.d.d. nor c.d.d. This result is linked to (6.29) as 0 cannot then lie in any closed Geršgorin disc, so that 0 is not an eigenvalue.

(b) If \( R \) and \( S \) are any nonsingular \( n \times n \) matrices and \( RAS \) is a d.d. matrix, then \( A \) is nonsingular. Conversely, if \( A \) is nonsingular, there exist nonsingular matrices \( R \) and \( S \) such that \( RAS \) is d.d.

(c) Suppose each row, except one (say the \( k \)th row), has a strictly dominant diagonal, and suppose the \( k \)th row is such that \( 0 < |a_{kk}| = R_k \). Then \( A \) is nonsingular. A similar theorem exists for columns.

(c) If each column of \( A \) has a strictly dominant element, and each row contains one of the dominant elements, then \( A \) is nonsingular. This result also holds if each row has a strictly dominant element and these are in distinct columns.

(d) Suppose that for one value of \( j = 1, 2, \ldots, n \), say \( j = t \), either of the following equations hold, namely

\[
0 < |a_{tt}| < R_t \quad \text{and} \quad |a_{i'i}| : |a_{tt}| > R_i R_t \quad \text{for} \ i = 1, 2, \ldots, n; \ i \neq t
\]

\[
0 < |a_{tt}| < C_t \quad \text{and} \quad |a_{i'i}| : |a_{tt}| > C_i C_t \quad \text{for} \ i = 1, 2, \ldots, n; \ i \neq t,
\]

then \( A \) is nonsingular.

(e) Suppose that all the elements of \( A \) are nonzero. If \( A \) is diagonally dominant (i.e., not strictly so), and \( |a_{ii}| > R_i \) for at least one value of \( i = 1, \ldots, n \), then \( A \) is nonsingular.

8.53. (Positive Determinant) Let \( A \) be an \( n \times n \) real matrix that is d.d. and has positive diagonal elements.

(a) \( \det A > 0 \).
(b) If $A_r$ is any $r \times r$ principal submatrix, then $\det A_r > 0$.

(c) If the signs of any set of off-diagonal elements are changed, then $\det A > 0$.

(d) The real part of each eigenvalue of $A$ is positive. Thus all real eigenvalues are positive. If, instead, the diagonal elements of $A$ are all negative, then the real parts of all eigenvalues are negative.

(e) From (d) it follows that if $A$ is also Hermitian and all its main diagonal elements are positive, then all the eigenvalues of $A$ are real and positive.

8.54. If $A$ is $n \times n$ and $T'AT$ is d.d. with positive diagonal elements, where $T$ is any orthogonal matrix, then $\det A = \det |T|^2 \det A = \det(T'AT) > 0$ (by 8.6b). Note that $T$ could be a permutation matrix.

8.55. Let $A$ be an $n \times n$ matrix that is d.d., and let $D$ be a diagonal matrix with the same diagonal elements as $A$. Then $\rho(B) < 1$, where $B = I_n - D^{-1}A$ and $\rho$ is the spectral radius of $B$.

8.56. (Linear Equations) Let $A$ be an $n \times n$ real matrix with positive diagonal elements and nonpositive off-diagonal elements. For each $n \times 1$ vector $b$ with non-negative elements, there exists a unique vector $x$ with non-negative elements that is a solution to $Ax = b$ if $A$ is d.d.

Proofs. Section 8.4.


8.52. Graybill [1983: 251–256, here dominant means strictly dominant]; also Horn and Johnson [1985: 302 and 355, for (a) and (b) respectively].


8.5 HADAMARD MATRICES

Definition 8.15. An $n \times n$ Hadamard matrix $H$ is a matrix with elements all $\pm 1$ such that $H'H = HH' = nI_n$, that is, $n^{-1/2}H$ is orthogonal. If all the elements of the first column are equal to $+1$, then $H$ is called a seminormalized Hadamard matrix. If all the elements in the first row and column are equal to $+1$, then $H$ is said to be normalized. These matrices are closely linked to balanced incomplete block designs, group divisible designs, Youden designs, $2^n$ factorial experiments, optimal weighing designs, and response surface methodology. For further details and applications see Agaian [1985].
8.57. We have the following properties of an \( n \times n \) Hadamard matrix \( H \).

(a) \( H' \) and \( nH^{-1} \) are Hadamard matrices.

(b) If \( D_1 \) and \( D_2 \) are diagonal matrices with diagonal elements \( \pm 1 \), then \( D_1HD_2 \) is a Hadamard matrix. We can set \( D_i = I_n \) for \( i = 1 \) or 2.

(c) \( n \) must equal 1 or 2 or be a multiple of 4.

(d) From \( \det(H'H) = n^n \), \( \det H = \pm n^{n/2} \).

(e) (Hadamard) If \( A \) is a real \( n \times n \) matrix with \( |a_{ij}| \leq 1 \), then \( \det A \leq n^{n/2} \).

We find that the Hadamard family is the only family of matrices which attains the upper bound.

(f) If \( H_1 \) and \( H_2 \) are \( n_1 \times n_1 \) and \( n_2 \times n_2 \) Hadamard matrices, respectively, then \( H_1 \otimes H_2 \) (the Kronecker product) is an \( n_1n_2 \times n_1n_2 \) Hadamard matrix.

(g) Setting \( n = 2 \) and applying (f) repeatedly, we see that there is a \( 2^k \times 2^k \) Hadamard matrix for every positive integer \( k \).

(h) If an \( n \times n \) Hadamard matrix exists, then an \( n \times n \) normalized Hadamard matrix exists.

8.58. In digital signal processing, Hadamard matrices, \( H_n \) say, are restricted to be of order \( 2^n \) given by the recursion

\[
H_1 = \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}, \quad H_2 = \begin{pmatrix} H_1 & H_1 \\ H_1 & -H_1 \end{pmatrix} = H_1 \otimes H_1, \\
H_n = H_1 \otimes H_{n-1}.
\]

Also \( H_{2n} \) is symmetric so that \( H_{2n}^2 = 2^nI_{2n} \).

8.59. Let \( H_n \) be defined in (8.58) above, and consider the iteration

\[
x_1 = \begin{pmatrix} 1 \\ -1 + \sqrt{2} \end{pmatrix} \quad \text{and} \quad x_n = \begin{pmatrix} x_{n-1} \\ (-1 + \sqrt{2})x_{n-1} \end{pmatrix}.
\]

Then \( H_n \) has eigenvalues \( +2^{n/2} \) and \( -2^{n/2} \), each of multiplicity \( 2^{n-1} \), and an eigenvector \( x_n \) corresponding to the positive eigenvalue \( 2^{n/2} \).

8.60. If \( H \) is an \( m \times m \) Hadamard matrix that contains \( J_n = 1_n1_n' \), then \( m \geq n^2 \).

Proofs. Section 8.5.


8.6 IDEMPOTENT MATRICES

8.6.1 General Properties

**Definition 8.16.** An $n \times n$ real or complex matrix is said to be *idempotent* if $A^2 = A$. In Section 2.3 we called such a matrix a projection matrix. If $A$ is also real and symmetric (with $\langle x, y \rangle = x'y$), or Hermitian (with $\langle x, y \rangle = y^*x$), it represents an orthogonal projection matrix. Some other geometrical properties of such matrices are given in Section 2.3. We assume below that $A$ is real, unless otherwise stated, though many of the following results hold for complex matrices.

**8.61.** The following statements are equivalent.

1. An $n \times n$ matrix $P$ is idempotent.
2. $I - P$ is idempotent.
3. $\mathcal{C}(P) \cap \mathcal{C}(I_n - P) = 0$.
4. $\mathcal{C}(P) = \mathcal{N}(I_n - P)$.
5. $\mathcal{C}(I_n - P) = \mathcal{N}(P)$.

**8.62.** The following statements are equivalent.

1. $A$ is an $n \times n$ idempotent matrix of rank $r$ with Moore–Penrose inverse $A^+$. 
2. There exist orthogonal projection matrices $R$ and $S$ such that $A^+ = RS$.
3. $A^+A' = A^+$.
5. $A = BC'$, where $C'B = I_r$ with $B$ and $C$ being $n \times r$ matrices.
6. The Jordan canonical form of $A$ (cf. 16.7) can be written as

\[
\begin{pmatrix}
I_r & 0 \\
0 & 0
\end{pmatrix}
\]

For further results and discussion see Trenkler [1994].

**8.63.** If $A$ is an $n \times n$ idempotent matrix of rank $r$, then there exist nonsingular $R$ and unitary $U$ such that

\[
R^{-1}AR = \begin{pmatrix} I_r & 0 \\ 0 & 0 \end{pmatrix} \quad \text{and} \quad U^*AU = \begin{pmatrix} I_r & Q \\ 0 & 0 \end{pmatrix}
\]

for some $Q$. If $A$ is symmetric, we can replace $R$ by an orthogonal matrix.
8.64. An $n \times n$ matrix $A$ is idempotent if and only if $\text{rank } A + \text{rank}(I_n - A) = n$.

8.65. Let $A$ be an $n \times n$ idempotent (real or complex) matrix of rank $r$, then:

(a) $A$ has $r$ eigenvalues equal to 1 and $n - r$ eigenvalues equal to 0. Also, if $A$ is real and symmetric, then it is idempotent if and only if each eigenvalue of $A$ is 1 or 0.

(b) $\det A^2 = \det A$ and $\det A$ is 0 or 1. If $\det A = 1$ then, by (a), $A = I_n$.

(c) From (8.63) we have $\text{rank } A = \text{trace } A = r$.

(d) $I_n - A$ is idempotent and, from (c), $\text{rank}(I_n - A) = n - \text{rank } A$.

(e) $A$ can be expressed in the form $A = QR^*$, where $Q$ and $R$ are $n \times r$ and $R^*Q = I_r$.

(f) There exists a Hermitian positive definite matrix $C$ such that $A = C^{-1}A^*C$.

8.66. Let $A$ be an $n \times n$ matrix with Moore–Penrose inverse $A^+$. Then $A$ is a real symmetric idempotent matrix if and only if one of the following conditions is satisfied.

1. $A'A = A$.
2. $I - A$ is symmetric and idempotent.
3. $A$ is idempotent and $AA' = A'A$.
4. $A$ and $A'A$ are idempotent.
5. $AA' = A$ and $A$ is idempotent.
6. $A'AA' = A'$ and $A$ is idempotent.
7. $A$ and $\frac{1}{2}(A + A')$ are idempotent.
8. $AA' + A'A = A + A'$ and $A$ is idempotent.
9. $I_n - 2A$ is a symmetric, orthogonal matrix.
10. $A^2 = A'$ and $A$ is tripotent (i.e., $A^3 = A$).
11. $AA' = A'AA'$.
12. $A$ is idempotent and $\text{rank}(I_n - A'A) = n - \text{rank } A$.
13. $A$ is idempotent and $\|Ax\|_2 \leq \|x\|_2$ for all $x \in \mathbb{R}^n$.
14. $x'A'Ax = x'Ax$ for all $x \in \mathbb{R}^n$.
15. $A$ is idempotent and $x'Ax \geq 0$ for all $x \in \mathbb{R}^n$.
16. $\|y - Ay\|_2 \leq \|y - x\|_2$ for all $y \in \mathbb{R}^n$ and all $x \in \mathcal{C}(A)$.
17. $A$ is idempotent and $A = A^+$.
18. $A$ is idempotent and $AA' = AA^+$.
(19) \( A^+ = A \) and \( A^2 = A' \).
(20) \( A \) and \( A^+ \) are idempotent.
(21) There exists an \( n \times m \) matrix \( B \) such that \( A = BB^+ \).
(22) \( A = AA^+ \).
(23) \( A = B(B'B)^{-1}B \) for some \( n \times m \) matrix \( B \) of rank \( m \).

See Trenkler [1994] for these and further results of a similar nature. He also gives necessary and sufficient conditions that a symmetric matrix is idempotent.

**8.67. (Generalized Inverse and Idempotency)** Let \( A \) be \( m \times n \) with Moore–Penrose inverse \( A^+ \). Then the following conditions are equivalent.

1. \( A'A \) is idempotent (i.e., is an orthogonal projection matrix, because it is symmetric).
2. \( AA' \) is idempotent.
3. \( AA'A = A \), that is, \( A' \) is a weak inverse of \( A \).
4. \( A' = A^+ \).

**8.68.** If \( A \) is \( m \times n \) with any weak inverse \( A^- \), then \( \mathcal{N}(A) = C(I - A^-A) \).

**8.69.** If \( (CB)^{-1} \) exists, then \( B(CB)^{-1}C \) is idempotent.

**8.70.** Let \( A \) be an \( n \times n \) symmetric idempotent matrix, and let \( B \) be an \( n \times m \) matrix of rank \( m \).

(a) If \( AB = B \) and \( \text{rank} \ A = \text{rank} \ B \), then \( A = B(B'B)^{-1}B' \).

(b) If \( AB = 0 \) and \( \text{rank} \ A + \text{rank} \ B = n \), then \( A = I_n - B(B'B)^{-1}B' \).

**8.71. (Symmetric Matrix)** Let \( A \) be an \( n \times n \) symmetric idempotent matrix of rank \( r \), where \( r < n \). Then we have the following.

(a) \( 0 \leq a_{ii} \leq 1 \) for \( i = 1, 2, \ldots, n \).

(b) If \( a_{ii} = 0 \) or \( a_{ii} = 1 \), then \( a_{ij} = 0 \) for all \( j, j \neq i \).

(c) \( A \) is non-negative definite.

(d) If \( T \) is orthogonal, then \( P = T'AT \) is a symmetric idempotent matrix.

(e) If \( R \) is nonsingular, then \( P = R^{-1}AR \) is idempotent.

(f) \( Q = I_n - 2A \) is a symmetric orthogonal matrix.

(g) We can write \( A = T_rT_r' \), where \( T_rT_r' = I_r \), and the columns of \( T_r \) form an orthonormal basis for \( C(A) \). This result holds if \( A \) is Hermitian and we replace \( T' \) by \( T^* \).

(h) If \( V \) is positive definite, then

\[
\text{rank}(AVA) = \text{trace}(AV).
\]
8.72. Let $A$ be a symmetric matrix that satisfies $A^{k+1} = A^k$ for some positive integer $k$. Then $A$ is idempotent.

8.73. Let $A_1$ and $A_2$ be $n \times n$ symmetric idempotent matrices, and suppose $A_1 - A_2$ is non-negative definite.

(a) $A_1 A_2 = A_2 A_1 = A_2$.

(b) $A_1 - A_2$ is a symmetric idempotent matrix.

8.74. Suppose $A$ and $B$ are $n \times n$ matrices. If $AB = A$ and $BA = B$, then $A$ and $B$ are both idempotent.

8.75. (Kronecker Products) Let $A$ be $m \times n$ and $B$ be $m \times p$ real matrices. Let $A \otimes B$ be their Kronecker product, and denote by $P_A$, $P_B$, and $P_{A \otimes B}$ the symmetric idempotent matrices that project orthogonally onto $C(A)$, $C(B)$, and $C(A \otimes B)$. Then:

(a) $P_{A \otimes B} = P_A \otimes P_B$.

(b) $P_{A \otimes I} = P_A \otimes I$.

(c) If $Q = I - P$ in each case, then

$$Q_{A \otimes B} = Q_A \otimes Q_B + Q_A \otimes P_B + P_A \otimes Q_B.$$ 

8.76. Let $A$ and $B$ be $n \times n$ symmetric matrices, with $B$ positive definite. Then $AB$ is idempotent if and only if each eigenvalue of $AB$ is 0 or 1.

Proofs. Section 8.6.1.

8.61(2). Follows directly from (1).

8.61(3). Harville [1997: 384, lemma 17.2.6].

8.61(4). Let $P^2 = P$. If $y = Px$ then $(I_n - P)y = (I_n - P)Px = 0$ and $y \in \mathcal{N}(I_n - P)$. Conversely, if $(I_n - P)y = 0$ then $y = Py \in C(P)$.

8.61(5). Similar to (4); see Harville [1997: 146].

8.62. Trenkler [1994].


8.66. Trenkler [1994].


8.68. Harville [1997: 140].
8.69. Simply square the matrix.

8.70. Abadir and Magnus [2005: 236].

8.71a–b. Schott [2005: 399].

8.71c. Follows from $x'Ax = x'A'Ax = y'y$.

8.71d–e. We have $P^2 = P$.

8.71f. We show that $Q'Q = I_n$.


8.71h. Harville [2001: 82, exercise 10]. We have $\text{trace}(AVA) = \text{trace}(AV^{1/2}V^{1/2}A) = \text{trace}(V^{1/2}A^2V^{1/2}) = \text{trace}(V^{1/2}AV^{1/2}) = \text{trace}(AV)$.

8.72. Schott [2005: 399].

8.73. Seber and Lee [2003: 465].

8.74. Abadir and Magnus [2005: 236].


8.76. Schott [2005: 397].

8.6.2 Sums of Idempotent Matrices and Extensions

There are many results given for sums of idempotent matrices, and these are often expressed with different conditions. We give several versions of these below, and there is some overlap. For a very general investigation of a linear combination of two projectors see Baksalary and Baksalary [2004a] and the references therein. Questions relating to the nonsingularity of such combinations of idempotent matrices, including just sums and differences, are considered by Baksalary and Baksalary [2004b] and Koliha et al. [2004]. We assume below that all matrices are real, unless otherwise stated, though some of the results hold for complex matrices as well.

8.77. If $A$ and $B$ are $n \times n$ idempotent matrices, then $A + B$ is idempotent if and only if $AB = BA = 0$. We generalize this result below.

8.78. (Cochran’s Theorem) Suppose $A_1, A_2, \ldots, A_k$ is a sequence of symmetric $n \times n$ matrices such that $\sum_{i=1}^{k} A_i = I_n$. Then the following conditions are equivalent (i.e., each one implies the other two).

1. $A_i^2 = A_i$ for $i = 1, 2, \ldots, k$.

2. $A_iA_j = 0$ for all $i, j, i \neq j$.

3. $\sum_{i=1}^{k} \text{rank} A_i = n$.

This can be derived from (8.79) below.
8.79. Let \( A = \sum_{i=1}^{k} A_i \), where each \( A_i \) is a symmetric \( n \times n \) matrix. Any two of the following three conditions implies the third.

1. \( A = A^2 \).
2. \( A_i^2 = A_i \) for \( i = 1, 2, \ldots, n \).
3. \( A_i A_j = 0 \) for all \( i, j, i \neq j \).

From (8.80) we can include further results involving

4. \( \text{rank } A = \sum_{i=1}^{k} \text{rank } A_i \).

For example, any two of (1), (2), and (3) implies all four. Furthermore, (1) and (4) imply (2) and (3) (Rao [1973a: 28]). We can relate this theorem to the previous one by defining \( A_0 = I_n - A \) so that \( \sum_{i=0}^{k} A_i = I_n \). Alternatively, we can set \( A = I_n \).

8.80. Let \( A_i \) be an \( n \times n \) matrix \((i = 1, 2, \ldots, k)\), and let \( A = \sum_{i=1}^{k} A_i \).

(a) If \( A^2 = A \), then the following conditions are equivalent.

1. \( A_i A_j = 0 \), for all \( i, j, i \neq j \), and \( \text{rank } A_i^2 = \text{rank } A_i \) for \( i = 1, 2, \ldots, k \).
2. \( A_i^2 = A_i \) for \( i = 1, 2, \ldots, k \).
3. \( \text{rank } A = \sum_{i=1}^{k} \text{rank } A_i \).

If \( A = I_n \), then the condition on \( A \) is automatically satisfied and \( \text{rank } A = n \).
Furthermore, if each \( A_i \) is also symmetric, then \( A_i^2 = A_i'A_i \), which implies \( \text{rank } A_i^2 = \text{rank } A_i \), and condition (1) reduces to the condition

\[
A_i A_j = 0 \quad \text{for all} \quad i, j, i \neq j.
\]

(b) If the \( A_i \) are all idempotent and \( A_i A_j = 0 \) for all \( i, j, i \neq j \), then

(i) \( A^2 = A \).
(ii) \( \text{rank } A = \sum_{i=1}^{k} \text{rank } A_i \).

(c) Suppose \( V \) is an \( n \times n \) non-negative definite matrix, and let \( R \) be any matrix such that \( V = RR' \) (cf. 10.10). Then (a) and (b) still hold if we replace each \( A_i \) by \( RA_iR' \) throughout and \( A \) by \( RR' \).

8.81. Let \( A_i \) \((i = 1, 2, \ldots, k)\) be square (not necessarily symmetric) matrices, and let \( A = \sum_{i=1}^{k} A_i \). Consider the following conditions:

1. \( A_i^2 = A_i, \; i = 1, 2, \ldots, k \).
2. \( A_i A_j = 0 \) for all \( i \neq j \).
3. \( A^2 = A \).
4. \( \sum_i \text{rank } A_i = \text{rank } A \).
5. \( \text{rank } (A_i^2) = \text{rank } A_i, \; i = 1, 2, \ldots, k \).
Then

\[(1), (2) \rightarrow (3), (4), (5),\]
\[(1), (3) \rightarrow (2), (4), (5),\]
\[(2), (3), (5) \rightarrow (1), (4),\]
\[(3), (4) \rightarrow (1), (2), (5).\]

For references to extensions of these results see Tian and Styan [2006]. They also add a new rank subtractivity condition of the form \(\text{rank}(I_n - A) = n - \sum_{i=1}^{k} \text{rank} A_i.\)

8.82. Let \(A_i (i = 1, 2, \ldots, k)\) be \(p \times q\) matrices, and let \(A = \sum_{i=1}^{k} A_i.\) Consider the following conditions:

1. \(A_i A_i - A_i = A_i, i = 1, 2, \ldots, k.\)
2. \(A_i A_i - A_j = 0\) for all \(i, j, i \neq j.\)
3. \(\text{rank}(A_i A_i - A_i) = \text{rank} A_i, i = 1, 2, \ldots, k.\)
4. \(\sum_i \text{rank} A_i = \text{rank} A,\)

for some weak inverse \(A^-\) of \(A.\) Then

\[(1) \rightarrow (2), (3), (4),\]
\[(2), (3) \rightarrow (1), (4),\]
\[(4) \rightarrow (1), (2), (3).\]

If (1) or if (2) and (3) hold for some weak inverse \(A^-,\) then (1), (2), and (3) hold for every weak inverse \(A^-\).

8.83. Let \(A_i (i = 1, 2, \ldots, k)\) be an \(n \times n\) matrix, let \(A = \sum_{i=1}^{k} A_i,\) and let \(V\) be a non-negative definite matrix.

(a) If \(V A_i V A_j V = V A_i V\), then each of the following three conditions implies the other two.

1. \(V A_i V A_j V = 0\) for all \(i, j, i \neq j,\) and \(\text{rank}(V A_i V A_j V) = \text{rank}(V A_i V)\) for \(i = 1, 2, \ldots, k.\)
2. \(V A_i V A_i V = V A_i V\) for \(i = 1, 2, \ldots, k.\)
3. \(\text{rank}(V A_i V) = \sum_{i=1}^{k} \text{rank}(V A_i V).\)

When the \(A_i\) are symmetric, condition (1) reduces to \(V A_i V A_j V = 0\) for all \(i, j, i \neq j.\)

(b) If \(V A_i V A_i V = V A_i V\) for all \(i\) and \(V A_i V A_j V = 0\) for all \(i, j, i \neq j,\) then:

1. \(V A_i V A_i V = V A_i V,\)
2. \(\text{rank}(V A_i V) = \sum_{i=1}^{k} \text{rank}(V A_i V).\)

A generalization of the above results involving rectangular matrices and an arbitrary rectangular \(V\) is given by Tian and Styan [2006]. For related results see Tian and Styan [2005].
8.84. Let \( A \) be an \( n \times n \) symmetric idempotent matrix, and let \( \mathbf{B} \) be a non-negative definite \( n \times n \) matrix. If \( \mathbf{I}_n - \mathbf{A} - \mathbf{B} \) is non-negative definite, then \( \mathbf{A} \mathbf{B} = \mathbf{B} \mathbf{A} = \mathbf{0} \).

8.85. Let \( \mathbf{A}_i \) be a symmetric idempotent \( n \times n \) matrix of rank \( r_i \) \( (i = 1, 2, \ldots, k) \), and let \( \mathbf{A}_{k+1} \) be an \( n \times n \) non-negative definite matrix such that \( \mathbf{I}_n = \sum_{i=1}^{k+1} \mathbf{A}_i = \mathbf{A} + \mathbf{A}_{k+1} \), say. Then:

(a) \( \mathbf{A}_i \mathbf{A}_j = \mathbf{0} \) for all \( i, j = 1, 2, \ldots, k+1, i \neq j \).

(b) \( \mathbf{A}_{k+1} \) is symmetric and idempotent of rank \( n - \sum_{i=1}^{k} r_i \).

8.86. Let \( \mathbf{A} = \sum_{i=1}^{k} \mathbf{A}_i \), where each \( \mathbf{A}_i \) is an \( n \times n \) non-negative definite matrix \( (i = 1, 2, \ldots, k) \), and let \( \mathbf{A}^2 = \mathbf{A} \). If

\[
\text{trace} \mathbf{A} \leq \text{trace} \left( \sum_{i=1}^{k} \mathbf{A}_i^2 \right),
\]

then:

(a) \( \mathbf{A}_i^2 = \mathbf{A}_i \) for \( i = 1, 2, \ldots, k \).

(b) \( \mathbf{A}_i \mathbf{A}_j = \mathbf{0} \) for all \( i, j, i \neq j \).

8.87. Let \( \mathbf{A}_i \) \( (i = 1, 2, \ldots, k) \) be symmetric idempotent matrices such that

\[
\mathbf{A}_i \mathbf{A}_j = \mathbf{0}, \text{ all } i, j, (i \neq j), \text{ and } \sum_{i=1}^{k} \mathbf{A}_i = \mathbf{I}_n.
\]

Then, for positive \( \alpha_i \) \( (i = 1, 2, \ldots, k) \), \( \sum_{i=1}^{k} \alpha_i \mathbf{A}_i \) is positive definite.

8.88. Let \( \mathbf{A}_i \) \( (i = 1, 2, \ldots, k) \) be symmetric idempotent matrices such that \( \mathbf{A}_i \mathbf{A}_j = \mathbf{0} \) for all \( i, j, i \neq j \), and let \( \alpha_i, i = 0, 1, \ldots, k \), be positive scalars. Then:

(a) \( \mathbf{V} = \alpha_0 \mathbf{I}_n + \sum_{i=1}^{k} \alpha_i \mathbf{A}_i \) is positive definite.

(b) \( \mathbf{V}^{-1} = \beta_0 \mathbf{I}_n + \sum_{i=1}^{k} \beta_i \mathbf{A}_i \), where

\[
\beta_0 = \alpha_0^{-1} \text{ and } \beta_i = \frac{-\alpha_i}{\alpha_0 (\alpha_0 + \alpha_i)}, \quad i = 1, 2, \ldots, k.
\]

8.89. Let \( \mathbf{A} \) be any \( n \times n \) symmetric matrix of rank \( r \) with nonzero eigenvalues \( \lambda_i \) \( (i = 1, 2, \ldots, r) \). Then, since \( \mathbf{A} \) is diagonalizable, \( \mathbf{A} \) can be expressed in the form (cf. 16.17)

\[
\mathbf{A} = \sum_{i=1}^{r} \lambda_i \mathbf{E}_i,
\]

where, for each \( i = 1, 2, \ldots, r \), \( \mathbf{E}_i \) is symmetric and idempotent and \( \mathbf{E}_i \mathbf{E}_j = \mathbf{0} \) for all \( i, j, i \neq j \). If \( \mathbf{A} \) is also idempotent, then

\[
\mathbf{A} = \sum_{i=1}^{r} \mathbf{E}_i.
\]
8.90. Let $A_i$ be an $n \times n$ symmetric idempotent matrix of rank $r_i$ ($i = 1, 2, \ldots, k$) such that $\sum_{i=1}^{k} A_i = I_n$, and let $C_i$ ($i = 1, 2, \ldots, k$) be a $p \times p$ square matrix (possibly complex). If

$$\Omega_1 = \sum_{i=1}^{k} (A_i \otimes C_i) \quad \text{and} \quad \Omega_2 = \sum_{i=1}^{k} (C_i \otimes A_i)$$

are $np \times np$, then:

(a) From (8.78) we have $A_i A_j = 0$ for all $i \neq j$, and $\sum_{i=1}^{k} r_i = n$.

(b) The eigenvalues of $\Omega_1$ and $\Omega_2$ are the eigenvalues of $C_1, \ldots, C_k$ with respective algebraic multiplicities $r_1, \ldots, r_k$.

(c) $\det \Omega_1 = \det \Omega_2 = \prod_{i=1}^{k} (\det C_i)^{r_i}$.

(d) The matrices $\Omega_1$ and $\Omega_2$ are nonsingular if and only if all the $C_i$ ($i = 1, 2, \ldots, k$) are nonsingular, in which case

$$\Omega_1^{-1} = \sum_{i=1}^{k} \left( A_i \otimes C_i^{-1} \right) \quad \text{and} \quad \Omega_2^{-1} = \sum_{i=1}^{k} \left( C_i^{-1} \otimes A_i \right).$$

This result is used in multivariate error component analysis.

Proofs. Section 8.6.2.


8.81. Anderson and Styan [1982: 3].

8.82. Anderson and Styan [1982: 4].


8.84. $C = A(I_n - A - B)A = -ABA = 0$ as $C$ is non-negative definite. Then $AB^{1/2} = 0$ and $AB = 0$.

8.85. Quoted by Graybill [1983: : 423]. For (a) we consider $I_n - A_i - A_j = (A - A_i - A_j) + A_k$, which is non-negative definite for all $i, j = 1, 2, \ldots, k+1$, ($i \neq j$), as each $A_i$ is non-negative definite, and then use (8.84). For (b), $A_{k+1} = I_n - A$, where $A$ is idempotent with rank $A = \text{trace} A$.


8.6.3 Products of Idempotent Matrices

8.91. Every singular $n \times n$ matrix can be written as the product of idempotent matrices.

8.92. If $A$ and $B$ are $n \times n$ idempotent matrices, then $AB$ is idempotent if $AB = BA$.

Proofs. Section 8.6.3.

8.91. Ballantyne [1978].


8.7 TRIPOTENT MATRICES

Definition 8.17. An $n \times n$ matrix is said to be tripotent if $A^3 = A$. A nonsingular tripotent matrix $A$ is called a involutionary matrix and satisfies $A^2 = I_n$. An idempotent matrix is also tripotent.

8.93. (General Properties) Let $A$ be an $n \times n$ tripotent matrix.

(a) $\text{rank } A = \text{trace}(A^2)$.

(b) The eigenvalues of $A$ are $\pm 1$ or 0. If $n_1$ are equal to $+1$, $n_2$ equal to $-1$ and $n_3$ equal to 0, then:

(i) $\frac{1}{2} \text{trace}(A^2 + A) = n_1$.

(ii) $\frac{1}{2} \text{trace}(A^2 - A) = n_2$.

(iii) $\text{trace}(I_n - A^2) = n_3$.

(iv) $\text{trace } A = n_1 - n_2$.

(c) $A$ is equal to a weak inverse of itself if and only if $A$ is tripotent.

(d) If $A$ is nonsingular, then:

(i) $A^{-1} = A$.

(ii) $A^2 = I_n$.

(iii) $(A + I_n)(A - I_n) = 0$.

(e) If $T$ is orthogonal, then $T'AT$ is tripotent.

(f) If $R$ is nonsingular, then $R^{-1}AR$ is tripotent.

(g) $A^2$ is idempotent.

(h) $-A$ is tripotent.

8.94. Let $A$ and $B$ be $n \times n$ matrices.

(a) If $A$ is symmetric, then $A$ is tripotent if and only if its eigenvalues can only take the values $+1$, $-1$, or 0.
(b) If $A$ is symmetric, then $A$ is tripotent if and only if there exists two symmetric $n \times n$ idempotent matrices $C$ and $D$ such that $A = C - D$ and $CD = 0$. These two matrices are unique with $C = \frac{1}{2}(A^2 + A)$ and $D = \frac{1}{2}(A^2 - A)$. This result has been generalized by Baksalary et al. [2002], and they give conditions for when a linear combination of an idempotent and tripotent matrices is idempotent.

(c) $A$ is tripotent if and only if $A^2$ is idempotent.

(d) If $A$ is symmetric, then $A$ is tripotent if and only if $\text{rank } A = \text{rank}(A + A^2) + \text{rank}(A - A^2)$.

(e) If $A$ and $B$ are symmetric idempotent matrices and $AB = BA$, then $A - B$ is a symmetric tripotent matrix.

8.95. Let $A_i$ ($i = 1, 2, \ldots, k$) be square matrices (not necessarily symmetric), and let $A = \sum_{i=1}^{k} A_i$. Consider the following conditions:

1. $A_i^3 = A_i$, $i = 1, 2, \ldots, k$.
2. $A_iA_j = 0$, for all $i \neq j$.
3. $A^3 = A$.
4. $\sum_i \text{rank } A_i = \text{rank } A$.
5. $A_iA = A_i^2$, $i = 1, 2, \ldots, k$.
6. $A_i^2A = A_i$, $i = 1, 2, \ldots, k$.
7. $A_iA = AA_i$, $i = 1, 2, \ldots, k$.

Then (1) and (2) hold if and only if (3), (4), and (5) hold. Condition (5) may be replaced by (6) or (7). Anderson and Styan [1982] prove the above result and a similar result for symmetric matrices. An extension is also given to $r$-potent matrices, which have the property that $A^r = A$, where $r$ is a positive integer.

**Proofs.** Section 8.7.


8.94c. If $A^3 = A$, then $(A^2)^2 = A^2$. Conversely, if $A^2$ is symmetric and idempotent, its eigenvalues are 0 and there exists orthogonal $T$ such that

$$A^2 = T'AT'TAT = \begin{pmatrix} I_r & 0 \\ 0 & 0 \end{pmatrix},$$

and the eigenvalues of $A$ are 0, ±1; then use (a).

8.94d. Anderson and Styan [1982: 13].

8.94e. We multiply out $(A - B)^3$.
8.8 IRREDUCIBLE MATRICES

Definition 8.18. An \( n \times n \) matrix \( A \) is said to be reducible if and only if, by permuting a set of rows and the corresponding set of columns, \( A \) can be transformed to a matrix of the form

\[
B = \begin{pmatrix}
B_{11} & 0 \\
B_{12} & B_{22}
\end{pmatrix},
\]

or equivalently of the form

\[
B = \begin{pmatrix}
B_{11} & B_{12} \\
0 & B_{22}
\end{pmatrix},
\]

where \( B_{11} \) and \( B_{22} \) are square matrices, i.e., there exists a permutation matrix \( \Pi \) such that \( \Pi A \Pi' = B \). When \( n = 1 \) we have \( A = 0 \). A matrix that is not reducible is said to be irreducible.

8.96. Given \( \text{mod}(A) = (|a_{ij}|) \), where \( A \) is a real \( n \times n \) matrix (cf. Section 9.1.2), then \( A \) is irreducible if and only if \( (I_n + \text{mod}(A))^{n-1} > 0 \) (i.e., every element is positive) or, equivalently, if \( [I_n + \mathcal{I}(A)]^{n-1} > 0 \), where \( \mathcal{I}(A) \) is the indicator matrix of \( A \) (each nonzero element is replaced by 1).

8.97. Let \( A \) be any \( n \times n \) real matrix.

(a) If \( A \) has no zero elements, then it is irreducible.

(b) If \( A \) has zero diagonal elements and nonzero off-diagonal elements, then \( A \) is irreducible.

(c) If \( A \) is reducible, it must have at least \( n - 1 \) elements equal to zero.

(d) If \( A \) has at least one row (column) of zeros, then \( A \) is reducible.

8.98. Let \( A \) be an \( n \times n \) irreducible real matrix and let \( R_i \) be the sum of the absolute values of the off-diagonal elements of the \( i \)th row and \( C_j \) the same for the \( j \)th column. Suppose that either \( |a_{ii}| \geq R_i \) for \( i = 1, \ldots, n \) with \( |a_{ii}| > R_i \) for at least one value of \( i \), or \( |a_{jj}| \geq C_j \) for \( j = 1, \ldots, n \) with \( |a_{jj}| > C_j \) for at least one value of \( j \). Then \( A \) is nonsingular.

8.99. An \( n \times n \) (\( n \geq 2 \)) matrix \( A = (a_{ij}) \) is reducible if \( a_{ij} = 0 \) for \( i \in S \) and \( j \notin S \) for some nonempty proper subset \( S \) of \( \{1, 2, \ldots, n\} \).

8.100. The forward shift permutation matrix \( \Pi_0 = (e_n, e_1, \ldots, e_{n-1}) \) is irreducible.

8.101. A permutation matrix is irreducible if and only if it is permutation similar (cf. Definition 8.3 below (8.17)) to a forward shift permutation matrix.

8.102. An \( n \times n \) permutation matrix is irreducible if and only if its eigenvalues are \( 1, \omega, \ldots, \omega^{n-1} \), where \( \omega \) is the \( n \)th primitive root of unity.

Proofs. Section 8.8.

8.96. Horn and Johnson [1985: 361].


8.9 TRIANGULAR MATRICES

Definition 8.19. A matrix is lower-triangular if the elements above the main diagonal are all zero. The transpose of this is said to be upper-triangular. A triangular matrix need not be square. A unit triangular matrix is a triangular matrix with unit diagonal elements, and a strictly triangular matrix is a triangular matrix with zero diagonal elements.

8.103. (Basic Properties)
(a) The determinant of a square triangular matrix is the product of the diagonal elements.
(b) The eigenvalues of a square triangular matrix are the diagonal elements.
(c) The inverse of a nonsingular lower (respectively upper) triangular matrix is a lower (respectively upper) triangular matrix.
(d) The product of a finite number of square lower (respectively upper) triangular matrices of the same order is a lower (respectively upper) triangular matrix.
(e) The product of two square unit upper (respectively lower) triangular matrices is unit upper (respectively lower) triangular.
(f) If \( B \) is an \( n \times n \) triangular matrix with inverse \( C = B^{-1} \), then \( b_{ii}c_{ii} = 1 \) for \( i = 1, 2, \ldots, n \).

8.104. If \( K \) is a real lower (upper) triangular matrix and if \( K'K = KK' \), then \( K \) is a diagonal matrix.

8.105. (Factorization) Let \( A \) be a real square matrix such that every leading principal minor (excluding \( A \) itself) is nonzero.
(a) Then \( A \) can be written as the product of a real lower-triangular matrix \( L \) and a real upper-triangular matrix \( U \), that is,
\[
A = LU.
\]
Furthermore, if each of the diagonal elements of \( L \) (or \( U \)) is set equal to unity, then the two triangular matrices are unique. It should be noted that \( A \) does not need to be square to have such a factorization, and the reader is referred to Section 16.4 for further details.

(b) If \( A \) is also symmetric, then there exists a real upper-triangular matrix \( U \) and a diagonal matrix \( D \) with diagonal elements equal to \( \pm 1 \) such that
\[
A = U'DU.
\]

8.106. Every real square matrix \( A \) is similar to a triangular matrix (either upper or lower) whose diagonal elements are the eigenvalues of \( A \), that is, there exists a nonsingular matrix \( R \) (not necessarily real) such that \( R^{-1}AR = K \), where \( K \) is
triangular (and not necessarily real). If the eigenvalues of $A$ are real, then $R$ and $K$ are both real (cf. 16.1e).

8.107. If $A$ is a real $n \times n$ matrix with real eigenvalues, then there exists an orthogonal matrix $T$ such that $T'AT$ is upper-triangular with diagonal elements the eigenvalues of $A$ (cf. 16.37b).

8.108. (Block Triangular Matrices) An upper block triangular matrix takes the form

$$A = \begin{pmatrix}
A_{11} & A_{12} & \cdots & A_{1p} \\
0 & A_{22} & \cdots & A_{2p} \\
\vdots & \vdots & \ddots & \vdots \\
0 & 0 & \cdots & A_{pp}
\end{pmatrix},$$

where the diagonal blocks are all square matrices of possibly different sizes. We have that

$$\det A = \prod_{i=1}^{p} \det A_{ii}.$$ 

Thus $A$ is nonsingular if and only if all the $A_{ii}$ are nonsingular. In this case $A^{-1}$ is also upper block triangular. An algorithm for computing the inverse is given by Harville [1997: 94]. Similar results apply for lower block triangular matrices, as the inverse is also lower block triangular.

Proofs. Section 8.9.

8.103a. Simply expand the determinant by the first row or column depending on whether the matrix is lower- or upper-triangular, respectively.

8.103b. Follows from (a).

8.103c. We use the identity $AA^{-1} = I_n$.

8.103d. Prove for just two matrices first.

8.103e. Use $BC = I_n$.


8.10 HESSENBERG MATRICES

Definition 8.20. An $n \times n$ matrix $A$ is said to be an upper Hessenberg matrix if all its elements below the subdiagonal are zero (i.e., $a_{ij} = 0$ for $i > j + 1$). Its transpose is called a lower Hessenberg matrix. Upper Hessenberg matrices play an important role in the QR decomposition (Meyer [2000a: 536–538]). Many eigenvalue algorithms reduce their input to a Hessenberg form as a first step, and the latter play a similar role in the Schur decomposition (Golub and Van Loan [1996: section 7.4]). Hessenberg matrices appear elsewhere in this book.
8.11 TRIDIAGONAL MATRICES

**Definition 8.2.1.** An \( n \times n \) matrix \( A \) is *tridiagonal* if all its elements are zero except those in the middle three diagonals, (i.e., \( a_{ij} \neq 0 \) if \( |i - j| \leq 1 \) and \( a_{ij} = 0 \) if \( |i - j| > 1 \)). Tridiagonal matrices play a role in matrix decompositions and factorizations—for example, (16.43), (16.45), and (16.46b).

8.109. If \( A = (a_{ij}) \) is tridiagonal, then expanding \( c_n(\lambda) = \det(\lambda I_n - A) \) by the last column we find that

\[
\begin{align*}
c_0(\lambda) &= 1, \\
c_1(\lambda) &= (\lambda - a_{11}) \quad \text{and} \\
c_i(\lambda) &= (\lambda - a_{ii})c_{i-1}(\lambda) - a_{i,i-1}a_{i-1,i}c_{i-2}(\lambda), \quad i = 2, 3, \ldots, n.
\end{align*}
\]

8.110. Suppose that the \( n \times n \) tridiagonal matrix \( A \) is given by

\[
A = \begin{pmatrix}
a & b & 0 & 0 & 0 \\
c & a & b & 0 & 0 \\
0 & c & a & 0 & 0 \\
& & & & \\
0 & 0 & 0 & c & a \\
0 & 0 & 0 & 0 & c
\end{pmatrix},
\]

where \( a, b, \) and \( c \) are real or complex. This matrix is both a Toeplitz matrix and a regular circulant.

(a) Then

\[
\det A = \begin{cases} 
a^n & \text{if } bc = 0, \\
(n + 1)(a/2)^n & \text{if } a^2 = 4bc, \\
(\alpha^{n+1} - \beta^{n+1})/((\alpha - \beta) & \text{if } a^2 \neq 4bc,
\end{cases}
\]

where

\[
\alpha = \frac{a + \sqrt{a^2 - 4bc}}{2} \quad \text{and} \quad \beta = \frac{a - \sqrt{a^2 - 4bc}}{2}.
\]

(b) If \( a \) is real and \( bc > 0 \), the eigenvalues of \( A \) are

\[
\lambda_j = a + 2\sqrt{bc}\cos(j\pi/(n+1)), \quad j = 1, 2, \ldots, n.
\]

(c) Let \( b = c \) so that \( A \) is symmetric. Then \( A \) is positive definite if and only if the eigenvalues are positive (i.e., \( a + 2b\cos(j\pi/(n+1)) > 0 \) for \( j = 1, 2, \ldots, n \)). A sufficient condition is \( a > 0 \) and \( |b/a| \leq \frac{1}{2} \).

(d) If \( A \) is positive definite and \( b \neq 0 \), then \( B = A^{-1} \) is given by \( b_{ij} = b_{ji} \) for \( i > j \) and

\[
b_{ij} = \frac{(1 - \gamma^{2n-2j+2})(\gamma^{j+i+1} - \gamma^{i+1})}{(b/a)(1 - \gamma^2)(1 - \gamma^{2n+2})} \quad \text{for } i \leq j,
\]

where \( \gamma = \frac{b}{2a}(\sqrt{1 - 4(b/a)^2} - 1) \).

8.111. Given \( A \) in (8.110), with \( a \) real and \( bc > 0 \), then \( A \) has real eigenvectors.
8.112. The tridiagonal matrix

\[ A = \begin{pmatrix}
0 & 1 & 0 & 0 & 0 & 0 \\
-c_n & 0 & 1 & 0 & 0 & 0 \\
0 & -c_{n-1} & 0 & 0 & 0 & 0 \\
\cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\
0 & 0 & 0 & -c_1 & 0 & 1 \\
0 & 0 & 0 & 0 & -c_2 & c_1 \\
\end{pmatrix}, \]

is called the Schwartz matrix. It often arises in stability analysis. \( A \) is positive stable if and only if \( c_1 c_2 \cdots c_n > 0 \) (cf. Section 8.14.4).

8.113. The inverse of a symmetric \( n \times n \) matrix \( B \) is tridiagonal if and only if for \( i = 2, 3, \ldots, n, \)

\[ b_{ij}/b_{11} = \theta_i, \quad b_{ij} \neq 0 \quad \text{for} \quad i \leq j \leq n. \]

This condition means that all the elements on and to the right of the diagonal element in the \( i \)th row of \( B \) have a constant relation to the corresponding elements of the first row.

If \( B \) satisfies the above condition, then the inverse \( B^{-1} = (b^{ij}) \) is given by

\[ b^{11} = -\theta_2(b_{12} - \theta_2 b_{11})^{-1}, \]
\[ b^{rr} = -\frac{b_{r-1,r+1} - \theta_{r+1} b_{1,r}}{(b_{r-1,r} - \theta_r b_{1,r-1})(b_{r,r+1} - \theta_{r+1} b_{1,r})} \quad \text{for} \quad r = 2, 3, \ldots, n - 1, \]
\[ b^{nn} = -\frac{b_{1,n-1}}{b_{1,n}(b_{n-1,n} - \theta_n b_{1,n-1})}, \]
\[ b^{r,r-1} = b^{r-1,r} = (b_{r-1,r} - \theta_r b_{1,r-1})^{-1} \quad \text{for} \quad r = 2, 3, \ldots, n, \]
\[ b^{ij} = 0 \quad \text{for} \quad |i - j| > 1. \]

8.114. (Applications of the Above Result) In all of the following cases we can simply confirm that \( BB^{-1} = I. \)

(a) If

\[ B = \begin{pmatrix}
n & n-1 & n-2 & n-3 & \cdots & 1 \\
n-1 & 2(n-1) & 2(n-2) & 2(n-3) & \cdots & 2 \\
n-2 & 2(n-2) & 3(n-2) & 3(n-3) & \cdots & 3 \\
n-3 & 2(n-3) & 3(n-3) & 4(n-3) & \cdots & 4 \\
\cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\
1 & 2 & 3 & 4 & \cdots & n \\
\end{pmatrix}, \]

then \( B^{-1} \) is tridiagonal with \( b^{ii} = 2/(n+1) \) for \( i = 1, 2, \ldots, n, \) and \( b^{i-1,i} = b^{i,i+1} = -1/(n+1) \) for \( i = 2, 3, \ldots, n-1. \) (\( B \) is the variance matrix of ordered observations from a random sample of size \( n \) from a uniform distribution.)

(b) The autocorrelation matrix of an AR(1) time series is the symmetric Toeplitz matrix \( \sigma^2 B, \) where

\[ B = \begin{pmatrix}
1 & \rho & \rho^2 & \rho^3 & \cdots & \rho^{n-1} \\
\rho & 1 & \rho & \rho^2 & \cdots & \rho^{n-2} \\
\rho^2 & \rho & 1 & \rho & \cdots & \rho^{n-3} \\
\cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\
\rho^{n-1} & \rho^{n-2} & \rho^{n-3} & \rho^{n-4} & \cdots & 1
\end{pmatrix}. \]
and \(|\rho| < 1\), that is, \(b_{ij} = \rho^{i-j}\). Then

\[
B^{-1} = (1 - \rho^2)^{-1} \begin{pmatrix}
1 & -\rho & 0 & \cdots & 0 & 0 \\
-\rho & 1 + \rho^2 & -\rho & \cdots & 0 & 0 \\
0 & -\rho & 1 + \rho^2 & \cdots & 0 & 0 \\
\cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\
0 & 0 & 0 & \cdots & -\rho & 1
\end{pmatrix}.
\]

Also \(B^{-1} = (1 - \rho^2)^{-1} L'L\), where

\[
L = \begin{pmatrix}
\sqrt{1 - \rho^2} & 0 & 0 & \cdots & 0 & 0 \\
-\rho & 1 & 0 & \cdots & 0 & 0 \\
\cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\
0 & 0 & 0 & \cdots & -\rho & 1 \\
0 & 0 & 0 & \cdots & 0 & -\rho
\end{pmatrix}.
\]

Then \(\det L = \sqrt{1 - \rho^2}\) and \(\det B = (1 - \rho^2)^{n-1}\).

(c) If

\[
B = \sigma^2 \begin{pmatrix}
1 & 1 & 1 & 1 \\
1 & 2 & 2 & 2 \\
1 & 2 & 3 & 3 \\
1 & 2 & 3 & 4 \\
\cdots & \cdots & \cdots & \cdots \\
1 & 2 & 3 & 4 \\
\end{pmatrix}
\]

then

\[
B^{-1} = (\sigma^2)^{-1} \begin{pmatrix}
2 & -1 & 0 & \cdots & 0 \\
-1 & 2 & -1 & \cdots & 0 \\
0 & -1 & 2 & \cdots & 0 \\
\cdots & \cdots & \cdots & \cdots & \cdots \\
0 & 0 & 0 & \cdots & -1 \\
0 & 0 & 0 & \cdots & 2
\end{pmatrix}.
\]

(d) If

\[
B = \begin{pmatrix}
a_1^2 b_1 & a_2 a_1 b_1 & \cdots & a_n a_1 b_1 \\
a_1 a_2 b_1 & a_2^2 (b_1 + b_2) & \cdots & a_n a_2 (b_1 + b_2) \\
a_1 a_3 b_1 & a_2 a_3 (b_1 + b_2) & \cdots & a_n a_3 (b_1 + b_2 + b_3) \\
\cdots & \cdots & \cdots & \cdots \\
a_1 a_n b_1 & a_2 a_n (b_1 + b_2) & \cdots & a_n^2 (b_1 + \cdots + b_n)
\end{pmatrix},
\]

where none of the \(a_i\) or \(b_j\) is zero, then

\[
B^{-1} = \begin{pmatrix}
\frac{1}{a_1^2} (\frac{1}{b_1} + \frac{1}{b_2}) & -\frac{1}{a_1 a_2 b_2} & 0 & \cdots & 0 \\
-\frac{1}{a_1 a_2 b_2} & \frac{1}{a_2^2} (\frac{1}{b_2} + \frac{1}{b_3}) & -\frac{1}{a_2 a_3 b_3} & \cdots & 0 \\
0 & -\frac{1}{a_2 a_3 b_3} & \frac{1}{a_3^2} (\frac{1}{b_3} + \frac{1}{b_4}) & \cdots & 0 \\
\cdots & \cdots & \cdots & \cdots & \cdots \\
0 & 0 & 0 & \cdots & -\frac{1}{a_n-1 a_n b_n} \\
0 & 0 & 0 & \cdots & \frac{1}{a_n^2 b_n}
\end{pmatrix}.
\]
Also, \( \det \mathbf{B} = \Pi_{i=1}^{n} (a_i^2 b_i) \). A special case of the above result holds for the variance matrix of order statistics for a random sample of size \( n \) from an exponential distribution by setting
\[
a_1 = a_2 = \cdots = a_n = 1 \quad \text{and} \quad b_i = 1/(n - i + 1)^2 \quad (i = 1, 2, \ldots, n).
\]

**Proofs.** Section 8.11.

8.112. Quoted by Horn and Johnson [1991: 111, exercise 9].
8.114c. We check that \( \mathbf{B} \mathbf{B}^{-1} = \mathbf{I} \).

### 8.12 VANDERMONDE AND FOURIER MATRICES

#### 8.12.1 Vandermonde Matrix

**Definition 8.22.** Let \( a_1, a_2, \ldots, a_n \) be a set of real numbers, and let
\[
\mathbf{V} = \begin{pmatrix}
1 & 1 & 1 & \cdots & 1 \\
1 & a_1 & a_2 & a_3 & \cdots & a_n \\
1 & a_1^2 & a_2^2 & a_3^2 & \cdots & a_n^2 \\
\vdots & \vdots & \vdots & \vdots & & \vdots \\
1 & a_1^{n-1} & a_2^{n-1} & a_3^{n-1} & \cdots & a_n^{n-1}
\end{pmatrix}.
\]

Then \( \mathbf{V} \) and \( \mathbf{V}' \) are called \( n \times n \) **Vandermonde matrices**. The matrix \( \mathbf{V}' \) arises in relation to the **Lagrange interpolation polynomial** (Meyer [2000a: 186]). Note that every \( k \times k \) leading principal submatrix is also a Vandermonde matrix. A helpful notation on occasion is \( \mathbf{V}(a_1, a_2, \ldots, a_n) \), which we shall use below.

8.115. \( \det \mathbf{V} = \prod_{1 \leq i < j \leq n} (a_j - a_i) \).

8.116. If there are \( r \) distinct \( a_i \) values, then rank \( \mathbf{A} = r \).
8.117. If $V_n$ is an $n \times n$ Vandermonde matrix, then
\[ \det V_n = (a_n - a_1)(a_n - a_2) \cdots (a_n - a_{n-1}) \det V_{n-1}. \]

8.118. Let $V$ be an $n \times n$ Vandermonde matrix with distinct $a_i$ (i.e., the inverse exists), and define
\[
P_i(x) = \prod_{j=1; j \neq i}^{n} (x - a_j), \text{ for } i = 1, 2, \ldots, n
\]
\[
= \sum_{j=1}^{n} b_{ij} x^{j-1}, \text{ say.}
\]
If $C = V^{-1}$, then $c_{ij} = b_{ij}/P_i(a_i)$.

8.119. (Extended Vandermonde Matrix) Let
\[
V = \begin{pmatrix}
1 & 1 & 1 & \cdots & 1 \\
a_1 & a_2 & a_3 & \cdots & a_n \\
a_1^2 & a_2^2 & a_3^2 & \cdots & a_n^2 \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
a_1^{p-1} & a_2^{p-1} & a_3^{p-1} & \cdots & a_n^{p-1}
\end{pmatrix}
\]
be an $p \times n$ matrix ($n \geq p$). Then $\text{rank} V = \min(p, d)$, where $d$ is the number of distinct values of $a_i$. Note that $V'$ is the regression matrix for a $(p-1)$th-degree polynomial regression model.

Proofs. Section 8.12.1.


8.116. Suppose $a_1, \ldots, a_r$ are distinct, then the leading principal $r \times r$ sub-matrix is nonsingular (by 8.115).

8.117. Harville [1997: section 13.6].

8.118. Graybill [1983: 270]. For another formulation of this result see Zhang [1999: 114].


8.12.2 Fourier Matrix

Definition 8.23. Let $\omega = e^{2\pi i/n} = \cos(2\pi/n) + i \sin(2\pi/n)$, where $i = \sqrt{-1}$, so that $\overline{\omega} = e^{-2\pi i/n}$; also $\omega^r = \cos(2\pi r/n) + i \sin(2\pi r/n)$. Then
\[
F = n^{-1/2} V(1, \overline{\omega}, \omega^2, \ldots, \omega^{n-1})
\]
is defined to be a Fourier matrix. Since $F$ is symmetric, we have
\[
F^* = \overline{F} = \frac{1}{\sqrt{n}} \begin{pmatrix}
1 & 1 & 1 & \cdots & 1 \\
1 & \omega & \omega^2 & \cdots & \omega^{n-1} \\
1 & \omega^2 & \omega^4 & \cdots & \omega^{2n-2} \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
1 & \omega^{n-1} & \omega^{2n-2} & \cdots & \omega^{(n-1)(n-1)}
\end{pmatrix}
\]
The \((i,j)\)th element is \(n^{-1/2}\omega^{(i-1)(j-1)}\). Note that \(\omega^n = 1\), \(\overline{\omega} = \omega^{-1}\), \(\omega^{2n-2} = \omega^{n-2}\), \(\omega^{(n-1)(n-1)} = 1\), \(\omega^{-i} = \omega^{n-i}\), \(\omega^r = \cos(2\pi r/n) + is\sin(2\pi r/n)\), and we have \(\sum_{j=0}^{n-1} \omega^{ij} = 0\) if \(n > 1\) and \(i\) is an integer such that \(0 < i < n\) \((\omega^0 = 1)\). Note that Graybill [1983: 271] interchanges \(\omega\) and \(\overline{\omega}\) in his notation so that \(F\) looks like \(F^*\) above, although it is not. Schott [2005: 331] interchanges \(F\) and \(F^*\), while Meyer [2000a: 357] uses \(\overline{\omega} = \omega^{-1}\) and omits \(n^{-1/2}\) as a multiplier.

8.120. Suppose \(F\) is defined above.

(a) \(F\) and \(F^*\) are both symmetric.

(b) \(F\) is unitary, i.e., \(FF^* = I_n\).

(c) \(F^{-1} = \overline{F}\).

(d) \(F^2 = F^{*2} = \Pi\), where \(\Pi\) is the \(n \times n\) permutation matrix

\[
\Pi = (e_1, e_n, e_{n-1}, \ldots, e_2),
\]

and \(e_i\) is the \(i\)th column of \(I_n\).

(e) \(F^4 = F^{*4} = I_n\).

(f) \(F^*\) can be written as \(n^{1/2}F^* = C + iS\), where \(C\) and \(S\) are real matrices with

\[
c_{ij} = \cos[2\pi(i - 1)(j - 1)/n] \quad \text{and} \quad s_{ij} = \sin[2\pi(i - 1)(j - 1)/n].
\]

Also \(CS = SC\) so that from \(nFF^*\) we get \(C^2 + S^2 = nI_n\).

(g) The eigenvalues of \(F\) are \(\pm 1\) and \(\pm i\) with appropriate algebraic multiplicities.

8.121. Let \(c_n(\lambda) = \det(\lambda I_n - F^*).\) Then

\[
n \equiv 0(\text{mod} 4) : \quad c_n(\lambda) = (\lambda - 1)^2(\lambda - i)(\lambda + 1)(\lambda^4 - 1)^{(n/4) - 1},
\]

\[
n \equiv 1(\text{mod} 4) : \quad c_n(\lambda) = (\lambda - 1)(\lambda^4 - 1)^{(1/4)(n-1)},
\]

\[
n \equiv 2(\text{mod} 4) : \quad c_n(\lambda) = (\lambda^2 - 1)(\lambda^4 - 1)^{(1/4)(n-2)},
\]

\[
n \equiv 3(\text{mod} 4) : \quad c_n(\lambda) = (\lambda - i)(\lambda^2 - 1)(\lambda^4 - 1)^{(1/4)(n-3)}.
\]

**Definition 8.24.** Let \(y\) and \(z\) be \(n\)-dimensional vectors, and let \(F\) be an \(n \times n\) Fourier matrix. Then \(y = Fz\) is known as the *discrete Fourier transform* of the elements of \(z\). Typically, \(z = (z(0), z(1), \ldots, z(n - 1))'\), a times series sequence, or else \(z = z(t)\) \((t = 0, 1, \ldots, T - 1)\), where \(z(t)\) is vector time series. The Fourier transform can be computed using a so-called *Fast Fourier Transform Algorithm* in which one reduces the calculation of the discrete Fourier transform for a long stretch of data to the calculation of successive transforms of shorter sets of data (cf. Brillinger [1975: section 3.5] and Meyer [2000a: section 5.8]). One can also make use of the fact that a Fourier matrix of order \(2^n\) can be expressed as Kronecker products (Davis [1979: 36–37]).

Other applications of the transform include the convolution of two time series, computing filtered values from a transfer function, the estimation of the mixing distribution of a compound distribution, and the determination of the cumulative distribution of a random variable from its characteristic function (Brillinger [1975: 67–69]).
8.122. If \( y = Fz \) then \( z = F^{-1}y = F^*z \).

8.123. Let \( p(z) = a_0 + a_1z + a_2z^2 + \cdots + a_{n-1}z^{n-1} \) be a polynomial of degree \( n - 1 \). It will be determined uniquely by specifying its values \( p(z) \) at \( n \) distinct points \( z_k \) \((k = 1, 2, \ldots, n)\) in the complex plane. Suppose we select these points as the \( n \) roots of unity, namely, \( 1, \omega, \omega^2, \ldots, \omega^{n-1} \). Then

\[
\frac{1}{\sqrt{n}} F^* \begin{pmatrix} a_0 \\ a_1 \\ \vdots \\ a_{n-1} \end{pmatrix} = \begin{pmatrix} p(1) \\ p(\omega) \\ \vdots \\ p(\omega^{n-1}) \end{pmatrix},
\]

so that

\[
\begin{pmatrix} a_0 \\ a_1 \\ \vdots \\ a_{n-1} \end{pmatrix} = n^{1/2} F \begin{pmatrix} p(1) \\ p(\omega) \\ \vdots \\ p(\omega^{n-1}) \end{pmatrix}.
\]

This gives a relationship between the coefficients of \( p(z) \) and its values.

**Proofs.** Section 8.12.2.

8.120. Davis [1979: 31–37] and Graybill [1983: 272–273, with corrections in MI.]

8.121. Carlitz [1959].

8.13 **ZERO–ONE (0,1) MATRICES**

A matrix whose elements are all 0 or 1 is called a \((0,1)\) matrix. I have highlighted this topic as such matrices occur widely throughout statistics. Examples of such matrices are the permutation matrices in this chapter as well as the various vec-permutation and commutation matrices in Chapter 11. There is also the so-called incidence matrix discussed in (8.124) below, and there are Boolean matrices, both of which occur in combinatorial and graph theory. Zero-one matrices play an important role in the solution of equations with large sparse matrices (e.g., Duff et al. [1986]).

8.124. (Incidence Matrix)

(a) (Experimental Design) The incidence matrix for a block design has a row for each treatment and a column for each block. Thus a 1 for the \((i, j)\)th element of the matrix tells us that the \(i\)th treatment is applied to the \(j\)th block (cf. John and Williams [1995: chapter 1]).

(b) (Non-negative Matrix) As noted by Seneta [1981: 55], many properties of a non-negative matrix \( A \) depend only on the positions of the positive and zero elements within the matrix, and not on the actual size of the positive elements. Also, those positions will determine the corresponding positions in all powers \( A^k \), with \( k \) a positive integer. This means that in the investigation
of the properties of irreducibility and primitivity, the classification of indices into essential and inessential (cf. Section 9.3), and the periodicity of indices that communicate with each other, depend only on the location of the positive elements of $A$. Therefore given a non-negative matrix $A$ (i.e., all its elements are non-negative), then the matrix obtained by replacing each positive element by 1 is called the \textit{incidence matrix} of $A$. Particular matrices for which incidence matrices have useful applications are stochastic and Leslie matrices. A related $(0,1)$ matrix is the \textit{indicator} matrix, whereby the nonzero elements of any matrix are replaced by 1. For a non-negative matrix, the indicator matrix is the same as the incidence matrix.

\textbf{8.125.} Let $A$ be an $n \times n$ $(0,1)$ matrix. If $J_n = 1_n 1_n'$ and

$$AA' = kI_n + J_n$$

for some positive integer $k$, then $A$ is a normal matrix, that is, $AA' = A'A$.

\textbf{8.126.} If $A$ and $B$ are $n \times n$ $(0,1)$ matrices such that $AB = J_n - I_n$, then $AB = BA$.

\textbf{Definition 8.25.} (Boolean Matrix) The \textit{binary Boolean algebra} $B$ consists of the set $\{0, 1\}$, together with the usual operations of addition and multiplication (i.e., $1 + 0 = 1$, $0 + 0 = 0$, $1 \times 0 = 0$, $0 \times 0 = 0$, $1 \times 1 = 1$), except that $1 + 1 = 1$. A \textit{Boolean matrix} is a $(0,1)$ matrix over $B$. Boolean matrices have some properties that differ from matrices over $\mathbb{R}$; for example, the row rank need not equal the column rank. Some properties of Boolean matrices and Boolean vector spaces are given by Bapat and Raghavan [1997: section 5.6].

\textbf{8.127.} If $T$ is the incidence matrix of the non-negative matrix $A$, then $T^k$ is the incidence matrix of $A^k$ when $T$ is a Boolean matrix.

\textbf{Proofs.} Section 8.13.


\section*{8.14 SOME MISCELLANEOUS MATRICES AND ARRAYS}

\subsection*{8.14.1 Krylov Matrix}

\textbf{Definition 8.26.} If $x \in \mathbb{R}^n$ and $A$ is an $n \times n$ matrix, then the matrix

$$(x, Ax, A^2x, \ldots, A^{n-1}x)$$

is called a \textit{Krylov matrix}. This matrix arises in the so-called Lanczos method of obtaining approximations for some eigenvalues and eigenvectors, especially for large sparse matrices (Slapničar [2007: chapter 42, 8]). The column space of the Krylov matrix is called \textit{Krylov subspace}, and it is associated with the solution of linear equations (Greenbaum [2007: section 41.1]).
8.14.2 Nilpotent and Unipotent Matrices

**Definition 8.27.** An \( n \times n \) real or complex matrix is **nilpotent** if \( A^k = 0 \) for some positive integer \( k \), and is **unipotent** if \( A^2 = I_n \). For example,

\[
A = \begin{pmatrix}
I & B \\
0 & -I
\end{pmatrix}
\]

is unipotent. For a nilpotent matrix, the smallest \( k \) such that \( A^k = 0 \) is called the **index of nilpotency**.

8.128. The eigenvalues of a nilpotent matrix are all zero.

8.129. Let \( A \) be a real or complex \( n \times n \) singular matrix with matrix index \( k \) (cf. Section 3.8) such that \( \text{rank}(A^k) = r \). Then there exists a nonsingular matrix \( R \) such that

\[
R^{-1}AR = \begin{pmatrix}
C & 0 \\
0 & N
\end{pmatrix},
\]

where \( C \) is a nonsingular \( r \times r \) matrix and \( N \) is nilpotent with \( k \) its index of nilpotency.

8.130. If \( A \) and \( B \) are nilpotent matrices, then so is \( A + B \).

8.131. Any Jordan block \( J_m(\lambda) \) (cf. Definition 16.2) can written as \( J_m(\lambda) = \lambda I_m + A_m \), where \( A_m \) is nilpotent as \( (A_m)^m = 0 \).

More generally, a Jordan matrix can be written as \( J = D + N \), where \( D \) is diagonal matrix whose main diagonal is the same as that of \( J \), and \( N = J - D \). Here \( N \) is nilpotent as \( N^k = 0 \), where \( k \) is the order of the largest Jordan block in \( J \).

8.132. Any strictly upper-triangular \( n \times n \) matrix \( A \) is nilpotent with index of nilpotency at most \( n \) (as \( A^n = 0 \)). If \( r_j = \text{rank}(A^j) \), then \( r_{j+1} < r_j \) if \( r_j > 0 \).

**Proofs.** Section 8.14.2.

8.128. \( Ax = \lambda x \) implies that \( x \neq 0 \) and \( 0 = A^kx = \lambda^kx \).

8.129. Meyer [2000a: 397].

8.130. \( A^r = 0 \) and \( B^s = 0 \) for some \( r \) and \( s \), which imply \( (A + B)^{r+s} = 0 \).


8.14.3 Payoff Matrix

**Definition 8.28.** Suppose we have a game consisting of two players I and II. At each stage of the game, Player I chooses a strategy \( j \) with probability \( y_j \) (\( j = 1, 2, \ldots, n \)), where \( \sum_{j=1}^n y_j = 1 \), and Player II independently chooses a strategy \( i \) with probability \( x_i \) (\( i = 1, 2, \ldots, m \)), where \( \sum_{i=1}^m x_i = 1 \). Player II then pays Player I the amount \( a_{ij} \), or if \( a_{ij} \) is negative Player I pays Player II \( (-a_{ij}) \). The \( m \times n \) matrix \( A = a_{ij} \) is called a **payoff matrix**. (Some authors reverse the roles of the two players so that Player I chooses a strategy \( i \), etc.) The **expected income** to
Player I is $\sum_{j=1}^{n} a_{ij} y_j$, and the game is called a \textit{matrix game}. Optimal strategies exist for each player, as is proved in (8.133) below.

Let $x = (x_1, x_2, \ldots, x_m)'$ and $y = (y_1, y_2, \ldots, y_n)'$. If $x$ has more than one nonzero element, then the strategy is called a \textit{mixed} strategy. If all the elements are positive (i.e., $x > 0$), the strategy is said to be \textit{completely mixed}. A matrix game is called a \textit{completely mixed game} if every optimal strategy $x$ for Player II and $y$ for Player I are completely mixed. For further details see Bapat and Raghaven [1997: chapter 1].

8.133. (Minimax Theorem—von Neumann) Let $A$ be an $m \times n$ payoff matrix. There exists a unique constant $v$, called the \textit{value of the matrix game} $A$, and mixed strategies $x$ for Player II and $y$ for Player I such that

$$\sum_{j=1}^{n} a_{ij} y_j \geq v, \quad i = 1, 2, \ldots, m, \quad \text{and} \quad \sum_{i=1}^{n} a_{ij} x_i \leq v, \quad j = 1, 2, \ldots, n.$$ 

The strategy $x$ is called an \textit{optimal strategy} for Player II and $y$ is called an optimal strategy for Player I.

8.134. Let $v$ be the value of a matrix game $A$, and suppose some optimal strategy of Player II is completely mixed. Then, for any optimal strategy $y$ of Player I, $Ay = v1$.

8.135. Let the value of the $m \times n$ matrix game $A$ be zero (i.e., $v = 0$), and suppose that every optimal strategy for Player II is completely mixed. Then $m - 1 \leq \text{rank } A \leq n - 1$. If $\text{rank } A = m - 1$, then the optimal strategy for Player II is unique.

8.136. Let $A$ be an $n \times n$ matrix with cofactors $A_{ij}$. If the matrix game $A$ is completely mixed, then $\sum_{i=1}^{n} \sum_{j=1}^{n} A_{ij}$ is nonzero and the value $v$ of the game is given by

$$v = \frac{\det A}{\sum_{i=1}^{n} \sum_{j=1}^{n} A_{ij}}.$$ 

\textbf{Proofs.} Section 8.14.3.

8.133. Parthasarathy and Raghaven [1971].


\section*{8.14.4 Stable and Positive Stable Matrices}

\textbf{Definition 8.29.} An $n \times n$ real or complex matrix $A$ is said to be \textit{stable} if every eigenvalue of $A$ has a negative real part. The matrix is said to be \textit{positive stable} if every eigenvalue has a positive real part. These concepts are related to the long-term equilibrium of a dynamical system, and are discussed in detail by Horn and Johnson [1991: chapter 2]. For a further discussion see Meyer [2000a: section 7.4].

8.137. $\exp(At) \rightarrow 0$ as $t \rightarrow \infty$ if and only if $A$ is stable (cf. Section 19.6).
8.138. If $A$ is an $n \times n$ real or complex matrix and

$$\Re(a_{ii}) < - \sum_{j=1; j \neq i}^{n} |a_{ij}|, \quad i = 1, 2, \ldots, n,$$

where $\Re$ is the real part, then $A$ is stable.

8.139. Suppose $A$ is a positive stable matrix.

(a) $A^{-1}$, $A^*$ and $A'$ are all positive stable.

(b) $\det A > 0$.

(c) $\Re(\text{trace } A) > 0$.

(d) $\det(A^k) > 0$ for any positive integer $k$.

8.140. If $A$ is Hermitian positive definite, then $A$ is positive stable.

8.141. (Lyapunov's Equation) Suppose $X$, $A$, and $C$ are all $n \times n$ matrices such that $XA + A^*X = C$ (see also (13.17c) for further details).

(a) $A$ is positive stable if and only if there exists an Hermitian positive definite solution $X$ such that $C$ is Hermitian positive definite.

(b) Suppose $X$ and $C$ are Hermitian and $C$ is positive definite. Then $A$ is positive stable if and only if $X$ is positive definite.

(c) If $A$ is positive stable, then given $C$, there is a unique solution $X$ to Lyapunov's equation. If $C$ is Hermitian, then $X$ is Hermitian, while if $C$ is Hermitian positive definite, then $X$ is Hermitian positive definite.

(d) A special case of the above is when $C = I_n$, which is Hermitian and positive definite.

Horn and Johnson [1991: 96–98] give a number of generalizations of the above theory.


8.137. Horn and Johnson [1991: 92].

8.138. Marcus and Minc [1964: 159].

8.139. Horn and Johnson [1991: 93].

8.140. Horn and Johnson [1991: 95].

8.14.5 P-Matrix

**Definition 8.30.** An $n \times n$ real matrix $A$ is called a P-matrix if all its $k \times k$ principal minors are positive for $k = 1, 2, \ldots, n$.

8.142. Let $A$ be an $n \times n$ P-matrix. Then:

(a) $A'$ is also a P-matrix.

(a) $DA$ and $AD$ are also P-matrices, where $D$ is a diagonal matrix with positive diagonal elements.

(b) Every principal submatrix of $A$ is also a P-matrix.

(c) $a_{ii} > 0$ for $i = 1, 2, \ldots, n$.

(d) If $\Pi$ is any $n \times n$ permutation matrix, then $\Pi' A \Pi$ is a P-matrix.

(e) $A + D$ is a P-matrix, where $D$ is a diagonal matrix with non-negative diagonal elements.

8.143. Let $A$ be a real $n \times n$ matrix. Each of the following conditions is necessary and sufficient for $A$ to be a P-matrix.

1. For every $n \times 1$ vector $x$, there is an element in $x$ (say the $q$th) and the corresponding element in $y = Ax$ such that $x_q y_q > 0$.

2. For every $x \neq 0$, there exists a diagonal matrix $D$, a function of $x$, with positive diagonal elements such that $x' D A x > 0$.

3. For every $x \neq 0$, there exists a diagonal matrix $D$, a function of $x$, with non-negative diagonal elements such that $x' D A x > 0$.

4. Every real eigenvalue of $A$ and of each principal submatrix of $A$ is positive.

**Proofs.** Section 8.14.5.

8.142. These results quoted by Graybill [1983: 376] follow directly from the definition.


8.14.6 Z- and M-Matrices

**Definition 8.31.** An $n \times n$ real matrix $A = (a_{ij})$ for which $a_{ij} \leq 0$ for all $i, j$, $i \neq j$ is called a Z-matrix. Note that if $B$ is an ML-matrix (cf. Definition 9.11 above (9.43)) then $A = -B$ is a Z-matrix, and vice versa.

A Z-matrix $A$ is called a (nonsingular) M-matrix if it is a nonsingular Z-matrix and $A^{-1} \geq 0$ (i.e., has non-negative elements). This was the definition introduced by Ostrowski in 1937. An equivalent definition used by Horn and Johnson [1991: 113] is that $A$ is an M-matrix if it is a Z-matrix and positive stable (cf. Section 8.14.4). I have included the word "nonsingular" to avoid ambiguity as definitions vary in the literature. For example, Bapat and Raghavan [1997: section 1.5] allow an M-matrix to be singular and use a different definition. For general references
relating to M-matrices see Varga [1962] and Berman and Plemmons [1994]. Non-singular M-matrices arise in game theory (Bapat and Raghavan [1997: section 1.5]).

8.144. A is a Z-matrix if and only if \( A = sI_n - B \) for some \( B \geq 0 \) and some real \( s \).

8.145. Let \( A \) be an \( n \times n \) Z-matrix such that \( A = LU \), where \( L \) is lower-triangular and \( U \) is upper triangular, both with positive diagonal elements. Then:

(a) \( A \) has positive leading principal minors including \( \det A \) itself.

(b) \( L \) and \( U \) are nonsingular.

(c) The off-diagonal elements of both \( L \) and \( U \) are nonpositive.

(d) No element of \( L^{-1} \) or \( U^{-1} \) is negative, and the diagonal elements of \( L^{-1} \) and \( U^{-1} \) are all positive.

8.146. Let \( A \) be an \( n \times n \) Z-matrix such that each real eigenvalue of \( A \) is positive. Let \( B \) be a Z-matrix such that \( A \leq B \) (i.e., \( a_{ij} \leq b_{ij} \) for all \( i, j \)). Then:

(a) \( A \) and \( B \) are nonsingular.

(b) \( 0 \leq B^{-1} \leq A^{-1} \) (i.e., \( A^{-1} - B^{-1} \geq 0 \)).

(c) Each real eigenvalue of \( B \) is positive.

(d) \( \det B \geq \det A > 0 \).

8.147. (Equivalence of Definitions) Let \( A \) be a Z-matrix. Then \( A \) is an M-matrix if and only if \( \Re(\lambda) > 0 \) (where \( \Re \) is the real part) for all eigenvalues \( \lambda \), that is, if and only if \( A \) is stable.

8.148. Let \( A \) be a Z-matrix. Then each of the following conditions is necessary and sufficient for \( A \) to be an M-matrix.

(1) All principal minors of \( A \) are positive, including \( \det A \); that is, \( A \) is a P-matrix.

(2) The leading principal minors of \( A \) are all positive, including \( \det A \).

(3) Every real eigenvalue of \( A \) is positive.

(4) \( A + tI_n \) is nonsingular for all \( t \geq 0 \).

(5) \( A + D \) is nonsingular for every non-negative diagonal matrix \( D \).

(6) There exists an \( x > 0 \) such that \( Ax > 0 \).

(7) \( Ax \geq 0 \) implies \( x \geq 0 \).

8.149. If \( A \) is a Z-matrix, then it is a (nonsingular) M-matrix if and only if it can be expressed in the form \( A = sI_n - B \), where \( B \geq 0 \) and \( s > \rho(B) \), with \( \rho(B) \) being the spectral radius of \( B \).

8.150. If \( A \) is an M-matrix, then so is every principal submatrix.
8.151. If $A$ is an M-matrix, it is also a P-matrix.

8.152. Let $A$ and $B$ be $n \times n$ Z-matrices. If $A$ is an M-matrix and $B \geq A$ (i.e., $b_{ij} \geq a_{ij}$ for all $i,j$), then:

(a) $B$ is an M-matrix.
(b) $A^{-1} \geq B^{-1} \geq 0$.
(c) $\det B \geq \det A > 0$.
(d) The matrix $A$ satisfies the Hadamard inequality

$$\det A \leq a_{11}a_{22}\cdots a_{nn}.$$ 

(e) $A^{-1}B \geq I_n$ and $BA^{-1} \geq I_n$.
(f) $B^{-1}A \leq I_n$ and $AB^{-1} \leq I_n$.
(g) $AB^{-1}$ and $B^{-1}A$ are M-matrices

8.153. Let $A$ be an M-matrix. Then there exists a positive eigenvalue of $A$, $\lambda_0$ say, such that the real part of any eigenvalue of $A$ is greater than or equal to $\lambda_0$.


8.144. Horn and Johnson [1991: 113]. Take $c_{ij} = \max\{-a_{ij}, 0\}$ and $s \geq \max_i\{a_{ii}\}$ so that $A = sI_n - (C + sI_n - \text{diag}(a_{11}, \ldots, a_{nn})$.


8.147. Meyer [2000a: 626].

8.148. For further equivalent conditions and details see Horn and Johnson [1991: 114–115]. Some proofs are also given by Graybill [1983: section 11.3] and Meyer [2000a: 626]. A game theoretic proof for some of the results like these are given by Bapat and Raghavan [1991: 25–28].


8.152. Graybill [1983: 386, (a)–(g) except (d)] and Horn and Johnson [1991: 117, (a)–(d)].

Three-Dimensional Arrays

In nonlinear regression models, the expected value of a random response variable \(y_i\) is usually of the form \(f_i(x_i; \theta)\), and this leads to looking at \(\partial f_i/\partial \theta_j \partial \theta_k\), which is a 3-dimensional array. Such arrays have been used for a wide variety of models including nonlinear models (cf. Seber and Wild [1989] and Wei [1997]) and multinomial models (e.g., Seber and Nyangoma [2000] and Wei [1997: section 7.2]).

**Definition 8.32.** Consider the \(n \times p \times p\) array \(W = \{(w_{rs})\}\) made up of a \(p \times p\) array of \(n\)-dimensional vectors \(w_{rs}\) \((r, s = 1, 2, \ldots p)\). If \(w_{irs}\) is the \(i\)th element of \(w_{rs}\), then the matrix of \(i\)th elements \(W_i = (w_{irs})\) is called the \(i\)th face of \(W\). We now define two types of multiplication. Firstly, if \(B\) and \(C\) are \(p \times p\) matrices, then

\[ V = \{(v_{rs})\} = BWC \]

denotes the array with \(i\)th face \(V_i = BW_iC\), i.e.,

\[ v_{rs} = \sum_{\alpha} \sum_{\beta} b_{\alpha r} w_{\alpha \beta} c_{\beta s}. \]

Secondly, if \(D\) is a \(q \times n\) matrix, then we define square bracket multiplication by the equation

\[ [D][W] = \{(Dw_{rs})\}, \]

where the right-hand side is a \(q \times p \times p\) array.

We can also define trace \(W\), a vector with \(i\)th element \(\text{trace}(W_i)\), and vec \(W\), which is a \(p^2 \times n\) matrix with \(i\)th column vec \(W_i\).

**8.154.** Using the above notation, we have the following.

(a) \([I_n][W] = W\).

(b) \([\alpha B + \beta C][W] = \alpha[B][W] + \beta[C][W]\).

(c) \(\text{trace}(BW) = \text{trace}(WB)\).

(d) \(B\text{trace}(W) = \text{trace}([B][W])\).

(e) \(\text{vec}([B][W]) = (\text{vec}W)B'\).

(f) \([D][BW]C = B[D][W]C\).

(g) \(\text{vec}([BW]C) = (C' \otimes B)\text{vec}W\), where "\(\otimes\)" is the Kronecker product.

(h) \([DB][W] = [D][((BW)_{rs})] = [D][[B][W]]\).

(i) \(d'Wb = \sum_u \sum_v a_u b_v w_{uv}\).

(j) \([d'][W]\) is a matrix with \((r, s)\)th element \(\sum_i d_i w_{irs}\).

**Proofs.** Section 8.14.7.
Any matrix of probabilities has non-negative entries and is therefore a non-negative matrix. Consequently, such matrices play a varied role in probability and statistics. For example, they are used in genetic and population growth models, general stochastic processes, and various scaling problems. Such matrices are also encountered in the previous chapter where a number of matrices were mentioned such as permutation matrices, where the elements are zero or one. Non-negative matrices also play an important role in combinatorics (e.g., Sachkov and Tarakonov [2002]). In this chapter we look at a wide range of such matrices. For a concise reference to the subject see Rothblum [2007: chapter 9].

9.1 INTRODUCTION

Definition 9.1. A nonzero matrix $A = (a_{ij})$ is said to be non-negative (positive) if $a_{ij} \geq 0 (> 0)$ for all $i, j$. We write $A \geq 0 (> 0)$. Also we say that $A \leq 0 (< 0)$ if $a_{ij} \leq 0 (< 0)$. The same definition applies to vectors, namely $a \geq 0$ if $a_i \geq 0$ for all $i$, and $a \neq 0$. Finally we say that $A \leq B$ if and only if $B - A \geq 0$.

In most applications, $A$ is square. Unless stated otherwise, we shall assume that $A$ is $n \times n$. Although certain aspects of the general theory of non-negative matrices extend to countably infinite matrices, we shall consider only infinite stochastic matrices (Section 9.6.3).
9.1. (Frobenius–König) If \( A \geq 0 \), then \( \text{per}(A) = 0 \), where \( \text{per}(A) \) is the permanent of \( A \) (cf. Section 4.5), if and only if \( A \) has an \( r \times s \) zero submatrix with \( r + s = n + 1 \).

Proofs. Section 9.1.


9.1.1 Scaling

Definition 9.2. Let \( A \geq 0 \) be an \( m \times n \) matrix. The problem of scaling \( A \) to obtain a non-negative \( m \times n \) matrix \( B \) with prescribed row and column sums will be called the scaling problem.

\( A \) and \( B \) are said to have the same pattern if \( a_{ij} = 0 \) if and only if \( b_{ij} = 0 \) for all \( i, j \).

The procedure whereby we alternatively scale the rows of \( A \) to give the required rows sums, then scale the columns sums of the new \( A \) to give the required column sums (this will upset the row sums), and then continuing to repeat these two operations, we shall call the iterative scaling algorithm. Under certain conditions, this procedure converges to give a solution to the scaling problem. Of related interest is the doubly stochastic matrix discussed in Section 9.7.

Scaling problems arise in many contexts. For example, Bapat and Raghavan [1997: chapter 6] mention budget allocations, probability estimation in Markov chains, Leontief input–output systems, estimating cell entries in contingency tables, and transportation planning.

9.2. (Bacharach) Let \( A \geq 0 \) be \( m \times n \) with no zero row or column, and let \( I \) and \( J \) be subsets of \( \{1, 2, \ldots, m\} \) and \( \{1, 2, \ldots, n\} \), respectively, with complements \( I^c \) and \( J^c \). Let \( x \) and \( y \) be fixed \( m \times 1 \) and \( n \times 1 \) positive vectors, respectively. Then there exists an \( m \times n \) matrix \( B \geq 0 \) such that \( a_{ij} = 0 \Rightarrow b_{ij} = 0 \), with \( B1_m = x > 0 \) and \( 1_n^T B = y' > 0' \) if and only if

\[
  a_{ij} = 0 \text{ for all } i \in I^c, j \in J^c \quad \text{implies} \quad \sum_{i \in I^c} x_i \leq \sum_{j \in J^c} y_j \text{ and } \sum_{i \in I} x_i \geq \sum_{j \in J} y_j.
\]

Here \( a_{ij} \) is to be understood as zero if \( i \) or \( j \in \phi \), as is summation over an empty set. Using a concept relating to the elements of \( A \) called "connectedness," Seneta [1981: 70–77] gives a number of general theorems to establish the convergence of the iterative scaling algorithm to the matrix \( B \) described above with prescribed row and column sums. If \( A > 0 \), then \( A \) is connected, and the theory simplifies. A different approach to this problem is embodied in the next two results.

9.3. Let \( K \) be a nonempty, bounded polyhedron given by

\[
  K = \{ \pi \in \mathbb{R}^n : c \geq 0, C \pi = b \},
\]

where \( C = (c_{ij}) \) is an \( m \times n \) matrix and \( b \in \mathbb{R}^m \) is a nonzero vector. Let \( y \in K \). Then, for any \( x \geq 0 \) with the same pattern as \( y \), there exist \( z_i > 0 \) (\( i = 1, 2, \ldots, m \)) and \( \pi \in K \) such that

\[
  \pi_j = x_j \prod_{i=1}^{m} z_i^{c_{ij}}, \quad j = 1, 2, \ldots, n.
\]
Furthermore, any \( \pi \in K \) of the above type is unique. Bapat and Raghavan [1997: 247] show how to use this theorem to prove the existence of a solution to the scaling problem.

9.4. Let \( A \) and \( B \) be any pair of positive \( m \times n \) matrices. Then there exists a unique matrix \( C = D_1AD_2 \), where \( D_1 \) and \( D_2 \) are diagonal matrices with positive diagonal entries, and \( C \) and \( B \) have the same row and column sums. Also the iterative scaling algorithm applied to \( A \) converges to \( C \).

**Proofs.** Section 9.1.1.


### 9.1.2 Modulus of a Matrix

**Definition 9.3.** The *modulus* of any a real or complex matrix \( A = (a_{ij}) \) is the matrix of absolute values, namely \( \text{mod}(A) = (|a_{ij}|) \). Thus \( \text{mod}(A) \geq 0 \). Schott [2005: 318] uses the term \( \text{abs}(A) \).

9.5. Clearly \( A \preceq \text{mod}(A) \).

9.6. The following are readily proved using (5.1).

(a) If \( A \) and \( B \) are any two conformable matrices, then

\[
\text{mod}(AB) \leq \text{mod}(A)\text{mod}(B).
\]

Here \( B \) could also be a vector.

(b) If \( A \) is square, \( \text{mod}(A^k) \leq [\text{mod}(A)]^k \).

(c) If \( A \) and \( B \) are \( n \times n \) matrices such that \( \text{mod}(A) \preceq \text{mod}(B) \), then

\[
\|\text{mod}(A)\|_F \leq \|\text{mod}(B)\|_F,
\]

where \( \| \cdot \|_F \) represents the Frobenius norm.

**Proofs.** Section 9.1.2.


### 9.2 SPECTRAL RADIUS

#### 9.2.1 General Properties

We recall that the spectral radius \( \rho(A) \) of a square matrix \( A \) is the maximum of the absolute values of the eigenvalues of \( A \). Note that \( \rho(A) \) need not be an eigenvalue of \( A \), though we note below that it can be an eigenvalue in the case of
non-negative matrices. Although the emphasis is on non-negative matrices in this chapter, further results concerning the spectral radius are given in Section 4.6.2 (e.g., 4.68a) on matrix norms.

9.7. Let \( A = (a_{ij}) \) be a complex matrix and \( B = (b_{ij}) \geq 0 \) be a real matrix, both \( n \times n \), such that \( \text{mod}(A) \leq B \). Then:

(a) \( \rho(A) \leq \rho[\text{mod}(A)] \leq \rho(B) \).

(b) (Ky Fan) Every eigenvalue of \( A \) lies in the region

\[ \bigcup_{i=1}^{n} \{ z \in \mathbb{C} : |z - a_{ii}| \leq \rho(B) - b_{ii} \}. \]

9.8. Let \( A \) and \( B \) be \( n \times n \) non-negative matrices. If \( 0 \leq A \leq B \), then

\[ \rho(A) \leq \rho(B); \]

that is, \( \rho(\cdot) \) is monotonically increasing on the set of all \( n \times n \) non-negative matrices.

9.9. Let \( A \geq 0 \) be an \( n \times n \) matrix.

(a) If \( C \) is a principal submatrix of \( A \), then \( \rho(C) \leq \rho(A) \). In particular,

\[ \max_{1 \leq i \leq n} a_{ii} \leq \rho(A). \]

(b) Let \( r_i \) be the row sum of row \( i \) and \( c_j \) be the column sum of column \( j \). Then:

(i) \( \min_{1 \leq i \leq n} r_i \leq \rho(A) \leq \max_{1 \leq i \leq n} r_i. \)

(ii) \( \min_{1 \leq j \leq n} c_j \leq \rho(A) \leq \max_{1 \leq j \leq n} c_j. \)

(iii) If \( r_i = \alpha \) for all \( i \), then \( \rho(A) = \alpha \). If \( c_j = \beta \) for all \( j \), then \( \rho(A) = \beta \).

(c) Let \( x = (x_1, x_2, \ldots, x_n)' > 0 \). Then:

(i) \( \min_{1 \leq i \leq n} \frac{1}{x_i} \sum_{j=1}^{n} a_{ij}x_j \leq \rho(A) \leq \max_{1 \leq i \leq n} \frac{1}{x_i} \sum_{j=1}^{n} a_{ij}x_j. \)

(ii) \( \min_{1 \leq j \leq n} x_j \sum_{i=1}^{n} \frac{a_{ij}}{x_i} \leq \rho(A) \leq \max_{1 \leq j \leq n} x_j \sum_{i=1}^{n} \frac{a_{ij}}{x_i}. \)

(iii) If \( A \) has a positive right eigenvector, then

\[ \rho(A) = \max_{x > 0} \min_{1 \leq i \leq n} \frac{1}{x_i} \sum_{j=1}^{n} a_{ij}x_j = \min_{x > 0} \max_{1 \leq i \leq n} \frac{1}{x_i} \sum_{j=1}^{n} a_{ij}x_j. \]

(d) \( \rho(I_n + A) = 1 + \rho(A) \).

9.10. Let \( A > 0 \) with maximum and minimum row sums of \( R \) and \( r \), respectively, and let \( m = \min_{i,j} a_{ij} \). Then

\[ r + m(h - 1) \leq \rho(A) \leq R - m(1 - g^{-1}), \]
where
\[
g = \frac{R - 2m + \sqrt{R^2 - 4m(R - r)}}{2(r - m)}, \quad h = \frac{-r + 2m + \sqrt{r^2 + 4m(R - r)}}{2m}.
\]

There exist matrices for which the bounds are attained.

**Proofs.** Section 9.2.1.


### 9.2.2 Dominant Eigenvalue

**Definition 9.4.** If \(|\lambda_1| > |\lambda_2| \geq \cdots \geq |\lambda_n|\), then \(\lambda_1\) is called the **dominant eigenvalue** of \(A\). We note that \(|\lambda_1|\) is also the spectral radius \(\rho(A)\) of \(A\).

**9.11.** (Perron–Frobenius Theorem for Non-negative Matrices) If \(A \geq 0\), then the following hold.

(a) \(A\) has a real eigenvalue \(\rho \geq 0\).

(b) With \(\rho\) can be associated non-negative left and right eigenvectors (which need not be unique even when scaled to have unit length).

(c) If \(A\) has a positive eigenvector, then the corresponding eigenvalue is \(\rho\); that is, if \(Ax = \lambda x\) and \(x > 0\), then \(\lambda = \rho\).

(d) \(|\lambda| \leq \rho\) for any eigenvalue \(\lambda\) of \(A\), i.e., \(\rho\) is the spectral radius of \(A\).

(d) If \(0 \leq B \leq A\) and \(\beta\) is an eigenvalue of \(B\), then \(|\beta| \leq \rho\).


There is a corresponding theorem, originally proved by Perron in 1907 for positive matrices; for recent proofs see Bapat and Raghavan [1997: 5–6], Rao and Rao [1998: 473] and Schott [2005: section 8.8]. However, when \(A \geq 0\), \(A\) is also irreducible and primitive (see below for definitions), so that a more general theorem is therefore
given in (9.30). For completeness, we give some related results for $A > 0$ below in (9.16) from Horn and Johnson [1985] and Schott [2005].

9.12. If $A \geq 0$ and $s > \rho$, where $\rho$ is defined in (9.11) above, then $(sI_n - A)$ has an inverse and

$$(sI_n - A)^{-1} \geq 0.$$  

9.13. Let $A \geq 0$ with spectral radius $\rho$, and let $\text{adj}(A)$ denote the adjoint matrix. Then:

(a) $B(s) = \text{adj}(sI_n - A) \geq 0$ for $s > \rho$.
(b) $\frac{dB(s)}{ds} \geq 0$ for $s > \rho$.
(c) $B(\rho) \geq 0$.
(d) $\frac{d}{ds}(sI_n - A)^{-1}|_{s=\rho} \geq 0$.

9.14. Let $A \geq 0$ have spectral radius $\rho$.

(a) Suppose $x > 0$ and $\alpha, \beta \geq 0$. Then:

(i) If $\alpha x \leq Ax \leq \beta x$, then $\alpha \leq \rho \leq \beta$.
(ii) If $\alpha x < Ax$, then $\alpha < \rho$
(iii) If $Ax < \beta x$, then $\rho < \beta$.

(b) If $x \geq 0$ ($x \neq 0$) and $Ax \geq \alpha x$ for some $\alpha$, then $\rho \geq \alpha$.

9.15. Let $A \geq 0$.

(a) $(I_n - A)^{-1}$ exists and is non-negative if and only if there exists $x \geq 0$ such that $x > Ax$.

(b) If each of the row sums of $A$ is less than 1, then $(I_n - A)^{-1}$ exists and is non-negative. The same is true if each of the columns sums is less than 1.

(c) Consider the equation $(I_n - A)y = b$, where $b \geq 0$. If $(I_n - A)^{-1}$ exists and is non-negative, then there is a unique non-negative solution $y = (I_n - A)^{-1}b$. This result applies, for example, to Leontief’s input–output economic model.

An irreducible version of the above theorem is given in (9.36) below.

9.16. (Perron’s Theorem for Positive Matrices, with Additions) Suppose $A > 0$ with spectral radius $\rho = \rho(A)$. Then:

(a) $\rho$ is positive and is an eigenvalue.

(b) There are positive right and left eigenvectors $A$ corresponding to $\rho$.

(c) Suppose $|\lambda| = \rho$, with any corresponding eigenvector $x$. Then:

(i) $A \text{mod}(x) = \rho \text{mod}(x)$, where “mod” is defined in Definition 9.3 above.
(ii) There exists an angle $\theta$ such that $e^{-i\theta}x > 0$.

(d) The eigenvalue $\rho$ has algebraic and geometric multiplicity both equal to 1.
(e) If $\lambda$ is an eigenvalue of $A$ and $\lambda \neq \rho$, then $|\lambda| < \rho$.

(f) Suppose $x$ and $y$ are positive vectors such that $Ax = \rho x$, $y'A = \rho y'$, and $x'y = 1$. Then:

(i) $(A - \rho xy')^k = A^k - \rho^k xy'$, for $k = 1, 2, \ldots$.

(ii) Each nonzero eigenvalue of $A - \rho xy'$ is an eigenvalue of $A$.

(iii) $\rho$ is not an eigenvalue of $A - \rho xy'$.

(iv) $\rho(A - \rho xy') < \rho$.

(v) $\lim_{k \to \infty}(\rho^{-1}A)^k = xy'$.

Proofs. Section 9.2.2.


9.3 CANONICAL FORM OF A NON-NEGATIVE MATRIX

Definition 9.5. Let $A = (a_{ij}) \geq 0$ be $n \times n$, and define $A^m = (a_{ij}^{(m)})$. If $a_{ij}^{(m)} > 0$ for some positive integer $m$ (a function of $i$ and $j$), we say that $i$ leads to $j$ or $i$ can reach $j$ (or state $i$ can reach state $j$ in the case of a Markov chain and its transition matrix; see Definition 9.16 in Section 9.6), or $j$ is accessible from $i$, and we write $i \to j$. If $i \to j$ and $j \to i$, we say that the $i$ and $j$ communicate and write $i \leftrightarrow j$. If $i \leftrightarrow i$, the period of index $i$ is defined to be $d(i) = \gcd\{k : a_{ii}^{(k)} > 0\}$—that is, the greatest common divisor of those positive integers $k$ such that $a_{ii}^{(k)} > 0$. If $d(i) > 1$, then $i$ is said to be periodic (cyclic), while if $d(i) = 1$, then $i$ is said to be aperiodic (acyclic). Clearly, if there exists at least one $j$ such that $i \leftrightarrow j$, we must have $i \leftrightarrow i$.

The indices can be classified as essential or inessential. If $i \to j$, but $j \not\to i$ for some $j$, then $i$ is called inessential, and an index which leads to no index at all is also called inessential; otherwise, an index is called essential. Essential indices can be divided into self-communicating classes where all the indices within the class communicate with each other, but do not communicate with any indices outside the class. Similarly, inessential indices (if any) can also be divided into self-communicating classes in which an index in a class can reach another index outside the class, but can’t get back, together with a class of individuals that communicate with no index (Seneta [1981: 12]).

9.17. If $A \geq 0$ has at least one positive entry in each row, then it possesses at least one essential class of indices.
9.18. If \( A = (a_{ij}) \geq 0 \) and \( i \leftrightarrow j \), then \( d(i) = d(j) \).

9.19. (Canonical Form) Given \( A \geq 0 \), there exists a permutation matrix \( \Pi \) such that

\[
B = \Pi' A \Pi = \begin{pmatrix}
A_1 & 0 & \cdots & 0 & | & 0 \\
0 & A_2 & \cdots & 0 & | & 0 \\
\vdots & \vdots & \ddots & \vdots & | & \vdots \\
0 & 0 & \cdots & A_r & | & 0
\end{pmatrix},
\]

where the \( A_i \) (\( i = 1, 2, \ldots, r \)) correspond to the \( r \) self-communicating classes of essential indices, and \( Q \) corresponds to the inessential indices, with \( R \neq 0 \) in general. The matrix \( B \) is simply \( A \) with the indices reordered, and \( Q \) has a structure similar to \( A \), except that there may be nonzero elements to the left of any of its diagonal blocks, that is,

\[
Q = \begin{pmatrix}
Q_1 & 0 & \cdots & 0 \\
0 & Q_2 & \cdots & 0 \\
\vdots & \vdots & \ddots & \vdots \\
C & Q_s
\end{pmatrix}.
\]

In practice the matrix \((R | Q)\) in \( B \) may be missing from \( B \) and we could have \( r = 1 \). Also

\[
B^k = \begin{pmatrix}
A_1^k & 0 & \cdots & 0 & | & 0 \\
0 & A_2^k & \cdots & 0 & | & 0 \\
\vdots & \vdots & \ddots & \vdots & | & \vdots \\
0 & 0 & \cdots & A_r^k & | & 0
\end{pmatrix} \quad \text{and} \quad Q^k = \begin{pmatrix}
Q_1^k & 0 & \cdots & 0 \\
0 & Q_2^k & \cdots & 0 \\
\vdots & \vdots & \ddots & \vdots \\
C_k & Q_s^k
\end{pmatrix}.
\]

Proofs. Section 9.3.


9.4 IRREDUCIBLE MATRICES

9.4.1 Irreducible Non-negative Matrix

In Section 8.8 we introduced the concept of irreducibility for general matrices. In this section we concentrate on non-negative matrices, the major application of irreducibility, and recall the following definition.

**Definition 9.6.** An \( n \times n \) non-negative matrix \( A \) is said to be reducible if there exist a permutation matrix \( \Pi \) such that

\[
B = \Pi A \Pi' = \begin{pmatrix}
B_{11} & 0 \\
B_{12} & B_{22}
\end{pmatrix},
\]

where \( B_{11} \) and \( B_{22} \) are square matrices. A matrix which is not reducible is said to be irreducible. We note that if \( B \) has the general canonical form (9.19), then it is
reducible. Some authors use the equivalent definition

\[ B = \begin{pmatrix} B_{11} & B_{12} \\ 0 & B_{22} \end{pmatrix}. \]

An equivalent but more useful definition of irreducibility in the present context is as follows. The \( n \times n \) matrix \( A \geq 0 \) is irreducible if and only if every pair of indices in its index set communicate, that is, for every pair \( i, j \) there exists a positive integer \( m (\leq n) \), a function of \( i \) and \( j \), such that \( a_{ij}^{(m)} > 0 \). The equivalence of the two definitions is proved by Bapat and Raghavan [1997: 2-4].

An irreducible non-negative matrix is said to be periodic (cyclic) with period \( d \) if the period of any one (and so of each one, by (9.18)) of its indices satisfies \( d > 1 \), and it is said to be aperiodic (acyclic) if \( d = 1 \).

9.20. An irreducible non-negative matrix cannot have a zero row or column.

9.21. If the matrix \( A = (a_{ij}) \geq 0 \) is reducible, then so is \( A^k \) for any positive integer \( k \).

9.22. An \( n \times n \) non-negative matrix \( A \) is irreducible if and only if \( (I_n + A)^{n-1} > 0 \).

9.23. If \( A \) is irreducible, then so is \( A' \).

**Definition 9.7.** The matrix \( A \geq 0 \) is said to be primitive if there exists a positive integer \( p \) such that \( A^p > 0 \). (Thus if \( A \) is primitive, it is irreducible as \( a_{ij}^{(p)} > 0 \) for all \( i, j \).) Clearly, if \( A > 0 \), then \( A \) is primitive.

An alternative but equivalent definition is that \( A \geq 0 \) is primitive if it is irreducible and it has only one eigenvalue of maximum modulus. The equivalence follows from (9.26) below.

The smallest positive integer \( q \) such that \( A^q > 0 \) is called the index of primitivity.

9.24. If \( A \geq 0 \) is primitive, then \( A^k \) is non-negative, irreducible, and primitive for all \( k = 1, 2, \ldots \).

9.25. If \( A \geq 0 \) is primitive, then \( A^k > 0 \) for some integer \( k \leq (n - 1)n^n \).

9.26. A non-negative matrix \( A \) is primitive if and only if it is irreducible and aperiodic.

9.27. If \( A \geq 0 \) has \( a_{ii} > 0 \) for all \( i \), then \( A^{n-1} > 0 \) and \( A \) is primitive.

9.28. (Limit Theorem for Primitive Matrices) Let \( A \) be an \( n \times n \) primitive non-negative matrix with distinct eigenvalues \( \rho, \lambda_2, \ldots, \lambda_t \) (\( t \leq n \)), where \( \rho > |\lambda_2| \geq |\lambda_3| \geq \cdots \geq |\lambda_t| \). In the case \( |\lambda_2| = |\lambda_3| \) (\( \lambda_2 \neq \lambda_3 \)) we stipulate that the algebraic multiplicity \( m_2 \) of \( \lambda_2 \) is at least as great as that of \( \lambda_3 \) and of any other eigenvalues having the same modulus as \( \lambda_2 \). By (9.30) there exist positive vectors \( x \) and \( y \) such that \( Ax = \rho x, \ y'A = \rho y' \) and \( x'y = 1 \). We then have the following:

(a) Suppose \( \lambda_2 \neq 0 \).

(i) As \( k \to \infty \),

\[ A^k = \rho^k xy' + O(k^s|\lambda_2|^k) \]

elementwise, where \( s = m_2 - 1 \).
\( \lim_{k \to \infty} \frac{A^k}{\rho^k} = xy'. \)

(b) Suppose \( \lambda_2 = 0 \), then for \( k \geq n - 1 \),

\[ A^k = \rho^k xy'. \]

For matrix limits see Section 19.2.

**Definition 9.8.** An irreducible non-negative matrix that is periodic is said to be *imprimitive*. Thus irreducible matrices can be subdivided into primitive or imprimitive matrices depending on whether they are aperiodic or periodic.

**9.29.** The powers of an imprimitive matrix may be studied in terms of powers of primitive matrices.

**9.30.** (Perron–Frobenius Theorem for Irreducible Matrices) Let \( A \geq 0 \) be an irreducible matrix. Then we have the following.

(a) \( A \) has a real positive eigenvalue \( \rho \).

(b) With \( \rho \) can be associated strictly positive left and right eigenvalues.

(c) \( |\lambda| \leq \rho \) for any eigenvalue \( \lambda \) of \( A \). Thus \( \rho \) is the spectral radius of \( A \).

(d) \( \rho \) has geometric multiplicity 1, that is, the left and right eigenvectors associated with \( \rho \) are unique to constant multiples.

(e) \( \rho \) has algebraic multiplicity 1, that is, \( \rho \) is a simple root of the characteristic equation.

(f) If \( 0 \leq B \leq A \) and \( \beta \) is an eigenvalue of \( B \), then \( |\beta| \leq \rho \). Moreover, \( |\beta| = \rho \) implies \( B = A \) so that \( \rho \) increases when any element of \( A \) increases.

(g) (Primitive matrices) If \( A \) is primitive then (a)-(f) still hold except that (c) is replaced by \( |\lambda| < \rho \) for any eigenvalue \( \lambda \neq \rho \).

**Definition 9.9.** We call \( \rho \) the *Perron–Frobenius eigenvalue* of an irreducible non-negative matrix, and its corresponding positive eigenvectors are called the *Perron–Frobenius eigenvectors*. As noted above, \( \rho \) is the spectral radius.

**9.31.** Let \( A \geq 0 \) be an irreducible \( n \times n \) matrix with Perron–Frobenius eigenvalue \( \rho \), and let \( x \) and \( y \) be the right and left Perron–Frobenius eigenvectors of \( A \) satisfying \( x'y = 1 \). Then:

(a) \( y'Ax = \rho \leq x'Ay \).

(b) (Limit Theorem) If \( L = xy' \), then

\[ \lim_{N \to \infty} \frac{1}{N} \sum_{k=1}^{N} (\rho^{-1} A)^k = L. \]
9.32. (Subinvariance Theorem and Variations) Let \( A \geq 0 \) be an irreducible matrix with Perron–Frobenius eigenvalue \( \rho \). Let \( c > 0 \).

(a) If \( Ax \leq cx \) for any nonzero \( x \geq 0 \), then \( \rho \leq c \) and \( x > 0 \). Furthermore, \( \rho = c \) if and only if \( Ax = cx \).

(b) If \( Ax \geq cx \) for any nonzero \( x \geq 0 \), then \( \rho \geq c \). Also \( \rho = c \) if and only if \( Ax = cx \).

(c) If \( Ax \leq cx \) (\( \neq cx \)) for some \( x \geq 0 \), then \( \rho < c \).

(d) If \( Ax \geq cx \) (\( \neq cx \)) for some \( x \geq 0 \), then \( \rho > c \).

9.33. (Bounds on \( \rho \)) Let \( A \geq 0 \) be irreducible with Perron–Frobenius eigenvalue \( \rho \). Then (9.9b) holds with \( \rho(A) = \rho \). In the case of (i) and (ii), equality on one side implies equality on both sides, that is, \( \rho \) can only be equal to a maximal or minimal row (respectively column) sum if all the row (respectively column) sums are equal. The same is true for (c)(i).

9.34. Let \( \mathcal{P} = \{ x : x > 0 \} \). Then:

(a) \[
\sup_{x \in \mathcal{P}} \min_i \left\{ \frac{\sum_{j=1}^{n} a_{ij} x_j}{x_i} \right\} = \rho = \inf_{x \in \mathcal{P}} \max_i \left\{ \frac{\sum_{j=1}^{n} a_{ij} x_j}{x_i} \right\}.
\]

There also exists an \( x \in \mathcal{P} \) for which both the supremum and the infimum are attained.

(b) \[
\sup_{x \in \mathcal{P}} \left\{ \inf_{y \in \mathcal{P}} \frac{y'Ax}{y'x} \right\} = \rho = \inf_{x \in \mathcal{P}} \left\{ \sup_{y \in \mathcal{P}} \frac{y'Ax}{y'x} \right\}.
\]

9.35. Let \( A \geq 0 \) be irreducible with Perron–Frobenius eigenvalue \( \rho \), and let \( E \geq 0 \) (\( E \neq 0 \)). If \( \delta > 0 \), then \( B = A + \delta E \) is irreducible with a Perron–Frobenius eigenvalue that, by a suitable choice of \( \delta \), may be made equal to any positive number exceeding \( \rho \).

9.36. Let \( A \geq 0 \) be irreducible with Perron–Frobenius eigenvalue \( \rho \).

(a) A necessary and sufficient condition for a solution \( x \) (\( x \geq 0, x \neq 0 \)) to the equation \( (sI_n - A)x = c \) to exist for any \( c \geq 0 \) (\( c \neq 0 \)) is that \( s > \rho \). In this case, there is only one solution \( x \) that is strictly positive, and it is given by \( x = (sI_n - A)^{-1}c \).

(b) Of those real numbers \( s \) for which the inverse exists, \( (sI - A)^{-1} > 0 \) if and only if \( s > \rho \).

(c) If \( s = 1 \), then \( \rho < 1 \) if none of the row (or column) sums of \( A \) exceed 1, and at least one is less than 1. For applications see Leontief's input-output economic model and an extension described by Bapat and Raghavan [1997: chapter 7], Rao and Rao [1998: 477–481], and Seneta [1981: chapter 2].
9.37. Let $A \geq 0$ be irreducible with Perron–Frobenius eigenvalue $\rho = 1$. Then the sequence $\{A^k\}$ converges if and only if $A$ is primitive.

9.38. If $A \geq 0$ is irreducible with Perron–Frobenius eigenvalue $\rho$, and $A^k = (a_{ij}^{(k)})$, then for each pair $(i, j)$ the power series

$$A_{ij}(s) = \sum_{k=0}^{\infty} a_{ij}^{(k)} s^k$$

all have the same radius of convergence $R = \rho^{-1}$.

9.39. Suppose $A \geq B \geq 0$ and $A \neq B$. If $A + B$ is irreducible, then $\rho(A) > \rho(B)$, where $\rho(\cdot)$ is the dominant eigenvalue of the appropriate matrix.

Proofs. Section 9.4.1.


9.21. We take powers of $B$ in the definition (e.g., $B^2 = \Pi A \Pi' \Pi A \Pi' = \Pi A^2 \Pi'$).


9.23. This follows from either definition of irreducibility.


9.27. Horn and Johnson [1985: 517].


9.30. Bapat and Raghavan [1997: 17, proved the result using the theory of completely mixed matrix games], Horn and Johnson [1985: 508, for (a)–(e)], Schott [2005: 325–326, for (a)–(e)], and Seneta [1981: 22, 3–7].

9.31a. Bapat and Raghavan [1997: 121, with $x$ and $y$ interchanged].

9.31b. Horn and Johnson [1985: 524].


9.32c–d. Debreu and Hurstein [1953].

9.33. Quoted by Seneta [1981: 27, exercise 1.7].


9.4.2 Periodicity

**Definition 9.10.** If \( A \geq 0 \) is irreducible, then by (9.18) each index \( i \) has the same period, \( d \), say, which we call the period of \( A \).

9.40. Let \( A \geq 0 \) be an irreducible matrix with \( h \) eigenvalues whose moduli are equal to the spectral radius \( \rho \). We know from (9.30c) that \( h \geq 1 \). Then \( h = d \), the period of \( A \) (cf. (9.41b) below).

9.41. Let \( A \geq 0 \) be an \( n \times n \) irreducible matrix with period \( d \).

(a) \( A \) is primitive if and only if \( d = 1 \).

(b) If \( d > 1 \), there exist \( d \) distinct eigenvalues with \( |\lambda| = \rho \), where \( \rho \) is the spectral radius. These eigenvalues are \( \rho \exp(i(2\pi k/d)) \), \( k = 0, 1, \ldots, d - 1 \), the \( d \) roots of \( \lambda^d - \rho^d = 0 \).

(c) If \( \lambda \neq 0 \) is any eigenvalue of \( A \), then the numbers \( \lambda \exp[i(2\pi k/d)] \), \( k = 0, 1, \ldots, d - 1 \), are also eigenvalues.

(d) The set of \( n \) eigenvalues when plotted as points in the complex \( \lambda \)-plane is invariant under a rotation of the plane through the angle \( 2\pi/d \).

(e) Combining (b) and (c),

\[
\det(\lambda I - A) = \lambda^m (\lambda^d - \rho^d) \prod_{i=1}^{r} (\lambda^d - \lambda_i^d),
\]

where \( |\lambda_i| < \rho \) for \( i = 1, 2, \ldots, r \) and \( m = n - (r + 1)d \).

9.42. Let \( A \geq 0 \) be irreducible with period \( d \) (\( d > 1 \)).

(a) There exists a permutation matrix \( \Pi \) such that

\[
\Pi A \Pi' = \begin{pmatrix}
0 & B_{12} & 0 & \cdots & 0 \\
0 & 0 & B_{23} & \cdots & 0 \\
\vdots & \vdots & \ddots & \cdots & \vdots \\
0 & 0 & 0 & \cdots & B_{d-1,d} \\
0 & 0 & 0 & \cdots & 0
\end{pmatrix}
\]

(\( = B \)),

where the zero submatrices on the main diagonal are square. Note that \( \Pi \) permutes the rows, while \( \Pi' \) permutes the columns in the same order.

(b) Conversely, suppose \( A \geq 0 \) and there exists a permutation matrix such that \( \Pi A \Pi' = B \), as defined in (a). If \( A \) has no zero rows or columns and \( B_{12}B_{23}\cdots B_{d-1,d}B_{d1} \) is irreducible, then \( A \) is irreducible.
Proofs. Section 9.4.2.


9.41e. Bapat and Raghavan [1997: 43].


9.4.3 Non-negative and Nonpositive Off-Diagonal Elements

Definition 9.11. An \( n \times n \) real matrix \( B = (b_{ij}) \) for which \( b_{ij} \geq 0 \), for all \( i, j \) \((i \neq j)\) is called an \textit{ML-matrix}. This matrix arises in the theory of Markov processes.

9.43. If \( B \) is an ML-matrix, there exists a non-negative \( \alpha \) sufficiently large so that

\[ T = \alpha I_n + B \geq 0. \]

Definition 9.12. An ML-matrix \( B \) is said to be an \textit{irreducible ML-matrix} if \( T = \alpha I_n + B \geq 0 \) is irreducible. By taking \( \alpha > \max_i |b_{ii}| \), we can make the irreducible \( T \) aperiodic and primitive.

9.44. Suppose \( B \) is an \( n \times n \) irreducible ML-matrix. Then there exists an eigenvalue \( \tau \) with the following properties.

(a) \( \tau \) is real.

(b) With \( \tau \) are associated strictly positive left and right eigenvectors, which are unique to constant multiples.

(c) \( \tau \) is greater than the real part of any other eigenvalue \( \lambda \) of \( B \), \( \lambda \neq \tau \).

(d) \( \tau \) is a simple root of the characteristic equation of \( B \).

(e) \( \tau \leq 0 \) if and only if there exists \( y \geq 0 \) \((y \neq 0)\) such that \( By \leq 0 \), in which case \( y > 0 \); and \( \tau < 0 \) if and only if there is a strict inequality in at least one position in \( By \leq 0 \).

(f) \( \tau < 0 \) if and only if \( \Delta_i > 0, i = 1, 2, \ldots, n \), where \( \Delta_i \) is the principal minor of \( -B \) formed from the first \( i \) rows and columns of \( -B \).

(g) \( \tau < 0 \) if and only if \( -B^{-1} > 0 \).

9.45. An ML-matrix \( B \) is irreducible if and only if \( e^{Bt} > 0 \) for all \( t > 0 \) (see Section 19.6 for matrix exponentials). In this case

\[ e^{Bt} = e^{\mu t} wv' + O(e^{\lambda t}) \]
elementwise as $t \to \infty$, where $w$ and $v'$ are the positive right and left eigenvectors of $B$ corresponding to the dominant eigenvalue $\rho$ of $B$, normed so that $v'w = 1$, and having $t_1 < \rho$.

**Proofs.** Section 9.4.3.

9.43. Choose $\alpha = \max_i |b_{ii}|$.


### 9.4.4 Perron Matrix

**Definition 9.13.** An $n \times n$ matrix $A$ is said to be a Perron matrix (polynomially positive matrix) if $f(A) > 0$ for some polynomial $f$ with real coefficients. A matrix $A$ is called a *power-positive matrix* if $A^k > 0$ for some positive integer $k$.

9.46. If $A$ is an irreducible ML-matrix, then it is is a Perron matrix. Also $B = -A$ is a Perron matrix.

9.47. If $A \geq 0$ is irreducible, then $f(A) = \sum_{i=1}^{n} A^i > 0$ and $A$ is a Perron matrix.

9.48. A power-positive matrix is a Perron matrix. Setting $k = 1$, we see that this includes positive matrices.

9.49. If $A$ is a Perron matrix, then there exists an eigenvalue $\tau$ such that:

(a) $\tau$ is real.

(b) With $\tau$ can be associated strictly positive left and right eigenvectors, which are unique to constant multiples.

(c) $\tau$ is a simple root of the characteristic equation of $A$.

9.50. Let $A$ be a Perron matrix with $\tau$ defined above, and let adj denote an adjoint matrix.

(a) (i) $\min_i \sum_j a_{ij} \leq \tau \leq \max_i \sum_j a_{ij}$

(ii) $\min_j \sum_i a_{ij} \leq \tau \leq \max_j \sum_i a_{ij}$.

(b) Either $\text{adj}(\tau I_n - A) > 0$ or $-\text{adj}(\tau I_n - A) > 0$.

(c) If $Ax \leq cx$ for some nonzero $x \geq 0$ and scalar $c$, then $c \geq \tau$; $c = \tau$ if and only if $Ax = cx$.

**Proofs.** Section 9.4.4.

9.46. From Definition 9.12 we see that $A$ can be written in the form $T - \alpha I_n$, $\alpha > 0$, where $T$ is non-negative and primitive, so that for some positive integer $k$, $(A + \alpha I_n)^k > 0$, which is a real polynomial.


9.48. Set $f(x) = x^k$.


9.4.5 Decomposable Matrix

Definition 9.14. An square matrix $A$ is called partly decomposable if there exist permutation matrices $\Pi_1$ and $\Pi_2$ such that

$$\Pi_1 A \Pi_2 = \begin{pmatrix} B_{11} & 0 \\ B_{12} & B_{22} \end{pmatrix},$$

where $B_{11}$ and $B_{22}$ are square matrices. A matrix is said to be fully indecomposable if it is not partly decomposable. Clearly an irreducible matrix is also fully indecomposable, but not necessarily vice versa. A major role of indecomposability is in investigating the combinatorial properties of non-negative matrices.

9.51. If $A \geq 0$ is $n \times n$ and fully indecomposable, then $A^{n-1} > 0$.

9.52. If $A$ and $B$ are non-negative $n \times n$ fully indecomposable matrices, then so is $AB$. (This result is not necessarily true for irreducible matrices.)

Proofs. Section 9.4.5.


9.5 LESLIE MATRIX

Definition 9.15. A $k \times k$ Leslie matrix for population growth in animal or human populations is a matrix $A$ of the form

$$A = \begin{pmatrix} f_1 & f_2 & f_3 & \cdots & f_{k-1} & f_k \\ p_1 & 0 & 0 & \cdots & 0 & 0 \\ 0 & p_2 & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & p_{k-1} & 0 \end{pmatrix},$$

where, for $i = 1, 2, \ldots, k$, $f_i$ is the average number of daughters born to a single female during the time she is in age class $i$, and $p_i$ is the proportion of females in the $i$th age class expected to survive and pass into the next age class. (Some authors start the sequences with $f_0$ and $p_0$.) These fertility and survival rates are said to be age-specific. Here each $f_i \geq 0$ and $0 < p_i \leq 1$, so that $A \geq 0$. In some cases $i$ may refer to a state (stage) rather than age class, and the model is then stage-specific.

The matrix $A$, and those like it that describe population growth, are sometimes called population projection matrices. Typically, they will contain further non-negative elements such as down the diagonal.

9.53. Let $n(t) = (n_1(t), n_2(t), \ldots, n_k(t))'$, where $n_i(t)$ is the number of females in the $i$th age class at time $t$ ($t$ a positive integer). Then

$$n(t) = An(t - 1) = A'n(0),$$
where $A$ is a population projection matrix. The case when $A$ is singular and we require $n(t - 1)$ from $n(t)$ is considered by Campbell and Meyer [1979: 184–187].

9.54. A sufficient condition for the Leslie matrix $A$ to be primitive is that two consecutive $f_i$'s, say $f_j$ and $f_{j+1}$, are positive.

9.55. Suppose $A$ is primitive (i.e., $A^p > 0$ for some positive integer $p$). In fact, most population projection matrices are primitive, and the only significant exceptions are age-classified matrices with a single reproductive age class (Caswell [2001: 81]).

(a) By (9.30g), there is a positive dominant eigenvalue $\rho$ that is simple with $|\lambda| < \rho$ for every eigenvalue $\lambda$ different from $\rho$.

(b) Setting $x_1 = 1$ and successfully solving $Ax = \rho x$ using the second through to the $k$th rows, a positive right eigenvector corresponding to $\rho$ is

$$x = (1, p_1 \rho^{-1}, p_1 p_2 \rho^{-2}, \ldots, p_1 p_2 \cdots p_{k-1} \rho^{-(k-1)})'.$$

(c) Let $y$ be the positive left eigenvector corresponding to $\rho$ and scaled so that $x'y = 1$. Then, from (9.28),

$$\lim_{t \to \infty} \frac{A^t}{\rho^t} n(0) = xy'n(0) = kx, \text{ say.}$$

Thus for large $t$, $n(t) = A^n(0) \approx \rho^t kx$, and $n(t) \approx \rho n(t - 1)$.

(d) If $n(t) = kx$, then

$$n(t + 1) = An(t) = kAx = k\rho x,$$

and a population with age distribution determined by $x$ is said to have a stable age distribution as the age structure remains unchanged. According to (c), we see that as $t \to \infty$ the age distribution tends to the stable age distribution irrespective of the starting age distribution. Once the population reaches the stable age distribution, it increases, decreases, or remains constant in size depending on whether $\rho > 1$, $\rho < 1$, or $\rho = 1$. When $\rho = 1$, the population is said to be stationary. Also, $r = \ln \rho$ is called the intrinsic rate of increase.

9.56. (Diffusion Model) Suppose we have two identical patches of organisms coupled by diffusion. Suppose there are $s$ stages and that the within-patch demography is described by the population projection matrix $A$. Let $D = \text{diag}(d_1, d_2, \ldots, d_s)$ be an $s \times s$ diffusion matrix, where $d_i$ is the probability that an individual in stage $i$ leaves its patch to go to the other patch. If $n_i(t)$ is the stage abundance vector in patch $i$, then

$$\begin{pmatrix} n_1(t + 1) \\ n_2(t + 1) \end{pmatrix} = \begin{pmatrix} I_s - D & D \\ D & I_s - D \end{pmatrix} \begin{pmatrix} A & 0 \\ 0 & A \end{pmatrix} \begin{pmatrix} n_1(t) \\ n_2(t) \end{pmatrix}$$

$$= (K \otimes DA + I_s \otimes A) \begin{pmatrix} n_1(t) \\ n_2(t) \end{pmatrix}, \quad K = \begin{pmatrix} -1 & 1 \\ 1 & -1 \end{pmatrix}$$

$$= B \begin{pmatrix} n_1(t) \\ n_2(t) \end{pmatrix},$$
where $B \geq 0$ and "⊗" is the Kronecker product. For a general modeling method for patches and stages, see Hunter and Caswell [2005].

An important application of the above theory is the life cycle graph described, for example, by Caswell [2001: chapter 4], where a matrix like $A$ or $B$ is constructed from the graph. A life cycle can also be described as an absorbing finite-state Markov chain, which involves a transition matrix (described below). Caswell [2006] discussed this demographic role of Markov chains in ecology.

Proofs. Section 9.5.

9.54. Demetrius [1971].


9.6 STOCHASTIC MATRICES

9.6.1 Basic Properties

Definition 9.16. A non-negative matrix with each of its row sums equal to 1 is called a (row) stochastic matrix. A common application is the transition matrix of a finite (discrete time) Markov chain in which the $i, j$th element of the matrix is the probability of going from state $i$ to state $j$. In what follows, $P$ is an $n \times n$ stochastic matrix with $P1_n = 1_n$. When the Markov chain is homogeneous, we are interested in powers $P^k$ of $P$. For example, if $p_{i0}$ is the probability that the Markov chain is initially in state $i$, then $p_{(0)} = (p_{10}, p_{20}, \ldots, p_{n0})'$ is the initial probability distribution; after $k$ transitions, the corresponding probability distribution is $p_{(k)}$, where $p_{(k)} = p_{(0)} P^k$. If, as $k \to \infty$, $p_{(k)}$ tends to a limit that does not depend on the initial probability distribution, we say that the process has the ergodic property. Ergodicity and the so-called coefficient of ergodicity play an important role in more general processes such as inhomogeneous Markov processes and products of inhomogeneous non-negative matrices (cf. Seneta [1981].) The matrix $I - P$ is called the Markovian kernel of the chain, and it has a useful group inverse as well as the usual weak inverse.

If $p_{(0)}$ is such that $p_{(k)} = p_{(0)}$ for all $k$, we say that $p_{(0)}$ is stationary, and a Markov chain with such an initial distribution is said to be stationary. We shall denote this stationary distribution by $\pi$, where (setting $k = 1$) $\pi'P = \pi'$ and $\pi'1_n = 1$.

9.57. If $P = (p_{ij})$ is a stochastic matrix and $p = \min_i (p_{ii})$, then any eigenvalue $\lambda_j$ of $P$ satisfies $|\lambda_j - p| \leq 1 - p$. If $p_{ii}$ and $p_{jj}$ are the smallest main diagonal elements, then all the eigenvalues of $P$ lie in the interior or on the boundary of the oval

$$|x - p_{ii}||x - p_{jj}| \leq (1 - p_{ii})(1 - p_{jj}).$$

9.58. A stochastic matrix $P$ is irreducible and aperiodic if and only if $P^k > 0$ for some positive integer $k$—that is, if and only if $P$ is primitive.

9.59. If $P$ is a stochastic matrix, then so is $P^m$ for any positive integer $m$. 
9.60. For any stochastic matrix $P$,

$$\lim_{k \to \infty} \frac{1}{k} (I_n + P + P^2 + \cdots + P^{k-1}) = R,$$

where $R$ is stochastic and $RP = PR = R = R^2$.

**Proofs.** Section 9.6.1.

9.57. Quoted by Marcus and Minc [1964: 161].


9.59. $P^m 1_n = P^{m-1} 1_n = \cdots = 1_n$.

9.60. Bapat and Raghavan [1997: 50].

### 9.6.2 Finite Homogeneous Markov Chain

There is a substantial literature on Markov chains, for example, Hunter [1983b], and more recently, Ching [2006], Hernández and Lasserre [2003], and Norris [1997], so that I shall consider just some basic results in this section.

9.61. Suppose $P$, the $n \times n$ transition matrix of a finite Markov chain, is irreducible.

(a) Since $P 1_n = 1_n$, $P$ has an eigenvalue equal to 1. However, since the row sums are all equal, it follows from (9.9b(iii)) that $\rho = 1$ with a positive right eigenvector of $1_n$. If $q$ is a positive left eigenvector (i.e., $q'P = q'$), we can scale $q$ such that $q' 1_n = 1$; thus $q$ represents a probability distribution.

(b) $q'P^k = q'P^{k-1} = \cdots = q'$.

(c) The irreducible Markov chain has a unique stationary distribution $\pi$, the solution of $\pi'P = \pi'$ and $\pi' 1_n = 1$. We can identify $\pi$ with $q$ of (a).

9.62. Suppose that the $n \times n$ transition matrix $P$ is irreducible with stationary distribution $\pi$. Then:

(a) If $t$ and $u$ are any $n \times 1$ vectors, then $(I_n - P + tu')$ is nonsingular if and only if $\pi't \neq 0$ and $u'1_n \neq 0$. If the latter conditions hold, then $(I_n - P + tu')^{-1}$ is a weak inverse of $I_n - P$. Furthermore, any weak inverse can be expressed in the form

$$(I_n - P + tu')^{-1} + 1_n f' + g\pi',$$

where $f$ and $g$ are arbitrary vectors.

(b) $A^+ = (I_n - P + \pi 1_n)'^{-1} + \frac{1_n \pi'}{n \pi' \pi}$.

In addition to the above weak and Moore–Penrose inverses, Hunter [1988] gives expressions for other types of generalized inverses. For further results see Hunter [1990, 1992].

9.63. Suppose $P$ is a primitive stochastic matrix (i.e., irreducible and aperiodic). Using the above notation, we have the following special case of (9.28).
(a) $\lim_{k \to \infty} P^k = 1_n \pi' (= Q_0$, say), where $\pi$ is the unique stationary distribution.

(b) If $p$ is a probability distribution (i.e., $p'1_n = 1$), then $\lim_{k \to \infty} p'P^k = p'1_n \pi' = \pi'$.

(c) $Q_0$ is idempotent.

(d) $PQ_0^n = Q_0P^m = Q_0$ for all integers $m \geq 1$.

(e) $Q_0(P - Q_0) = 0$.

(f) Every nonzero eigenvalue of $P - Q_0$ is also an eigenvalue of $P$.

9.64. Suppose that a general stochastic matrix $P$ is expressed in the canonical form of (9.19), where $Q \neq 0$. Here $Q$ refers to the submatrix of $P$ associated with transitions between the inessential states, and $P$ is reducible.

(a) $Q^k \to 0$ elementwise and geometrically fast as $k \to \infty$.

(b) $(I_n - Q)^{-1}$ exists. In finite absorbing chains, this matrix is sometimes called the fundamental matrix of absorbing chains.

Definition 9.17. An $n \times n$ stochastic matrix $P$ is said to be regular if its essential indices form a single class that is aperiodic. In this case $P$ can be expressed in the canonical form (cf. 9.19)

$$P = \begin{pmatrix} P_1 & 0 \\ R & Q \end{pmatrix},$$

where $P_1$ is a stochastic irreducible aperiodic (primitive) matrix.

9.65. Suppose $P$ is regular with canonical form described above. Let $q_1$ be the unique stationary distribution of $P_1$, and define $q' = (q_1, 0')$ to be an $1 \times n$ vector. Then, as $k \to \infty$,

$$P^k \to 1_n q'$$
elementwise, where $q'$ is the unique stationary distribution corresponding to the matrix $P$, the approach to the limit being geometrically fast. Thus the regularity of $P$ is a sufficient condition for ergodicity; it is also a necessary condition.

9.66. If an $n$-state homogeneous Markov chain contains at least two essential classes, then any weighted linear combination of the stationary distribution vectors corresponding to each class, each appropriately augmented by zeros to give an $n \times 1$ vector, is a stationary distribution of the chain.

Proofs. Section 9.6.2.


9.6.3 Countably Infinite Stochastic Matrix

In this section we consider a stochastic matrix with a countable (i.e., finite or denumerably infinite) index set \( \{1, 2, \ldots\} \), with our focus on the infinite case. The matrix \( P = (p_{ij}) \) will still represent a stochastic matrix, but with infinite row sums adding to unity. As matrix multiplication readily extends to infinite matrices, \( P^k = (p_{ij}^{(k)}) \) is well-defined for \( k = 1, 2, \ldots \), and it is also stochastic (Seneta [1981: chapter 5]). However, a more sensitive classification of indices is now required.

**Definition 9.18.** Let

\[
l_{ij}^{(1)} = p_{ij} \quad \text{and} \quad l_{ij}^{(k+1)} = \sum_{r \neq i} l_{ir}^{(k)} p_{rj}, \quad k = 1, 2, \ldots,
\]

with \( l_{ij}^{(0)} = 0 \), by definition, for all \( i, j \in \{1, 2, \ldots\} \). Define, for each \( i \) and \( j \),

\[
L_{ij} = \sum_{k=0}^{\infty} l_{ij}^{(k)} \quad \text{and} \quad \mu_i = \sum_{k=1}^{\infty} k l_{ii}^{(k)} \leq \infty.
\]

An index \( i \) (or state \( i \)) is said to be **recurrent** if \( L_{ii} = 1 \) and **transient** if \( L_{ii} < 1 \). A recurrent index \( i \) is said to be **positive- or null-recurrent** depending on whether \( \mu_i < \infty \) or \( \mu_i = \infty \), respectively. Here \( \mu_i \) is called the **mean recurrence measure** of \( i \). Note that in the Markov chain context, \( l_{ij}^{(k)} \) is the probability of going from state \( i \) to state \( j \) in \( k \) steps (or in time \( k \)), without revisiting \( i \) in the meantime. Thus \( L_{ii} \) can be regarded as the probability of staying in or returning to state \( i \) for the first time. Also \( \mu_i \) is the **mean recurrence time** of state \( i \). Thus a state \( i \) is recurrent if, starting from state \( i \), we will eventually return to state \( i \) with certainty. If state \( i \) is transient, then there is a positive probability that the system will never return to state \( i \).

**9.6.7.** An inessential index is transient and a recurrent index is essential.

**9.6.8.** If \( i \) is a recurrent aperiodic index and \( j \) is any index such that \( j \to i \) (cf. second part of Definition 9.5 in Section 9.4.1), then

\[
\lim_{k \to \infty} p_{ij}^{(k)} = \mu_i^{-1} L_{ij}.
\]

In particular

\[
\lim_{k \to \infty} p_{ii}^{(k)} = \mu_i^{-1}.
\]

**Proofs.** Section 9.6.3.


**9.6.4 Infinite Irreducible Stochastic Matrix**

The definition of irreducibility given by Definition 9.6 (second definition) applies to infinite matrices; that is, \( A \geq 0 \) is irreducible if and only if every pair of indices \( i \) and \( j \) communicate.
9.69. The following hold for an infinite irreducible stochastic matrix.

(a) Every index has the same period.

(b) The indices are all transient, or all null-recurrent, or all positive-recurrent.

**Definition 9.19.** In the light of (9.69) we say that an irreducible $P$ is a transient, or null-recurrent, or positive-recurrent matrix depending on whether any one of its indices is transient, or null-recurrent, or positive-recurrent.

If $v'P = v'$ and $v$ is a nonzero non-negative (countably infinite) vector, we call $v$ an invariant measure. Note that a multiple of such a measure is still a measure.

9.70. (General Ergodic Theorem) We have the following series of limits.

(a) Let $P$ be a primitive (i.e., irreducible and aperiodic) stochastic matrix. If $P$ is transient or null-recurrent, then for any pair of indices $i, j$, we have $p_{ij}^{(k)} \to 0$ as $k \to \infty$. If $P$ is positive-recurrent,

$$\lim_{k \to \infty} p_{ij}^{(k)} = \mu_j^{-1},$$

and the vector $x = (\mu_i^{-1})$ is the unique stationary distribution (invariant vector) satisfying $x'P = x'$ and $\sum_{i=1}^{\infty} x_i = 1$. The question of computing a finite dimensional approximation for $x$ is discussed by Seneta [1981: section 7.2].

(b) If $P$ is irreducible and periodic with period $d$, then

$$\lim_{k \to \infty} p_{ii}^{(dk)} = d/\mu_i.$$

9.71. If $P$ is an irreducible transient or null-recurrent matrix, then there exists no invariant measure $v'$ satisfying $v'1 < \infty$.

**Proofs.** Section 9.6.4.


9.70. Seneta [1981: 177 for (a); 196, exercise 5.1, for (b)].


9.7 DOUBLY STOCHASTIC MATRICES

**Definition 9.20.** A square $n \times n$ matrix $A = (a_{ij})$ is doubly stochastic if $A \geq 0$ and all its column sums and row sums are 1. Some examples of doubly stochastic matrices are given by Marshall and Olkin [1979: 45–48]. For a reference to doubly stochastic matrices see Bapat and Raghavan [1997: chapter 2].

**Definition 9.21.** The diagonal of a matrix $A$ associated with the permutation $\pi$ is the set $\{a_{1\pi(1)}, a_{2\pi(2)}, \ldots, a_{n\pi(1)}\}$, and the corresponding diagonal product is $\prod_{i=1}^{n} a_{i\pi(i)}$. A diagonal is said to be positive if each element $a_{i\pi(i)}$ in the diagonal is positive.
**Definition 9.22.** The matrix \( A \) is said to have a *doubly stochastic pattern* if there exists a doubly stochastic matrix with the same pattern of zeros as \( A \).

9.72. A doubly stochastic matrix has a positive diagonal. An algorithm for finding such a diagonal is also available.

9.73. Let \( A = (a_{ij}) \) be an \( n \times n \) doubly stochastic matrix, and let \( y_1 \geq y_2 \geq \cdots \geq y_n \). Then

\[
\sum_{i=1}^{k} y_i \geq \sum_{i=1}^{k} \sum_{j=1}^{n} a_{ij} y_j, \quad k = 1, 2, \ldots, n.
\]

9.74. The product of a finite number of doubly stochastic matrices is doubly stochastic.

9.75. If \( n \times n \) \( A \) is doubly stochastic and nonsingular, then \( A^{-1} \) has row and column sums equal to 1, but it need not have non-negative elements.

9.76. If \( A \geq 0 \) is an \( n \times n \) matrix with row totals and column totals not exceeding unity, then there exists a doubly stochastic \( n \times n \) matrix \( B \) such that \( B \geq A \).

9.77. (Scaling) If \( A \) is a non-negative \( n \times n \) matrix with doubly stochastic pattern, then there exist diagonal matrices \( D_1 \) and \( D_2 \) with positive diagonal elements such that \( C = D_1 A D_2 \) is doubly stochastic.

9.78. If \( A \) is non-negative definite and doubly stochastic and has \( a_{ii} \leq 1/(n - 1) \) for each \( i \), then the non-negative definite square root \( A^{1/2} \) (cf. 10.8) is doubly stochastic.

9.79. Every permutation matrix is a doubly stochastic matrix, because there is a single 1 in every row and column and the remaining elements are zero.

9.80. (Birkhoff–von Neumann) A matrix is doubly stochastic if and only if it is a convex combination of the permutation matrices.

9.81. The set of doubly stochastic matrices is the convex hull of all \( n \times n \) permutation matrices (of which there are \( n \)), and the latter constitute the extreme points of this set.

9.82. Let \( A = (a_{ij}) \) be a doubly stochastic \( n \times n \) matrix.

(a) The permanent (cf. Section 4.5) of \( A \) is positive.

(b) \( \text{per}(A) \geq \frac{n^n}{n^n} \),

with equality if and only if \( a_{ij} = n^{-1} \) for all \( i, j \).

9.83. The matrix \( (a_{ij}) = (n^{-1}) \) is the unique irreducible idempotent \( n \times n \) doubly stochastic matrix.

9.84. If \( T = (t_{ij}) \) is a real orthogonal matrix, then \( A = (t_{ij}^2) \) is doubly stochastic.

9.85. If \( A \geq 0 \) is \( n \times n \) \( (A \neq 0) \), then \( A \) has a doubly stochastic pattern if and only if every positive entry of \( A \) is contained in a positive diagonal.
**Definition 9.23.** A matrix $A = (a_{ij})$ is said to be orthostochastic if there exists an orthogonal matrix $T$ such that $a_{ij} = t_{ij}^2$. If there exists a unitary matrix $U = (u_{ij})$ such that $a_{ij} = |u_{ij}|^2$, then $A$ is said to be unitary-stochastic (Marshall and Olkin [1979: 23]).

**Definition 9.24.** A square matrix $A$ is said to be doubly substochastic if $A \geq 0$ and all row and column sums are at most 1.

9.86. The set of all $n \times n$ doubly substochastic matrices is a convex set.

9.87. From the definition we have that any square submatrix of a doubly substochastic matrix is doubly substochastic.

9.88. If $A = (a_{ij})$ is doubly substochastic, then there exists a doubly stochastic matrix $B = (b_{ij})$ such that $a_{ij} \leq b_{ij}$ for all $i, j$.

9.89. If $A = (a_{ij})$ and $B = (b_{ij})$ are doubly substochastic, then their Hadamard (Schur) product $A \circ B = (a_{ij}b_{ij})$ is doubly substochastic.

**Proofs.** Section 9.7.


9.73. Anderson [2003: 646].


9.75. $A1_n = 1_n$ implies $1_n = A^{-1}1_n$, and $A'1_n = 1_n$ implies $1_n = A^{-1}'1_n$.


9.84. Follows from the fact that the rows and columns of an orthogonal matrix each have unit length.


9.86. Follows immediately from the idea of a convex combination.


9.89. Since $b_{ij} \leq 1$, $a_{ij}b_{ij} \leq a_{ij}$. 
CHAPTER 10

POSITIVE DEFINITE AND NON-NEGATIVE DEFINITE MATRICES

Quadratic forms that are non-negative definite play an important role in statistical theory, particularly those related to chi-square distributions. They can also be used for establishing a wide variety of inequalities, such as those in Chapter 12.

10.1 INTRODUCTION

Definition 10.1. Let $A$ be an $n \times n$ Hermitian matrix, and let $x \in \mathbb{C}^n$. Then $x^*Ax$ is said to be a Hermitian non-negative definite (n.n.d.) quadratic form if $x^*Ax \geq 0$ for all $x$. If $x^*Ax$ is Hermitian n.n.d. we say that $A$ is Hermitian n.n.d. and we write $A \succeq 0$. (Some authors use the term positive semi-definite instead of n.n.d. We reserve the former for the following definition.)

If $A$ is Hermitian and n.n.d., and there exists $x, x \neq 0$ such that $x^*Ax = 0$, we say that $A$ is Hermitian positive semidefinite or positive indefinite. An alternative definition is that $A$ is n.n.d. and $\det A = 0$.

If $x^*Ax > 0$ for all $x \neq 0$, then we say that $A$ is Hermitian positive definite (p.d.) definite and write $A \succ 0$.

Given $n \times n$ Hermitian matrices $A$ and $B$, we say that $A \succeq B$ if $A - B \succeq 0$. Similarly we say that $A \succ B$ if $A - B \succ 0$. This is referred to as the (partial) Löwner ordering of matrices. There are many applications of Löwner ordering in statistics such as estimability and efficiency of estimation.

In most applications, $A$ is a real symmetric matrix, in which case we simply replace * by ′, assume $x \in \mathbb{R}^n$, and drop the term Hermitian in the above definitions.
and in what follows. Thus a positive definite matrix without the adjective Hermitian will always represent a real symmetric matrix. The same is true for a non-negative definite matrix.

10.1. The following matrices are all assumed to be Hermitian.

(a) \( A_1 \succeq B_1 \) and \( A_2 \succeq B_2 \) imply that \( A_1 + A_2 \succeq B_1 + B_2 \).

(b) If \( A \succeq B \) and \( B \succeq C \), then \( A \succeq C \).

(c) \( A_1 \succeq B_1 \) and \( A_2 \succeq B_2 \) do not necessarily imply that \( A_1 A_2 \succeq B_1 B_2 \), even if \( A_1 A_2 \) and \( B_1 B_2 \) are Hermitian. Thus \( A \succeq B \) does not necessarily imply that \( A^2 \succeq B^2 \).

Proofs. Section 10.1.

10.1a. Consider the corresponding quadratics.

10.1b. \( x^*(A - C)x = x^*(A - B + B - C)x = x^*(A - B)x + x^*(B - C)x \geq 0 \).

10.2 NON-NEGATIVE DEFINITE MATRICES

10.2.1 Some General Properties

In this section we assume that \( A \) is a Hermitian \( n \times n \) matrix, unless otherwise stated. The results hold for a real symmetric matrix if we replace * by '.

10.2. \( A \succeq 0 \) if and only if all its eigenvalues are real and non-negative .

10.3. If \( A \succeq 0 \), then from (10.2), \( \det A = \prod_i \lambda_i \geq 0 \).

10.4. If \( A \succeq 0 \), then \( \text{trace} A = \sum_i \lambda_i \geq 0 \).

10.5. Given \( A \succeq 0 \), then any principal submatrix of \( A \), including \( A \) itself, is non-negative definite. In particular, the diagonal elements of \( A \) are non-negative.

10.6. \( A \succeq 0 \) if and only if all principal minors (including \( A \) itself) of \( A \), and not just the leading ones, are non-negative. Note that \( A = \begin{pmatrix} 0 & 0 \\ 0 & -1 \end{pmatrix} \) has non-negative leading principal minors including \( A \) itself, but it is not non-negative definite.

10.7. (Fejer) \( A \succeq 0 \) if and only if

\[
\sum_{i=1}^{n} \sum_{j=1}^{n} a_{ij} b_{ij} \geq 0
\]

for all \( n \times n \) non-negative definite matrices \( B = (b_{ij}) \).

10.8. If \( A \succeq 0 \) and \( k \) is a positive integer, there exists a unique non-negative definite matrix \( A^{1/k} \succeq 0 \) such that \( (A^{1/k})^k = A \). In particular, if \( A = U \Lambda U^* \), where \( \Lambda = \text{diag}(\lambda_1, \ldots, \lambda_n) \) and the \( \lambda_i \) are the non-negative eigenvalues of \( A \), then \( A^{1/k} = U \Lambda^{1/k} U^* \), where \( \Lambda^{1/k} = \text{diag}(\lambda_1^{1/k}, \ldots, \lambda_n^{1/k}) \). The case \( k = 2 \) arises frequently in statistics. We note the following.
(a) $A$ and $A^{1/k}$ commute.
(b) The eigenvalues of $A^{1/k}$ are the $k$th roots of those of $A$.
(c) $\text{rank } A = \text{rank}(A^{1/k})$.
(d) If $A$ is real, then so is $A^{1/k}$.
(e) For $k = 2$ and $A$ real, another way of deriving $A^{1/2}$ is to obtain the Cholesky decomposition $A = RR'$. Then, if $R = \Sigma \Sigma'Q'$ is the singular value decomposition of $R$, we have $A^{1/2} = \Sigma \Sigma'P'$ as $(A^{1/2})^2 = \Sigma \Sigma'P' = RR'$.
(f) If $A > 0$, then $(A^{-1})^{1/2} = (A^{1/2})^{-1}$.

10.9. If $A \succeq 0$, then the matrix $(a_{ij}^k)$ for $k$ a positive integer is non-negative definite.

10.10. If $A$ is of rank $r$, then $A \succeq 0$ if and only if $A = RR^*$, where $R$ is $n \times n$ of rank $r$. The result is also true if we replace $R$ by an $n \times r$ matrix of rank $r$, as we have a full-rank factorization of $A$.

10.11. $A \succeq 0$ is of rank $r$ if and only if there exists an $n \times r$ matrix $S$ of rank $r$ such that $S^*AS = I_r$.

10.12. Let $A \succeq 0$.
(a) $CAC^* \succeq 0$.
(b) If $CAC^* = 0$, then $CA = 0$; in particular, $CC^* = 0$ implies that $C = 0$.
(c) $\text{rank}(C^*AC) = \text{rank}(AC)$.

10.13. If $A \succeq 0$ and $a_{ii} = 0$, then $a_{ij} = 0$ for all $j = 1, 2, \ldots, n$. Since $A$ is Hermitian, $a_{ii} = 0$ if and only if the row and column containing $a_{ii}$ consist entirely of zeros.

10.14. If $A \succeq 0$, then $A^k \succeq 0$ for $k$ a positive integer.

10.15. If $\text{trace } A \geq \Re \text{trace}(AU)$ for all unitary matrices $U$ (i.e., $U^*U = I_n$), then $A$ is non-negative definite. (Here $\Re$ denotes "real part of.")

10.16. Let $A$ be any $m \times n$ real matrix, and let $V$ be an $m \times m$ non-negative definite matrix. If $Z$ is any matrix such that $C(Z) = N(A')$ (i.e., the columns of $Z$ span the null space of $A'$), then $C(A) \cap C(VZ) = 0$ and

$$C(A, V) = C(A, VZ) = C(A) \oplus C(VZ).$$

We can express $Z$ in the form $Z = I - (A')^{-1}A'$.

10.17. Let $A = (a_{ij}) \succeq 0$. If $f(z) = a_0 + a_1z + a_2z^2 + \ldots$ is an analytic function with non-negative coefficients and radius of convergence $R > 0$, then the matrix with $(i, j)$th elements $f(a_{ij})$ is n.n.d. if all $|a_{ij}| < R$.

10.18. We have the following results.
(a) Given the real matrix $A \succeq 0$, then

$$C(BAB') = C(BA) \quad \text{and} \quad \text{rank}(BAB') = \text{rank}(BA) = \text{rank}(AB').$$
(b) If \( \begin{pmatrix} A & B \\ B' & C \end{pmatrix} \) is n.n.d., then \( C(B) \subseteq C(A) \) and \( C(B') \subseteq C(C) \).

10.19. Let \( A \) be an \( n \times n \) real symmetric idempotent matrix, and suppose that \( \{B_1, B_2, \ldots, B_k\} \) is a set of real \( n \times n \) non-negative definite matrices such that

\[
I_n = A + \sum_{i=1}^{k} B_i.
\]

Then \( AB_i = B_iA = 0 \) for \( i = 1, 2, \ldots, k \).

**Proofs.** Section 10.2.1.

10.5. Set appropriate elements of \( x \) in \( x^*Ax \) equal to zero.
10.7. Horn and Johnson [1985: 459].
10.8. Horn and Johnson [1985: 405 for (a–d)], Golub and Van Loan [1996: 149 for (e)], and Abadir and Magnus [2005: 221 for (f)],
10.9. Horn and Johnson [1985: 461].
10.10. Seber and Lee [2003: 460, real case]. We can also choose \( R \) such that \( R^*R = A \), where \( A \) is a diagonal matrix with diagonal elements the positive eigenvalues of \( A \). (cf. Abadir and Magnus [2005: 219]).
10.14. From (10.8) with \( B = A^{1/2} \), we have \( A^k = (B^2)^k = (B^k)^2 = C^2 \), say, where \( C \) is symmetric.
10.18. Sengupta and Jammalamadaka [2003: 45, \( A \) and \( B \) interchanged in (a)].
10.2.2 Gram Matrix

**Definition 10.2.** Let \( \{v_1, v_2, \ldots, v_k\} \) be a set of \( n \) vectors in an inner product space \( V \) with inner product \( \langle \cdot, \cdot \rangle \). Then the Gram matrix of the vectors \( v_i \) is the \( k \times k \) matrix \( G = (g_{ij}) \), where \( g_{ij} = \langle v_i, v_j \rangle \).

10.20. Let \( G \) be the Gram matrix of the vectors \( \{w_1, w_2, \ldots, w_k\} \) in \( \mathbb{C}^n \) with respect to the inner product \( \langle \cdot, \cdot \rangle \), and let \( W = (w_1, w_2, \ldots, w_k) \) be an \( n \times k \) matrix.

(a) \( G \) is Hermitian non-negative definite.

(b) \( G \) is nonsingular if and only if the vectors \( w_1, \ldots, w_k \) are linearly independent.

(c) There exists a Hermitian positive definite \( n \times n \) matrix \( A \) such that

\[
G = W^*AW.
\]

(d) If \( r \) is the maximum number of linearly independent vectors in the set of vectors \( \{w_1, \ldots, w_k\} \), then \( \text{rank } G = \text{rank } W = r \).

(e) If \( \langle x, y \rangle = x^*y \), then \( A = I_n \) in (c).

**Proofs.** Section 10.2.2.


10.2.3 Doubly Non-negative Matrix

**Definition 10.3.** A (real) non-negative definite matrix that is also non-negative (i.e., \( A \geq 0 \) with non-negative elements) is referred to as doubly non-negative matrix. A square matrix \( A \) is said to be completely positive if there exists an \( n \times k \) matrix \( B \) such that \( B \geq 0 \) and \( A = BB' \). (The smallest value of \( k \) is called the cp-rank of \( A \) and its properties are considered by Berman and Shaked-Monderer [2003: chapter 3].)

Completely positive matrices arise in relation to graph theory, block designs, some maximum efficiency-robust tests, and in a Markovian model for DNA evolution (cf. Berman and Shaked-Monderer [2003: 68-70], who also give further references). The following results make full use of (10.10).

10.21. It follows immediately from the definition that \( A \) is completely positive if and only if it can be expressed in the form

\[
A = \sum_{i=1}^k b_i b_i', \quad b_i \geq 0, \quad i = 1, \ldots, k,
\]

where \( b_i \) is the \( i \)th column of \( B \).

10.22. A completely positive matrix is doubly non-negative. However, the converse is not necessarily true, except in some cases. For example, a rank 1 or rank 2 doubly non-negative matrix is completely positive.
10.23. We have the following results for completely positive matrices.

(a) The sum of completely positive matrices is completely positive.

(b) The Kronecker product of two completely positive matrices is completely positive.

(c) If $A$ is a completely positive $n \times n$ matrix, and $C$ is an $m \times n$ non-negative matrix, then $CAC'$ is completely positive. Two special cases that are of interest when $m = n$ are when $C$ is a permutation matrix, or a diagonal matrix with non-negative elements.

(d) If $A$ is completely positive, then so is $A^k$, where $k$ is a positive integer.

(e) Let $A$ and $B$ be $n \times n$ completely positive matrices with columns $a_i$ and $b_i$, respectively. Then the Hadamard product

$$A \circ B = \sum_{i=1}^{n} \sum_{j=1}^{n} (a_i \circ b_j)(a_i \circ b_j)'$$

is also completely positive.

(f) The principal submatrices of a completely positive matrix are completely positive.

10.24. If $A$ is a symmetric $n \times n$ totally non-negative matrix (i.e. every minor is positive), then $A$ is completely positive. Furthermore, since $A = BB'$, we can choose $B$ to be either a non-negative upper-triangular matrix or a non-negative lower-triangular matrix.

**Proofs.** Section 10.2.3.

10.22. Berman and Shaked-Monderer [2003: 64].

10.23a. This follows from (10.21).

10.23b. This follows from $(BB') \otimes (CC') = (B \otimes C)(B \otimes C)'$.

10.23c. Since $A = BB'$, the result follows from $CBB'C' = (CB)(BC)'$.

10.23d. The result is obvious when $k = 2l$ and follows from (c) when $k = 2l+1$.

10.23e. This follows from (10.21) and the fact that $cc'$, where $c = a_i \circ b_j$, is non-negative definite and the sum of non-negative definite matrices is non-negative.


10.3 POSITIVE DEFINITE MATRICES

In this section we assume that $A$ is a Hermitian $n \times n$ matrix, unless otherwise stated. Note that the eigenvalues of a Hermitian matrix are real.

10.25. There exists a real number $a$ such that $I_n + aA \succ 0$.

10.26. (Kato) If $A$ has no eigenvalue in the interval $[a, b]$, then $(A - aI_n)(A - bI_n) \succ 0$.

10.27. If $A = (a_{ij}) \succ 0$, then so are $A'$, $\overline{A} = (\overline{a}_{ij})$, and $A^{-1}$.

10.28. Given the inner product $\langle x, y \rangle = x^*y$, then $A \succ 0$ if and only if $A$ is the Gram matrix (cf. Section 10.2.2) of $n$ linearly independent vectors.

10.29. $A \succ 0$ if and only if all its eigenvalues are positive.

10.30. $A \succ 0$ if and only if there exists a nonsingular matrix $R$ such that $A = RR^*$.

10.31. Let $A \succ 0$, and let $C$ be $p \times n$ of rank $q \ (q \leq p)$. Then:

(a) $CAC^* \succeq 0$.

(b) $\text{rank}(CAC^*) = \text{rank}(C)$.

(c) $CAC^* \succ 0$ if $q = p$.

(d) $B^*AB = 0$ if and only if $B = 0$.

10.32. If $A \succ 0$ and $k$ is a positive integer, then, arguing as in (10.8), there exists a unique $A^{1/k} \succ 0$ such that $(A^{1/k})^k = A$. A particularly useful case is $k = 2$.

10.33. Consider the quadratic $x^*Ax$, where $A$ is Hermitian.

(a) By relabeling the elements of $x$, we see that if $A \succ 0$, then so is any matrix obtained by interchanging any rows and the corresponding columns.

(b) By setting some of the $x_i$ equal to zero, we see that the principal submatrices of $A$ are all Hermitian p.d. In particular, the diagonal elements of $A$ are all positive.

10.34. If $A \succ 0$ then, since the diagonal elements are positive, we have:

(a) (Hadamard) $0 < \det A \leq a_{11}a_{22} \cdots a_{nn}$ with equality if and only if $A$ is diagonal (see also (12.27)).

(b) $\text{trace } A > 0$.

(c) $|a_{ij}| < \sqrt{a_{ii}a_{jj}} \leq \max\{a_{ii}, a_{jj}\}, i \neq j$.

10.35. $A \succ 0$ if and only if all the leading principal minors are positive (including $\det A$).

10.36. $A \succ 0$ if and only if the principal minors in any nested sequence of $n$ principal minors are positive.
10.37. If $A > 0$, then from (10.27) we have $A^{-1} = (a^{ij}) > 0$. Furthermore:

(a) $a^{ii}a_{ii} \geq 1$.

(b) If $A$ is real and $a_{ij} < 0$ for all $i \neq j$, then $a^{ij} > 0$ for all $i, j$.

(c) Let

\[
A = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} \quad \text{and} \quad A^{-1} = B = \begin{pmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{pmatrix},
\]

where $A_{11}$ and $B_{11}$ are $m \times m$ matrices. Then the $i$th diagonal element of $A_{11}$ is greater than or equal to the $i$th diagonal element of $B_{11}$.

10.38. If $A > 0$, then $A + A^{-1} \geq 2I_n$.

10.39. If $A > 0$ is a real $n \times n$ matrix, then

\[
\log(\det A) \leq \text{trace } A - n,
\]

with equality if and only if $A = I_n$.

10.40. If $A > 0$ is a real $n \times n$ matrix, $\alpha$ a real scalar, and $a$ a real $n \times 1$ vector, then

\[
\alpha A - aa' \succeq 0 \quad \text{if and only if} \quad a'A^{-1}a \leq \alpha.
\]

10.41. If $A$ is a real symmetric matrix, then there exists a scalar $t$ such that $A + tI_n > 0$.

10.42. If $A$ is any $m \times n$ matrix of rank $r$, then, from the corresponding quadratic form, $A'A$ is Hermitian n.n.d. of rank $r$ if $r < n$ and Hermitian p.d. if $r = n$.

10.43. (Ottowski-Taussky) If $A$ is any $n \times n$ matrix such that $B = \frac{1}{2}(A + A^*) > 0$, then

\[
\det B \leq | \det A |,
\]

with equality if and only if $A$ is Hermitian.

10.44. If $A$ is an $n \times n$ real symmetric matrix that is d.d. namely, strictly row or column diagonally dominant (cf. Section 8.4) and if $a_{ii} > 0$ for all $i = 1, 2, \ldots, n$, then it follows from (8.53b) and (10.35) that $A > 0$.

**Definition 10.4.** (Hilbert Matrix) The $n \times n$ matrix $H(n) = (h_{ij})$, where $h_{ij} = 1/(i + j - 1)$, is called a Hilbert matrix of order $n$. It is well known that $H(n)$ is highly ill-conditioned (e.g., Seber and Lee [2003: 166, 372]) and has a condition number of approximately $e^{1.5n}$ for large $n$. It arises in the fitting of polynomial regression models.

10.45. The Hilbert matrix $H(n)$ is positive definite.

**Proofs.** Section 10.3.

10.25. Abadir and Magnus [2005: 218].


10.27. We have $a_{ji} = \overline{a}_{ij}$ so that $\sum\sum(a_{ij} + \overline{a}_{ij})x_i x_j$ is unchanged if we replace $a_{ij}$ by $a_{ji}$ or $\overline{a}_{ij}$. Also, if $x = Ay$, then $x' A^{-1} x = y' A y$. 


10.34b. The eigenvalues are positive so that their sum (the trace) is positive.


10.36. Permute rows and corresponding columns and note that $II'AI \succ 0$ if and only if $A \succ 0$ for the permutation matrix $II$; see Horn and Johnson [1985: 404].


10.38. This follows from $U^*(A + A^{-1})U - 2I_n = \Lambda + \Lambda^{-1} - 2I_n \succeq 0$, since $\lambda_i + \lambda_i^{-1} - 2 = (\lambda_i^{1/2} - \lambda_i^{-1/2})^2 \geq 0$.


10.40. Farebrother [1976].


10.43. Horn and Johnson [1985: 481].

10.45. This follows from the fact that if $V$ is the space of continuous functions on $[0, 1]$, with inner product

$$\langle f, g \rangle = \int_0^1 f(x)g(x) \, dx,$$

then $H(n)$ is the Gram matrix of $f_i(x) = x^{i-1}, i = 1, \ldots, n$ (Berman and Shaked-Monderer [2003: 16]).

10.4 PAIRS OF MATRICES

10.4.1 Non-negative or Positive Definite Difference

In this and subsequent sections I give a number of results for pairs of matrices. I have tried to be systematic with the consequence that some of the results overlap.

10.46. Suppose $A$ and $B$ are Hermitian $n \times n$ matrices.

(a) $A \succeq B$ if and only if $R^*AR \succeq R^*BR$ for nonsingular $R$. 
(b) Let $S$ be any $n \times m$ matrix, then:

(i) $A \succeq B$ implies that $S^*AS \succeq S^*BS$.

(ii) If $m \leq n$ and rank $S = m$, then $A \succ B$ implies $S^*AS \succ S^*BS$.

10.47. Let $A$ and $B$ be $n \times n$ Hermitian matrices.

(a) If $A \succeq B$, then the following hold.

(i) $\lambda_i(A) \geq \lambda_i(B)$, where in each case the $\lambda_i$ are ordered $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_n$.

(ii) From (i) and (6.17b) we have $\text{trace } A \geq \text{trace } B$.

(iii) From (i) and (6.17a) we have $\|A\|_F \geq \|B\|_F$, where $\|\cdot\|_F$ is the Frobenius norm.

(iv) If $A \succ B$, then the above inequalities are strict.

(b) If $\lambda_i(A) \geq \lambda_i(B)$ for each $i$, then there exists a unitary matrix $U$ such that $U^*AU \succeq B$.

10.48. Let $A$ and $B$ be Hermitian non-negative $n \times n$ matrices. If $A \succeq B$, then the following hold.

(a) $\text{rank } A \geq \text{rank } B$.

(b) $\det A \geq \det B$.

(c) $A^{1/2} \succeq B^{1/2}$ (cf. 10.8).

(d) $\text{trace } A \geq \text{trace } B$.

(e) It is not true in general that $A^2 \succeq B^2$.

(f) Suppose $A$ and $B$ commute, then $A^k \succeq B^k$ for $k = 2, 3, \ldots$.

10.49. Suppose $A$ and $B$ are Hermitian $n \times n$ matrices. If $B \succ 0$ and $A \succeq B$, then:

(a) $A = A - B + B + O$.

(b) If $A_r$ is a principal submatrix of $A$ of order $r$ and $B_r$ is the corresponding submatrix of $B$, then $A_r \succeq B_r$.

10.50. Let $B \succ 0$ be Hermitian and $A$ be Hermitian n.n.d. (respectively p.d.).

(a) The eigenvalues of $AB^{-1}$, namely the roots of $\det(A - \lambda B) = 0$, are real and non-negative (respectively positive) because they are the same as those of $B^{-1/2}AB^{-1/2}$, which is n.n.d. (respectively p.d.)

(b) $B - A$ is n.n.d. (respectively p.d.) if and only if the eigenvalues $\lambda_i$ of $AB^{-1}$ all satisfy $\lambda_i \leq 1$ (respectively $\lambda_i < 1$).

10.51. Let $A$ and $B$ be $n \times n$ Hermitian p.d. matrices. Then:

(a) $A \succeq B$ if and only if $B^{-1} \succeq A^{-1}$. 
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(b) \( A \succ B \) if and only if \( B^{-1} \succ A^{-1} \).

(c) If \( A \succeq B \), then \( \lambda_{i}(A) \geq \lambda_{i}(B) > 0 \) (cf. 10.47a(i)).

(d) If \( A \succeq B \), then, from (c), trace \( A \geq \) trace \( B \) and (from 6.17c) \( \det A \geq \det B \). Equality occurs in each case if and only if \( A = B \).

10.52. Let \( A \) and \( B \) be \( n \times n \) real n.n.d. matrices.

(a) The following two statements are equivalent:

(1) \( A \succeq B \).

(2) \( C(B) \subseteq C(A) \) and \( \lambda_{\max}(BA^{-}) \leq 1 \), where \( \lambda_{\max}(BA^{-}) \) is independent of the choice of weak inverse \( A^{-} \). For example, we can choose \( A^{+} \), the Moore–Penrose inverse.

(b) If \( A \succeq B \succeq 0 \), then \( B^{+} \succ A^{+} \) if and only if \( C(A) = C(B) \).

10.53. If \( A \) and \( B \) are real symmetric \( n \times n \) nonsingular matrices and \( A \succ B \), then \( B^{-1} \succ A^{-1} \).

10.54. Given real \( n \times n \) matrices \( A \succ 0 \) and symmetric \( B = (b_{ij}) \), then \( A - B \succ 0 \) provided that the \( |b_{ij}| \) are all sufficiently small. In particular, \( A - tB \succ 0 \) for \( |t| \) sufficiently small. Similarly, for sufficiently small positive \( t \), \( A + tB \succeq 0 \).

10.55. (Regression) Let \( V \succ 0 \) be \( n \times n \), and let \( X \) be an \( n \times p \) matrix of rank \( p \). Then:

(a) \( V \succeq X(X'V^{-1}X)^{-1}X' \).

(b) \( X'VX \succeq (X'V^{-1}X)^{-1} \) for any \( X \) such that \( X'X = I_{p} \).

Proofs. Section 10.4.1.

10.46. Horn and Johnson [1985: 470]. We have \( x^{*}RARx = y^{*}Ay \) and \( x = 0 \) if and only if \( y = 0 \).

10.47a(i). Horn and Johnson [1985: 182, with \( A \) and \( B \) relabeled, \( B \) becoming \( A - B \succeq 0 \), and eigenvalues in the reverse order] and Zhang [1999: 227].


10.48. Abadir and Magnus [2005: 332, for (c), (e), and (f)] and Zhang [1999: 169–170, for (a)–(d)].

10.49a. We have \( x^{*}(A - B)x + x^{*}Bx \geq x^{*}Bx > 0 \).

10.49b. This follows by appropriately choosing \( x \) in \( x^{*}(A - B)x \).

10.50. Dhrymes [2000: 86–89, real case] and Horn and Johnson [1985: 471, with \( A \) and \( B \) interchanged].


10.52. Liski and Puntanen [1989].


10.4.2 One or More Non-negative Definite Matrices

In this section we consider a number of inequalities for non-negative definite matrices. For further such inequalities, the reader should refer to Chapter 12, and to Chapter 6 for those relating to eigenvalues.

10.56. Suppose \( A \) and \( B \) are \( n \times n \) Hermitian matrices with \( B \succeq 0 \).

(a) \( \lambda_i(A + B) \geq \lambda_i(A) \), \( i = 1, 2, \ldots, n \), where \( \lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_n \) are the (real) ordered eigenvalues of the particular matrix. If \( B \succ 0 \), then the inequality is strict.

(b) From (a) we have \( \text{trace}(A + B) \geq \text{trace } A \).

(c) \( \|A + B\|_F \geq \|A\|_F \), where \( \| \cdot \|_F \) is the Frobenius norm.

10.57. Let \( A \) and \( B \) be \( n \times n \) Hermitian matrices.

(a) The eigenvalues of \( AB \) are real if either \( A \) or \( B \) is Hermitian non-negative definite.

(b) If \( B \succ 0 \), then the roots of \( \det(A - \lambda B) = 0 \) are real.

10.58. Let \( A \succ 0 \) and \( B \succeq 0 \) be \( n \times n \) Hermitian matrices. Then:

(a) \( A + B \succeq 0 \).

(b) \( \det(A + B) \geq \det A \) with equality if and only if \( B = 0 \).

(c) If \( A - B \succ 0 \), then \( \det(A - B) < \det A \).

10.59. Suppose \( A \succeq 0 \) and \( B \succeq 0 \) are Hermitian \( n \times n \) matrices.

(a) The eigenvalues of \( AB \) are non-negative.

(b) \( \text{trace}(AB) \leq \text{trace } A \text{ trace } B \).

(c) \( \det(A + B) \geq \det A + \det B \) with equality if and only if \( A + B \) is singular or \( A = 0 \) or \( B = 0 \).

(d) \( \frac{1}{4}(A^{-1} + B^{-1}) \succeq (A + B)^{-1} \) if \( A \) and \( B \) are nonsingular, with equality if and only if \( A = B \).

10.60. Given a real symmetric matrix \( A \succ 0 \) and real skew-symmetric \( B \) (i.e., \( B' = -B \)), then \( \det(A + B) \geq \det A \) with equality if and only if \( B = 0 \).

10.61. Given real symmetric \( A \succ 0 \) and \( B \succ 0 \), then

\[
\alpha A^{-1} + (1 - \alpha)B^{-1} \succeq [\alpha A + (1 - \alpha)B]^{-1}
\]

for all \( 0 \leq \alpha \leq 1 \). A special case of historical interest is \( \alpha = \frac{1}{2} \) (cf. (10.59d)).

10.62. If \( A \succ 0 \) and \( A + B \succ 0 \) are real symmetric matrices, then

\[
\frac{\det(A + B)}{(\det A)} \leq \exp[\text{trace}(A^{-1}B)],
\]

with equality if and only if \( B = 0 \).
10.63. (Haynsworth) If $A$, $B$, and $A - B$ are all real $n \times n$ p.d. matrices, then
$$\det(A + B) > \det A + n \det B.$$  

10.64. (Hartfiel) If $A$ and $B$ are real $n \times n$ p.d. matrices, then
$$\det(A + B) \geq \det A + \det B + (2^n - 2)(\det A \cdot \det B)^{1/2}.$$  

10.65. (Olkin) If $A > 0$ and $B$ is symmetric with $\det(A + B) \neq 0$, then
$$A^{-1} - (A + B)^{-1} \succeq (A + B)^{-1}B(A + B)^{-1}.$$  

The inequality is strict if and only if $B$ is nonsingular.

10.66. Let $A$ and $B$ be $n \times n$ real non-negative definite matrices. Then any two of the following conditions implies the third.

1. $\text{rank } A = \text{rank } B$.

2. $A \succeq B \succeq 0$.

3. $B^+ \succeq A^+ \succeq 0$.

10.67. Let $C$ be any real symmetric matrix. There exist two unique matrices $A \succeq 0$ and $B \succeq 0$ such that $AB = 0$ and
$$C = A - B.$$  

**Proofs.** Section 10.4.2.


10.56c. Follows from (10.47a(iii)) by relabelling $B \rightarrow A$, $A - B \rightarrow B$ and $A \rightarrow A + B$.


10.58a. Use $x^*(A + B)x \geq x^*Ax$.

10.58b. Follows from (10.56a) as $\lambda_i(A) > 0$. Magnus and Neudecker [1999: 21, real case].

10.58c. We replace $A$ by $A - B$ in (b) and (a).


10.60. $\det(A + B) = \det A \det(I_n + A^{-1/2}BA^{-1/2}) \geq \det A$ by (5.24c), since $A^{-1/2}BA^{-1/2}$ is skew-symmetric.


10.64. Ouellette [1981: 218].


In order to handle a number of complicated manipulations, which typically arise for example in multivariate statistical analysis, a number of special products and operators have been developed, along with rules for using them. Being able to treat a matrix like a stacked vector is one such example that arises when one is finding derivatives and Jacobians in later chapters.

11.1 KRONECKER PRODUCT

11.1.1 Two Matrices

We shall consider a number of operators on pairs of matrices that have the following product properties shared by the real numbers, \( \mathbb{R} \).

(i) The product is associative, i.e., \( a(bc) = (ab)c \) for all \( a, b, c \in \mathbb{R} \).

(ii) The product is distributive with respect to addition, that is, \( a(b+c) = ab + ac \) and \( (a + b)c = ac + bc \) for all \( a, b, c \in \mathbb{R} \).

(iii) There exist 0 and 1 such that for all \( a \in \mathbb{R} \), \( a(0) = 0 \) and \( a(1) = a \).

The following product has these properties.
**Definition 11.1.** If $A$ is an $m \times n$ and $B$ is $p \times q$, then the **Kronecker product** of $A$ and $B$ is defined by the $mp \times nq$ matrix

$$A \otimes B = \begin{pmatrix}
    a_{11}B & a_{12}B & \cdots & a_{1n}B \\
    a_{21}B & a_{22}B & \cdots & a_{2n}B \\
    \vdots & \vdots & \ddots & \vdots \\
    a_{m1}B & a_{m2}B & \cdots & a_{mn}B \\
\end{pmatrix} = (a_{ij}B).$$

The matrices $A$ and $B$ may be complex and we note that, in general, $A \otimes B \neq B \otimes A$. Also $A$ and $B$ can be replaced by vectors in the above definition.

The terms **direct product** and **tensor product** are also used in the literature. It should be noted that Graybill [1982: 216] defines the direct product to be $A \times B$, which is actually $B \otimes A$ in our notation. Although Kronecker’s name is associated with the above product, Henderson et al. [1983] suggest that Zehfuss should perhaps have the honor (see also Horn and Johnson [1991: 254]). In addition to the following results, further properties are listed in this chapter under star product, vec and vech operators, vec-permutation matrix, Jacobians and matrix linear equations. Many of the proofs of the properties given below are straightforward, and details are given in Abadir and Magnus [2005: chapter 10], Brewer [1978], Harville [1997: chapter 16], Horn and Johnson [1991: section 4.2, complex case], Kollo and von Rosen [2005: chapter 1], Magnus and Neudecker [1999: chapter 2], and Schott [2005: chapter 8]. The product rule of (11.11a) is particularly useful.

Kronecker products have been used extensively in statistics—for example, in experimental design, analysis of variance modeling (e.g., Rogers [1984], Ryan [1996], and Schott [2005: 288-290]), and multivariate moment problems.

**Definition 11.2.** If $A_i$ is $n_i \times n_i$ ($i = 1, 2, \ldots, r$), then

$$\text{diag}(A_1, \ldots, A_r) = \begin{pmatrix}
    A_1 & 0 & \cdots & 0 \\
    0 & A_2 & \cdots & 0 \\
    \vdots & \vdots & \ddots & \vdots \\
    0 & 0 & \cdots & A_r \\
\end{pmatrix}$$

is said to be the **direct sum** of $A_1, \ldots, A_r$, and is sometimes written in the form $	ext{diag}(A_1, \ldots, A_r) = A_1 \oplus \cdots \oplus A_r$.

11.1. (General Properties)

(a) $c \otimes A = cA = A \otimes c$.

(b) $x' \otimes y = yx' = y \otimes x'$.

(c) $aA \otimes bB = abA \otimes B$.

(d) $I_m \otimes I_n = I_{mn}$.

(e) $(A \otimes B)' = A' \otimes B'$.

(f) $(A \otimes B) = \overline{A} \otimes \overline{B}$ and $(A \otimes B)^* = A^* \otimes B^*$. Here $\overline{A}$ is the complex conjugate of $A$ and $A^*$ is the conjugate transpose.

(g) $(A \otimes B)^{-} = A^{-} \otimes B^{-}$, where $A^{-}$ and $B^{-}$ are any weak inverses of $A$ and $B$, respectively.
(h) \((A \otimes B)^+ = A^+ \otimes B^+\), where \(A^+\) and \(B^+\) are Moore–Penrose inverses.

(i) If \(A\) and \(B\) are nonsingular, then so is \(A \otimes B\) and 
\((A \otimes B)^{-1} = A^{-1} \otimes B^{-1}\).

(j) \(B \otimes A = H_1 A \otimes BH_2\), where \(H_1\) and \(H_2\) are permutation matrices that are independent of \(A\) and \(B\) except for their sizes.

(k) \(\text{rank}(A \otimes B) = \text{rank}(A) \text{rank}(B)\).

(l) If \(A\) is \(m \times m\) and \(B\) is \(p \times p\), then 
\[ \det(A \otimes B) = (\det A)^p (\det B)^m. \]
\[ \text{trace}(A \otimes B) = \text{trace}(A) \text{trace}(B). \]

(m) \(\|A \otimes B\|_F = \|A\|_F \|B\|_F\), where \(\| \cdot \|_F\) is the Frobenius norm.

(n) \(I_n \otimes A = \text{diag}(A, A, \ldots, A)\), where there are \(n\) diagonal blocks.

(o) \((A \otimes B)^k = A^k \otimes B^k\), for positive integer \(k\).

11.2. (Direct Sum) \((A \oplus B) \otimes C = (A \otimes C) \oplus (B \otimes C)\). However, in general, \(A \otimes (B \oplus C) \neq (A \otimes B) \oplus (A \otimes C)\).

11.3. (Partitioned Matrices)

(a) \((A_1, A_2) \otimes B = (A_1 \otimes B, A_2 \otimes B)\).

(b) \((A \otimes x)B = (A \otimes x)(B \otimes 1) = AB \otimes x\).

(c) Suppose \(A\) is partitioned into submatrices, say
\[
A = \begin{pmatrix}
A_{11} & \cdots & A_{1s} \\
\vdots & \ddots & \vdots \\
A_{r1} & \cdots & A_{rs}
\end{pmatrix},
\]
then
\[
A \otimes B = \begin{pmatrix}
A_{11} \otimes B & \cdots & A_{1s} \otimes B \\
\vdots & \ddots & \vdots \\
A_{r1} \otimes B & \cdots & A_{rs} \otimes B
\end{pmatrix}.
\]

(d) If \(B = (B_1, B_2, \ldots, B_r)\), then \(a \otimes B = (a \otimes B_1, \ldots, a \otimes B_r)\).

11.4. (Singular Value Decomposition) Let \(A\) be an \(m \times n\) matrix of rank \(r_1\) with a singular value decomposition \(A = V_1 \Sigma_1 W_1^*\), and let \(B\) be a \(p \times q\) matrix of rank \(r_2\) with singular value decomposition \(B = V_2 \Sigma_2 W_2^*\), where \(V_i\) and \(W_i\) \((i = 1, 2)\) are unitary matrices. Let \(\sigma_i(C)\) be the \(i\)th singular value of \(C\) for \(C = A\) or \(B\). Then
\[
A \otimes B = (V_1 \otimes V_2)(\Sigma_1 \otimes \Sigma_2)(W_1 \otimes W_2)^*,
\]
where the nonzero singular values of \(A \otimes B\) are the \(r_1 r_2\) positive numbers \(\{\sigma_i(A)\sigma_j(B)\}\) \((i = 1, \ldots, r_1; j = 1, \ldots, r_2)\) (including multiplicities). Zero is a singular value of \(A \otimes B\) with multiplicity \(\min\{mp, nq\} - r_1 r_2\). In particular, the singular values of \(A \otimes B\) are the same as those of \(B \otimes A\), and \(\text{rank}(A \otimes B) = \text{rank}(B \otimes A) = r_1 r_2\).
11.5. (Eigenvalues and Vectors) Let \( \{\lambda_i\} \) and \( \{x_i\} \) be the eigenvalues and the corresponding right eigenvectors of the \( m \times m \) matrix \( A \), and \( \{\mu_j\} \) and let \( \{y_j\} \) be the eigenvalues and corresponding right eigenvectors for the \( n \times n \) matrix \( B \).

(a) \( A \otimes B \) has eigenvalues \( \{\lambda_i \mu_j\} \) (including algebraic multiplicities), and \( \{x_i \otimes y_j\} \) \((i = 1, 2, \ldots, m; j = 1, 2, \ldots, n)\) are right eigenvectors of \( A \otimes B \) (but not necessarily all of them). Note that \( B \otimes A \) also has eigenvalues \( \{\lambda_i \mu_j\} \). It should be noted that not every eigenvector of \( A \otimes B \) is of the form \( x \otimes y \), where \( x \) is an eigenvector of \( A \) and \( y \) is an eigenvector of \( B \). Abadir and Magnus [2005: 279] give a counterexample.

(b) The so-called Kronecker sum \( (A \otimes I_n + I_m \otimes B) \) has eigenvalues \( \{\lambda_i + \mu_j\} \) with corresponding right eigenvectors \( \{x_i \otimes y_j\} \).

11.6. Let \( A \) be \( m \times m \) and \( B \) be \( n \times n \) matrices. We have the following results, some of which are also listed elsewhere under the appropriate matrix topic.

(a) If \( A \) and \( B \) are both diagonal matrices, then so is \( A \otimes B \).

(b) If \( A \) and \( B \) are both upper (respectively lower) triangular matrices, then \( A \otimes B \) is also upper (respectively lower) triangular.

(c) If \( A \) and \( B \) are non-negative definite (respectively positive definite), then so is \( A \otimes B \).

(d) If \( A \) and \( B \) are both symmetric (respectively Hermitian), then so is \( A \otimes B \).

(e) If \( A \) and \( B \) are both orthogonal (respectively unitary), then so is \( A \otimes B \).

(f) If \( A \) and \( B \) are idempotent, then so is \( C = A \otimes B \). In fact

\[
P_C = P_A \otimes P_B,
\]

where \( P_C \) is the projection onto \( C(C) \).

11.7. If \( A \) and \( B \) are non-negative definite, then \( A \otimes A \succeq B \otimes B \) if and only if \( A \succeq B \), where \( A \succeq B \) means that \( A - B \) is non-negative definite.

11.8. If \( A \) and \( B \) are \( n \times n \) non-negative definite matrices, then:

(a) \( \text{trace}(A \otimes B) \leq \frac{1}{4}(\text{trace } A + \text{trace } B)^2 \).

(b) \( \text{trace}(A \otimes B) \leq \frac{1}{2} \text{trace}(A \otimes A + B \otimes B) \).

Definition 11.3. The function \( f \) is analytic in an open set if it can be expressed as a power series, namely \( f(z) = a_0 + a_1 z + a_2 z^2 + \cdots \).

11.9. If \( f \) is analytic and \( f(A) \) exists, where \( A \) is \( m \times m \), then:

(a) \( f(I_p \otimes A) = I_p \otimes f(A) \).

(b) \( f(A \otimes I_p) = f(A) \otimes I_p \).

For example,

(i) \( \exp(I_p \otimes A) = I_p \otimes \exp(A) \).
(ii) \((A \otimes I)^k = A^k \otimes I, k = 1, 2, \ldots\)

Proofs. Section 11.1.1.

11.1. For proofs see Abadir and Magnus [2005: section 101, Harville [1997: section 16.1], Rao and Rao [1998: chapter 6], and Schott [2005: section 8.2]. Some of the results follow using the product rule \((A \otimes B)(C \otimes D) = AC \otimes BD\) from (11.1a). For example, to prove (g), \((A \otimes B)(A^- \otimes B^-)(A \otimes B) = AA^-A \otimes BB^-B = A \otimes B; (h) is similar. For (i), \((A^{-1} \otimes B^{-1})(A \otimes B) = A^{-1}A \otimes B^{-1}B = I; (k) and (l) are proved by Schott [2005: 286–288]; and (m) is proved by Harville [2001: 143, exercise 9].


11.4. Horn and Johnson [1991: 246].


11.5b. Horn and Johnson [1991: 268–269, \(A\) and \(B\) interchanged].

11.6. The proofs follow by checking the appropriate property using (11.1) and applying the product rule (11.1a). For example, if \(A\) and \(B\) are orthogonal, then from (11.1e) we have \((A \otimes B)'(A \otimes B) = A'A \otimes B'B = I_{2n}\). For (c), use \(A = RR^*\), and so on, and apply (11.1f) and (11.1k). Also, for (d), \((A \otimes B)^* = A^* \otimes B^* = A \otimes B\). Harville [2001: 141, exercise 6] proves the second part of (f).

11.7. Abadir and Magnus [2005: 280].

11.8a. We use (11.1l(ii)), namely \(\text{trace}(A \otimes B) = \text{trace} A \text{trace} B\), and expand \((\text{trace} A - \text{trace} B)^2 \geq 0\).

11.8b. Use the trace of a sum is the sum of the traces, and apply \(\text{trace}(A \otimes B) = \text{trace} A \text{trace} B\).

11.9. Expand \(f(B)\) as a matrix power series, apply the product rule to each term, as for example in (ii), and then use (11.10b). For (i) we use the power series given in Section 19.6.

11.1.2 More than Two Matrices

The following apply to any conformable matrices, provided the appropriate products and additions exist.

11.10. (Distributive Rules)

(a) Let \(A\) be \(m \times n\), \(B\) be \(p \times q\), and \(C\) be \(r \times s\). Then

\[ A \otimes (B \otimes C) = (A \otimes B) \otimes C. \]

We can therefore write each expression as \(A \otimes B \otimes C\).
(b) Let $A$ and $B$ be $m \times n$, and let $C$ and $D$ be $p \times q$, then

$$(A + B) \otimes (C + D) = A \otimes C + A \otimes D + B \otimes C + B \otimes D.$$ 

Special cases follow by setting $A = 0$ or $C = 0$.

(c) $A \otimes (\sum_{i=1}^{r} B_i) = \sum_{i=1}^{r} (A \otimes B_i)$ and $(\sum_{i=1}^{r} A_i) \otimes B = \sum_{i=1}^{r} (A_i \otimes B)$.

(d) $(\sum_{i=1}^{r} A_i) \otimes (\sum_{j=1}^{r} B_j) = \sum_{i=1}^{r} \sum_{j=1}^{r} (A_i \otimes B_j)$.

11.11. (Mixed Product)

(a) (Product Rule) Let $A$, $B$, $C$, and $D$ be $m \times n$, $p \times q$, $n \times r$, and $q \times s$, respectively. Then

$$(A \otimes B)(C \otimes D) = AC \otimes BD.$$ 

This leads to the following special cases.

(i) From (11.15c), $(A \otimes b')(c \otimes D) = Acb'D$.

(ii) If $A$ is $m \times n$ and $B$ is $p \times q$, then

$$A \otimes B = (A \otimes I_p)(I_n \otimes B).$$

(b) $(A_1 \otimes B_1)(A_2 \otimes B_2) \cdots (A_k \otimes B_k) = A_1 A_2 \cdots A_k \otimes B_1 B_2 \cdots B_k$.

11.12. Let $L$ be a nonsingular $n \times n$ matrix $(n \geq 2)$, $A$ and $B$ be $m \times m$ matrices, and $a$ and $b$ be $n \times 1$ vectors. Then the $nm \times nm$ matrix

$$G = L \otimes B + ab' \otimes A$$

has determinant

$$\det G = (\det L)^m (\det B)^{n-1} \det C,$$

where

$$C = B + \alpha A \quad \text{and} \quad \alpha = b'L^{-1}a.$$ 

If $G$ is nonsingular, then

$$G^{-1} = L^{-1} \otimes B^{-1} - L^{-1}ab'L^{-1} \otimes E,$$

where

$$E = C^{-1}AB^{-1} = B^{-1}AC^{-1} = B^{-1}AB^{-1} \quad \text{if} \quad \alpha = 0,$$

$$= \frac{1}{\alpha}(B^{-1} - C^{-1}) \quad \text{if} \quad \alpha \neq 0.$$ 

**Definition 11.4.** The Kronecker power of an $m \times n$ matrix $A$ is defined as follows:

$$A^{[2]} = A \otimes A,$$

$$A^{[k]} = A \otimes A \otimes \cdots \otimes A = A \otimes A^{[k-1]} = A^{[k-1]} \otimes A,$$

for $k = 2, 3, \ldots$
11.13. \((AB)^{[k]} = A^{[k]}B^{[k]}\) for \(k = 1, 2, \ldots\).

11.14. If \(A\) and \(B\) are non-negative definite, then \(A - B\) is non-negative definite if and only if and \(A^{[2]} - B^{[2]}\) is non-negative definite.

**Proofs.** Section 11.1.2.

11.10. Prove directly from the definition of the Kronecker product (cf. Abadir and Magnus [2005: 275–276]).

11.11. Harville [1997: 337].


11.13. Follows from the product rule (11.11a).


### 11.2 VEC OPERATOR

**Definition 11.5.** Let \(A = (a_1, a_2, \ldots, a_n)\) be an \(m \times n\) matrix. Then \(\text{vec} A\) is a vector obtained by stacking the columns of \(A\), namely

\[
\text{vec} A = \begin{pmatrix}
a_1 \\
a_2 \\
\vdots \\
a_n
\end{pmatrix},
\]

an \(mn \times 1\) vector. Various other notations have been used for the above concept, and some history and references are given by Henderson and Searle [1981a]. Here \(\text{vec} A\) stands for "vector of columns of \(A\)."

Turkington [2002: 101] introduced the operator \(\text{devec} A\) that stacks the rows of \(A\) alongside each other so that \((\text{vec} A')' = \text{devec} A\).

The following properties are proved by Henderson and Searle [1979: 67]), except where labeled otherwise. We assume that \(A_{m \times n}\) is \(m \times n\), \(B_{n \times q}\) is \(n \times q\), and \(C_{q \times r}\) is \(q \times r\).

**11.15. (Some General Properties)**

(a) \(\text{vec} A = (I_n \otimes A)\text{vec} I_n = (A' \otimes I_m)\text{vec} I_m\).

(b) \(\text{vec} x = \text{vec} x' = x\).

(c) \(\text{vec} (xy') = y \otimes x\).

(d) From (c),

\[
\text{vec} [(Ax)(y'B)] = (B'y) \otimes (Ax) = (B' \otimes A)(y \otimes x) = (B' \otimes A)\text{vec} (xy').
\]

(e) If \(A\) is nonsingular, we apply (11.16b) to \(\text{vec} (A^{-1}AA^{-1})\) to get

\[
\text{vec} A^{-1} = (A^{-1'} \otimes A^{-1})\text{vec} A.
\]
\[ \text{vec} \left[ A(b_1, b_2, \ldots, b_q) \right] = \begin{pmatrix} Ab_1 \\ Ab_2 \\ \vdots \\ Ab_q \end{pmatrix}. \]

**11.16. (Products)**

(a) \[
\text{vec} (A_{m \times n} B_{n \times q}) = (I_q \otimes A) \text{vec} B = (B' \otimes A) \text{vec} I_n = (B' \otimes I_m) \text{vec} A.
\]

(b) We highlight the following result as it is used extensively.

\[ \text{vec} (A_{m \times n} B_{n \times q} C_{q \times r}) = (C' \otimes A) \text{vec} B. \]

(c) Using (a), we have

\[ \text{vec} (A_{m \times n} B_{n \times q} C_{q \times r}) = (I_r \otimes AB) \text{vec} C = (C'B' \otimes I_m) \text{vec} A. \]

(d) Using the above results, we obtain

\[ \text{vec} (A_{m \times n} B_{n \times q} C_{q \times r} D_{r \times s}) = (I \otimes ABC) \text{vec} D = (D' \otimes AB) \text{vec} C = (D'C' \otimes A) \text{vec} B = (D'C'B' \otimes I) \text{vec} A. \]

(e) Using (a), we have

\[ \text{vec} [(A + B)(C + D)] = [(I \otimes A) + (I \otimes B)][\text{vec} C + \text{vec} D] = [(C' \otimes I) + (D' \otimes I)][\text{vec} A + \text{vec} B]. \]

Clearly, (a), (b), and (c) can be deduced from (d) by replacing appropriate matrices by identity matrices. However, (a)--(c) are listed for convenient reference.

**11.17. (Trace)**

(a) \[ \text{trace}(A_{m \times n} B_{n \times q}) = (\text{vec } A')' \text{vec } B = (\text{vec } B')' \text{vec } A. \]

As noted by Henderson and Searle [1979: 67], the above can be expressed in an alternative form that is easier to remember, namely

\[ \text{trace}(A'B) = (\text{vec } A)' \text{vec } B. \]

This result can be used along with (11.16) to deduce the following.
(b) 

\[ \text{trace}(A_{m \times n}B_{n \times q}C_{q \times s}) = (\text{vec } A')'(I_s \otimes B)\text{vec } C \]
\[ = (\text{vec } B')'(I \otimes C)\text{vec } A \]
\[ = (\text{vec } C')'(I \otimes A)\text{vec } B \]
\[ = (\text{vec } A')'(C' \otimes I)\text{vec } B \]
\[ = (\text{vec } B')'(A' \otimes I)\text{vec } C \]
\[ = (\text{vec } C')'(B' \otimes I)\text{vec } A. \]

We can use such results as \( \text{trace}(ABC) = (\text{vec } A')'\text{vec } (BC) \) and \( \text{trace}(ABC) = \text{trace}(BCA) = \text{trace}(CAB) \).

(c) 

\[ \text{trace}(ABCD) = (\text{vec } A')'(D' \otimes B)\text{vec } C \]
\[ = \text{trace}(D(ABC)) = (\text{vec } D')'(C' \otimes A)\text{vec } B \]
\[ = \text{trace}(D'(C'B'A')) = (\text{vec } D')'(A' \otimes C')\text{vec } B'. \]

(d) From (c) and (11.16b) we have:

(i) \( \text{trace}(AXBX'C) = \text{trace}(X'CAXB) = (\text{vec } X)'(B' \otimes CA)\text{vec } X. \)

(ii) \( \text{trace}(AX'BXC) = \text{trace}(X'BXCA) = (\text{vec } X)'(A'C' \otimes B)\text{vec } X. \)

The above can also be transposed to obtain further results.

Proofs. Section 11.2.

11.15a. Follows from (11.16a) with \( A = I \) or \( B = I. \)

11.15d–e. Use (11.16b) with a suitable substitution.


11.16e. Expand and use (a).


11.17d. We use a result like \( \text{trace}(X'CAXB) = (\text{vec } X)'\text{vec } (CAXB) \) (Henderson and Searle [1979: 67]).
11.3 VEC-PERMUTATION (COMMUTATION) MATRIX

We now introduce a permutation matrix that is particularly useful for dealing with matrices of random variables and their moments.

**Definition 11.6.** Let \( A \) be an \( m \times n \) matrix. We define \( I_{(m,n)} \) as the the \( mn \times mn \) permutation matrix such that \( \text{vec} \ A = I_{(m,n)} \text{vec} A' \). Henderson and Searle [1979, 1981a], who give a useful historical background and a summary of its properties, call \( I_{(m,n)} \) the vec-permutation matrix. It is also called a commutation matrix by Abadir and Magnus [2005], Magnus and Neudecker [1999], and Schott [2005], who denote it by \( K_{nm} \) and, when \( m = n, K_n \); we shall mention both notations in our discussion. (Many of the results given in this section are also proved in Graybill [1983: section 9.3], though, as previously mentioned, he uses an alternative definition, namely \( A \times B \) instead of \( B \otimes A \.) The use of of the commutation matrix in statistics was discussed in Magnus and Neudecker [1979].

If \( A_{2 \times 3} = \left( \begin{array}{ccc} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \end{array} \right) \), then

\[
\text{vec} A_{2 \times 3} = \left( \begin{array}{c} a_{11} \\ a_{21} \\ a_{12} \\ a_{22} \\ a_{13} \\ a_{23} \end{array} \right) = \left( \begin{array}{cccccc} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{array} \right) \left( \begin{array}{c} a_{11} \\ a_{12} \\ a_{13} \\ a_{21} \\ a_{22} \\ a_{23} \end{array} \right) = I_{(2,3)} \text{vec} A'.
\]

Thus \( I_{(m,n)} \) is a rearrangement of \( I_{mn} \) obtained by taking every \( n \)th row starting at the first, then every \( n \)th row starting at the second, and so on. Thus \( I_{(2,3)} \) consists of rows 1, 4, 2, 5, 3, 6 of \( I_6 \). As a permutation matrix, it has all the standard properties of a permutation matrix (cf. Section 8.2).

11.18. (Some Basic Properties)

(a) \( I_{(m,n)} \) (\( = K_{nm} \)) is orthogonal, being a permutation matrix.

(b) \( I_{(m,n)} I_{(n,m)} = I_{mn} \) (i.e., \( K_{nm} K_{mn} = I_{mn} \)) so that

(i) \( I_{(m,n)}^{-1} = I_{(n,m)} \) (i.e., \( K_{nm}^{-1} = K_{mn} \)).

(ii) \( \text{vec} A' = I_{(n,m)} \text{vec} A \).

(iii) \( I_{(n,n)}^2 = I_{(n,n)} \).

(iv) \( I_{(n,n)}^r = I_{(n,n)} \).

(c) \( I_{(m,1)} = I_{(1,m)} = I_m \).

(d) If \( E_{ij} \) is the \( m \times n \) matrix with 1 in the the \( i, j \)th position and zeros elsewhere, then

\[
I_{(m,n)} = \sum_{i=1}^{m} \sum_{j=1}^{n} (E_{ij}' \otimes E_{ij}) \quad (= K'_{mn}).
\]
In particular (Harville [1997: 345, transposed]),

\[
I_{(m,n)} = \begin{pmatrix}
E_{11} & E_{21} & \cdots & E_{m1} \\
E_{12} & E_{22} & \cdots & E_{m2} \\
. & . & \cdots & . \\
E_{1n} & E_{2n} & \cdots & E_{mn}
\end{pmatrix}.
\]

As already noted,

\[
K_{mn} = \sum_{i=1}^{m} \sum_{j=1}^{n} (E_{ij} \otimes E_{ij}').
\]

This result can be used to define \(K_{mn}\), and Schott [2005: 308] proves the equivalence of the two definitions.

(e) If \(e_{i,m}\) is the \(i\)th column of \(I_m\) and \(e_{j,n}\) is the \(j\)th column of \(I_n\), then

\[
I_{(m,n)} = \sum_{i=1}^{m} (e'_{i,n} \otimes I_n \otimes e_{i,n})
\]

\[
= \sum_{j=1}^{n} (e_{j,m} \otimes I_m \otimes e'_{j,n}).
\]

(f) (i) \(\det I_{(m,n)} = (-1)^{\frac{1}{2}m(m-1)(n-1)} \det I_{(m,n-1)} = (-1)^{\frac{1}{2}m(m-1)n(n-1)}\).

(ii) \(\det I_{(n,n)} = (-1)^{\frac{1}{2}n(n-1)}\).

(g) (i) \(\text{trace}(I_{(m,n)}) = 1 + g(m - 1, n - 1)\),

where \(g(a, b)\) is the greatest common divisor of \(a\) and \(b\).

(ii) \(\text{trace} I_{(n,n)} = n\).

(h) \(I_{(n,n)}\) has eigenvalues \(\pm 1\) with respective multiplicities \(\frac{1}{2}n(n \pm 1)\).

11.19. Let \(A_{m \times n}\) and \(B_{p \times q}\) be \(m \times n\) and \(p \times q\) matrices, and let \(a\) and \(b\) be \(m \times 1\) and \(p \times 1\) vectors.

(a) \(I_{(m,p)}(A_{m \times n} \otimes B_{p \times q}) = (B_{p \times q} \otimes A_{m \times n})I_{(n,q)}\).

(b) \(I_{(m,p)}(A_{m \times n} \otimes B_{p \times q})I_{(q,n)} = B_{p \times q} \otimes A_{m \times n}\).

(c) We have the following special cases of the above.

(i) \(I_{(p,m)}(A_{m \times n} \otimes b_{p \times 1}) = b_{p \times 1} \otimes A_{m \times n}\).

(ii) Multiplying (i) on the left by \(I_{(p,m)}\) and using (11.18b) gives us

\[
I_{(p,m)}(b \otimes A) = A \otimes b.
\]

(iii) \((A_{m \times n} \otimes b'_{1 \times p})I_{(p,n)} = b' \otimes A\).

(iv) \((b' \otimes A)I_{(n,p)} = A \otimes b'\).

(v) \(I_{(m,p)}(a_{m \times 1} \otimes b_{p \times 1}) = b_{p \times 1} \otimes a_{m \times 1}\).

11.20. \(A_{m \times m} \otimes B_{p \times p} = I_{(p,m)}(I_p \otimes A_{m \times m})I_{(n,p)}(I_m \otimes B_{p \times p})\).
11.21. For handling more than two matrices, we introduce $I_{(ab,n)} = I_{(m,n)}(= K_{nm})$, where $m = ab$. Since $I_{(mp,s)} = I_{(pm,s)}$, we can interchange $m$ and $p$ in some of the following results.

(a) $I_{(p,ma)}I_{(m,ps)} = I_{(mp,s)} = I_{(m,p)}I_{(p,ms)}$.

(b) $I_{(mps)}I_{(ps,mp)} = I_{(mp,s)}$.

(c) $I_{(mp,s)} = (I_{(p,s)} \otimes I_{m})(I_{p} \otimes I_{(m,s)}) = (I_{(m,s)} \otimes I_{p})(I_{m} \otimes I_{(p,s)})$.

(d) Any two $I$ matrices with the same set of three indices commute, for example, $I_{(mp,s)}I_{(p,sm)} = I_{(ps,mp)}I_{(mp,sm)}$.

11.22.

$$C_{s \times t} \otimes A_{m \times n} \otimes B_{p \times q} = I_{(mp,s)}[(A_{m \times n} \otimes B_{p \times q}) \otimes C_{s \times t}]I_{(nt,q)}$$

$$= I_{(ps,m)}[B_{p \times q} \otimes (C_{s \times t} \otimes A_{m \times n})]I_{(nt,q)}.$$
Proofs. Section 11.3.


11.20. Use \((A \otimes I_p)(I_m \otimes B) = A \otimes B\) and (11.19b).


11.4 GENERALIZED VEC-PERMIUTATION MATRIX

Definition 11.7. Let \(I_{(n)}\) be the matrix obtained from \(I_r\) by taking every \(n\)th row starting with the first, then every \(n\)th row starting with the second, and so on (cf. Tracey and Dwyer [1969] and Henderson and Searle [1981a]). Then \(I_{(n)}\) is called a generalized vec-permutation matrix. For example, if \(r = 5\) and \(n = 3\), \(I_{(3)} = (e_1, e_4, e_2, e_5, e_3)\), where the \(e_i\) are the columns of \(I_r\).

We can apply the same procedure to any matrix \(M\) and obtain \(M_{(n)}\). In fact, \(M_{(n)} = I_{(n)} M\). We can also define \(M_{(m,n)} = I_{(m,n)} M\). When \(r = mn\), \(I_{(m,n)} = I_{(n)}\), and when \(M\) has \(mn\) rows, \(M_{(m,n)} = M_{(n)}\).

11.27. In the following, \(A\) is \(m \times n\), \(B\) is \(p \times q\), \(C\) is \(s \times t\), \(a\) is \(m \times 1\), and \(b\) is \(p \times 1\).

(a) \(\text{vec } A = (\text{vec } A')_{(m,n)}\).

(b) \((A \otimes B)_{(m,p)} = (B' \otimes A')_{(q,n)}\).

(c) \((a \otimes B)_{(m,p)} = I_{(m,n)} (a \otimes B) = B \otimes a\).

(d) \((A \otimes b)_{(m,p)} = I_{(m,p)} (A \otimes b) = b \otimes A\).

(e) \((a \otimes b')_{(m,p)} = I_{(m,p)} (a \otimes b) = b \otimes a\).

(f) \((a \otimes b' \otimes C)_{(m,s)} = (ab' \otimes C)_{(m,s)} = b' \otimes C \otimes a\).

11.28. \(I_{(m,n)} = (I_m \otimes I_n)_{(m,n)}\).
Proofs. Section 11.4.

11.27. Henderson and Searle [1981a: 283–284 and equation (49)]. Use (11.1b) for (f).

11.5 Vech Operator

Definition 11.8. If \( A \) is an \( n \times n \) matrix, then \( \text{vech} \, A \) (vector-half) is the \( k = n(n+1)/2 \) -dimensional vector obtained by stacking the columns of the lower triangle of \( A \), including the diagonal, one below the other; Magnus and Neudecker [1999] and Schott [2005] use the notation \( \nu(A) \). For example, if

\[
A = \begin{pmatrix}
a_{11} & a_{12} & a_{13} \\
a_{21} & a_{22} & a_{23} \\
a_{31} & a_{32} & a_{33}
\end{pmatrix}
\]

is symmetric, then

\[
\text{vech} \, A = \begin{pmatrix}
a_{11} \\
a_{21} \\
a_{31} \\
a_{22} \\
a_{32} \\
a_{33}
\end{pmatrix}
\]

This approach is useful for symmetric and lower-triangular matrices; for upper-triangular matrices we use \( \text{vech} \, (A') \).

11.5.1 Symmetric Matrix

A major application of the above definition is to symmetric matrices, so we now assume \( A = A' \). For this case, \( \text{vech} \, A \) lists all the distinct elements of \( A \). As the elements of \( \text{vec} \, A \) are those of \( \text{vech} \, A \) with some repetitions, it follows that \( \text{vec} \, A \) and \( \text{vech} \, A \) are linear transformations of one another. This leads to the following definitions.

Definition 11.9. We have \( \text{vech} \, A = H_n \, \text{vec} \, A \) and \( \text{vec} \, A = G_n \, \text{vech} \, A \). The matrix \( H_n \) is \( k \times n^2 \), and Magnus and Neudecker [1999: 48–51] call the \( n^2 \times k \) matrix \( G_n \) the duplication matrix \( D_n \) (see also Magnus [1988: chapter 4] and Schott [2005: section 8.7]). We shall also use the term duplication matrix. Examples of \( G_n \) and \( H_n \) for \( n = 3 \) (\( k = 6 \)) together with \( I_{(3,3)} \), with which they have several relationships, are

\[
D_3 = G_3(9 \times 6) = \begin{pmatrix}
1 & & & & & \\
& 1 & & & & \\
& & 1 & & & \\
\hline
& & & 1 & & \\
& & & & 1 & \\
& & & & & 1
\end{pmatrix}
\]
\[
H_3(6 \times 9) = \begin{pmatrix}
1 & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\
\alpha_1 & 1-\alpha_1 & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\
\alpha_2 & \cdots & 1-\alpha_2 & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\
\alpha_3 & \cdots & \cdots & \cdots & 1-\alpha_3 & \cdots & \cdots & \cdots & \cdots \\
\cdots & \cdots & \cdots & \cdots & \cdots & \cdots & 1 \\
\cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & 1
\end{pmatrix},
\]

and
\[
I_{(3,3)} = \begin{pmatrix}
1 & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\
\cdots & 1 & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\
\cdots & \cdots & 1 & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\
\cdots & \cdots & \cdots & \cdots & 1 & \cdots & \cdots & \cdots & \cdots \\
\cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\
\cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\
\cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\
\cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\
\cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & 1
\end{pmatrix},
\]

where the dots represent zeros and the \(\alpha_i\)'s are arbitrary, except for \(0 < \alpha_i < 1\) \((i = 1, 2, 3)\).

The matrix \(G_n\) can be described as follows (e.g., Harville [1997: 352, with a correction]). For \(i \geq j\), the \([(j - 1)n + i]\)th and \([(i - 1)n + j]\)th rows of \(G_n\) equal the \([(j - 1)(n - j/2) + i]\)th row of \(I_k\), that is, they equal the \(k\)-dimensional row vector whose \([(j - 1)(n - j/2) + i]\)th element is 1 and whose remaining elements are zero. For \(j \geq i\) the \([(j - 1)(n - j/2) + i]\)th column is an \(n^2\)-dimensional column vector whose \([(j - 1)n + i]\)th and \([(i - 1)n + j]\)th elements are 1 and whose remaining elements are 0.

Another related matrix is \(N_n\), where \(N_n = \text{vec}(\frac{1}{2}(A + A'))\) transforms \(A\) into a symmetric matrix. This matrix is called the symmetrizer. As shown below, \(N_n\) turns out to be symmetric and idempotent, so I shall also denote it by \(P_n\) to remind us that it represents an orthogonal projection (see also Schott [2005: 312]).

11.29. (General Properties) For handy reference, we frequently have in the literature \(G_n \equiv D_n, H_n \equiv D_n^+,\) and \(P_n \equiv N_n;\) also \(k = n(n + 1)/2.\)

(a) \(H_n\) is a left inverse of \(G_n,\) i.e., \(H_nG_n = I_k.\) Thus \(H_n\) is a weak inverse of \(G_n\) as \(G_nH_nG_n = G_n.\)

(b) Every row of \(G_n\) contains only one nonzero element, so that the columns of \(G_n\) are orthogonal.

(c) The \(n^2 \times k\) matrix \(G_n\) is unique, of rank \(k.\)

(d) \(I_{(n,n)}G_n = G_n\) (i.e., \(K_{nn}D_n = D_n).\)

(e) \(G_{n+1}'G_{n+1} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 2I_n & 0 \\ 0 & 0 & G_n'G_n \end{pmatrix}.\)

(f) \((G_{n+1}'G_{n+1})^{-1} = G_{n+1}'G_{n+1}' = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \frac{1}{2}I_n & 0 \\ 0 & 0 & (G_n'G_n)^{-1} \end{pmatrix}.\)
(g) The $k \times n^2$ matrix $H_n$ is not unique and has rank $k$.

(h) A useful form of $H_n$ is $H_n = G_n^+ = (G_n'G_n)^{-1}G_n'$, the Moore–Penrose inverse of $G_n$ (Schott [2005: 313]). (This is the form taken by $H_3(6 \times 9)$ above when all the $\alpha_i$'s are set equal to $\frac{1}{2}$.) Then:

(i) $G_n^+G_n = I_k$.

(ii) $G_nG_n^+ = \frac{1}{2}(I_{n^2} + I_{(n,n)}) = P_n$.

(iii) $G_n^+I_{(n,n)} = G_n^+$.

(i) $P_n = G_nG_n^+ = G_n(G_n'G_n)^{-1}G_n$. Then:

(i) $P_nG_n = G_n$ and $G_n^+P_n = G_n^+$.

(ii) $P_nvec A = vec [\frac{1}{2}(A + A')]$ for any $n \times n$ matrix $A$.

(iii) The symmetrizer $P_n$ is symmetric and idempotent, that is, a projection matrix projecting orthogonally onto $C(G_n)$.

(iv) rank $P_n = trace P_n = \frac{1}{2}n(n+1)$.

(v) $P_nI_{(n,n)} = P_n = I_{(n,n)}P_n$ (i.e., $N_nK_{nn} = N_n = K_{nn}N_n$).

(vi) If $A$ and $B$ are $n \times n$, then $P_n(A \otimes B)P_n = P_n(B \otimes A)P_n$ and $P_n(A \otimes A)P_n = P_n(A \otimes A) = (A \otimes A)P_n$.

For further properties of $G_n$, $G_n'$, $G_n^+$, $G_n'G_n$, and $G_nG_n'$, where $G_n = D_n$, see Abadir and Magnus [2005: section 11.3] and Magnus [1988: chapter 4].

11.30. Suppose $A$ and $X$ are both $n \times n$, and $X$ is symmetric, then

$$vech(AXA') = H_n vec(AXA)$$
$$= H(A \otimes A)vec X$$
$$= H_n(A \otimes A)G_n vec X$$
$$= Cvec X,$$ say.

Properties of $C$ are given in (11.31c) below.

11.31. Suppose $A$ is $n \times n$. Then:

(a) $G_nG_n^+(A \otimes A)G_n = (A \otimes A)G_n$.

(b) $G_nG_n^+(A \otimes A)G_n^+ = (A \otimes A)G_n^+$.

(c) Let $C = H_n(A \otimes A)G_n$, a $k \times k$ matrix, where $k = n(n+1)/2$. Then:

(i) $C$ is invariant with respect to the choice of $H_n$, so we can choose $H = G_n$ (cf. 11.29h).

(ii) $C$ is nonsingular if and only if $A$ is nonsingular. Then

$$C^{-1} = G_n^+(A^{-1} \otimes A^{-1})G_n.$$  

(iii) If $A$ is upper-triangular, lower-triangular, or diagonal, then $C$ is respectively upper-triangular, lower-triangular, or diagonal with diagonal elements $a_{ii}a_{jj}, i = 1, 2, \ldots, n; j = 1, 2, \ldots, n.$
(iv) The eigenvalues of $C$ are $\lambda_i \lambda_j$ ($1 \leq j \leq i \leq n$), where $\lambda_i$ ($i = 1, 2, \ldots, n$) are the eigenvalues of $A$.

(v) $\det C = \det\{G_n^+(A \otimes A)G_n\} = (\det A)^{n+1}$.

(vi) $\text{trace } C = \frac{1}{2}[(\text{trace } A)^2 + \text{trace}(A^2)]$.

(vii) $\text{rank } C = \frac{1}{2}[(\text{rank } A)^2 + \text{rank } A]$.

(viii) $C^{-} = H_n(A^{-} \otimes A^{-})G_n$ is a weak inverse of $C$.

(d) If $A$ is nonsingular, then:

(i) $[G_n'(A \otimes A)G_n]^{-1} = G_n^+(A^{-1} \otimes A^{-1})G_n^{+\prime}$.

(ii) $\det[G_n^+(A \otimes A)G_n^{+\prime}] = 2^{-n(n-1)/2}(\det A)^{n+1}$.

11.32. If $A$ is any $n \times n$ matrix, then the following hold.

(a) $(A \otimes A)G_n = G_n H_n(A \otimes A)G_n$.

(b) $G_n H_n(A \otimes A) = (A \otimes A)G_n H_n$.

(c) $H_n(A \otimes A) = H_n(A \otimes A)G_n H_n$.

We can set $H_n = G_n^+$ in the above.

For some properties of $G_n^+(I_n \otimes A + A \otimes I_n)G_n$, $G_n^+(A \otimes B)G_n$, and some related matrices (with $D_n = G_n$), including further relationships between $D_{n+1}$ and $D_n$, see Magnus [1988: 65–72].

Proofs. Section 11.5.1.

11.29a. $\text{vech } A = H_n \text{ vec } A = H_n G_n \text{ vech } A$ for all symmetric $A$. Henderson and Searle [1979: 69].

11.29b. Follows from the definition of $G_n$.

11.29c. Schott [2005: 313].

11.29d. Henderson and Searle [1979: 69].


11.29g. Henderson and Searle [1979: 69].


11.31c(i). Henderson and Searle [1979: 70].


11.31c(iii). Magnus [1988: 63].

11.31c(iv). Magnus [1988: 64].


11.5.2 Lower-Triangular Matrix

**Definition 11.10.** Let $A$ be an $n \times n$ lower-triangular matrix. If $k = n(n+1)/2$, the $k \times n^2$ matrix $L_n$ is called the *elimination matrix* if $\text{vec} A = L'_n \text{vech} A$. The difference between $G_n$ and $L'_n$ is that $\text{vec} A$ now contains some zeros. Thus $L'_n$ can be obtained from $G_n (= D_n)$ by replacing $n(n-1)/2$ rows of $G_n$ by zeros; (d) below gives a clearer picture.

11.33. We have the following properties for $L_n$.

(a) $L_n$ has full row rank $k$.

(b) $LL' = I_k$.

(c) $L'_n = L'_n$.

(d) From (b) we have $\text{vech} A = L_n \text{vec} A$, so that $L_n$ eliminates the zeros from $\text{vec} A$.

(e) $L_n G_n = I_k$, $k = n(n+1)/2$.

(f) $G_n L_n P_n = P_n$, where $P_n = \frac{1}{2}(I_{n^2} + I_{(n,n)})$ (i.e., $D_n L_n N_n = N_n$).

(g) $G_n^+ = L_n P_n$.

Similar properties apply to the situation where $A$ is strictly lower-triangular, that is lower-triangular but with zero diagonal elements (Schott 2005: 317–318). Triangular matrices, and in fact any patterned matrix can be handled using a general kind of vec operator (cf. Section 18.3.5).

**Proofs.** Section 11.5.2.

11.6 STAR OPERATOR

**Definition 11.11.** Let \( A = (a_{ij}) \) be \( m \times n \) and \( B = mp \times nq \). Then we define the \( p \times q \) matrix (MacRae [1974])

\[
A * B = \sum_{i=1}^{m} \sum_{j=1}^{n} a_{ij} B_{ij},
\]

where \( B_{ij} \) is the \((i,j)\)th submatrix of \( B \) when \( B \) is partitioned into submatrices of size \( p \times q \).

When \( A \) and \( B \) are the same size, \( A * B = \text{trace}(A'B) \).

11.34. If \( C \) is \( r \times s \), then \( (A * B) \otimes C = A * (B \otimes C) \).

11.35. \( A * B = B * (A \otimes \text{vec}_p(\text{vec}_q')' \).

11.36. If \( x \) is \( p \times 1 \) and \( y \) is \( q \times 1 \), then

\[
x'(A * B)y = A * (I_m \otimes x')B(I_n \otimes y)
\]

\[
= (I_m \otimes x)A(I_n \otimes y') * B.
\]

11.37.

\[
X_{m \times n} Y_{n \times p} Z_{p \times q} = Y * \text{vec} X(\text{vec} Z')'
\]

\[
= Y' * (Z \otimes I_m)I_{(m,q)}(X \otimes I_q).
\]

**Proofs.** Section 11.6.

11.34–11.37. MacRae [1974].

11.7 HADAMARD PRODUCT

We now consider a particular product that arises in a wide variety of mathematical applications such as covariance matrices for independent zero mean random vectors and characteristic functions in probability theory (Horn and Johnson [1985: 301, 393–394]). Further mathematical applications are described by Horn and Johnson [1985: 455–457] and Horn and Johnson [1991: chapter 5]. The Hadamard product appears in several places in this book. In this section \( A \preceq B \) means that \( A - B \) is non-negative definite.

**Definition 11.12.** If \( A = (a_{ij}) \) and \( B = (b_{ij}) \) are \( m \times n \) real or complex matrices, then their **Hadamard product** (also referred to as the **Schur product**) is the \( m \times n \) matrix \( A \circ B = (a_{ij}b_{ij}) \). The results below, where proofs are not referenced, follow from the definition by simply multiplying out the appropriate matrices.

11.38. Let \( A \) and \( B \) be \( m \times n \) matrices, and let \( e_i \) be the \( i \)th column of \( I_m \).

(a) Let \( \Phi_m = \sum_{i=1}^{m} e_i(e_i \otimes e_i)' = \sum_{i=1}^{m} e_i(\text{vec} E_{ii})' \), where \( E_{ii} = e_i e_i' \). Then:

(i) \( A \circ B = \Phi_m(A \otimes B)\Phi_n' \).
(ii) $\Psi_m \Psi'_m = I_m$.

(iii) If $C = (c_{ij})$ is $m \times m$, then

$$\Psi_m \text{vec } C = (c_{11}, c_{22}, \ldots, c_{mm})' = (\text{diag } C)1_m.$$ 

(iv) $\Psi_m I_{(m,m)} = \Psi_m$.

(b) $A \circ B$ is a submatrix of $A \otimes B$. In fact

$$A \circ B = (A \otimes B)_{\alpha,\beta},$$

where $(\alpha, \beta)$ denotes the submatrix formed by the intersection of the rows of $A \otimes B$ in $\alpha$ with the columns in $\beta$, where $\alpha = \{1, m + 2, 2m + 3, \ldots, m^2\}$ and $\beta = \{1, n + 2, 2n + 3, \ldots, n^2\}$.

(c) If $m = n$, then $A \circ B$ is a principal submatrix of $A \otimes B$.

The above results can be used to prove results about $A \circ B$ using $A \otimes B$.

11.39. Let $A$ and $B$ be $m \times n$ matrices. Then the following hold.

(a) $A \circ B = B \circ A$.

(b) $(A \circ B)' = A' \circ B'$.

(c) $\text{trace}(AB') = 1'_m (A \circ B)1_n$.

(d) $\text{rank}(A \circ B) \leq \text{rank } A \cdot \text{rank } B$.

11.40. If all matrices are the same size, then

$$(A + B) \circ (C + D) = A \circ C + A \circ D + B \circ C + B \circ D.$$ 

11.41. If $A$, $B$, and $C$ are all $m \times n$ matrices, then

$$\text{trace}[(A \circ B)C'] = \text{trace}[(A \circ C)B'].$$

11.42. (Multiplication by Diagonal Matrices) Suppose $A$ and $B$ are $m \times n$, $D$ is $m \times m$, and $E$ is $n \times n$, where $D$ and $E$ are diagonal matrices, then

$$D(A \circ B)E = (DAE) \circ B = (DA) \circ (BE) = (AE) \circ (DB) = A \circ (DBE).$$

11.43. If $A$ is square, then $A \circ 11' = A = 11' \circ A$.

11.44. (Quadratics) Let $A$ and $B$ be $n \times n$ matrices, and suppose $y, z \in \mathbb{C}^n$. Then

$$y^*(A \circ B)z = \text{trace}(D_y AD_z B'),$$

where $D_y = \text{diag}(y)$ and $D_z = \text{diag}(z)$.

11.45. If $A$ and $B$ are Hermitian matrices, then so is $A \circ B$.

11.46. Let $A$ and $B$ be Hermitian non-negative definite $n \times n$ matrices, that is, $A \succeq 0$ and $B \succeq 0$. Then:

(a) $A \circ B \succeq 0$. The same results apply to $A \circ A \circ \cdots \circ A$ to any number of terms.
(b) $\det(A \circ B) + \det A \cdot \det B \geq b_{11}b_{22} \cdots b_{nn} \det A + a_{11}a_{22} \cdots a_{nn} \det B$.

(c) $\prod_{i=1}^{n} a_{ii} b_{ii} \geq \det(A \circ B) \geq b_{11} b_{22} \cdots b_{nn} \det A \geq \det A \det B$.

(Note that $A$ and $B$ can be interchanged.) The left-hand side follows from (12.27).

(d) $A^2 \circ B^2 \succeq (A \circ B)^2$.

(e) If $A$ and $B$ are positive definite, then:

(i) $A \circ B$ is positive definite.

(ii) $A^{-1} \circ B^{-1} \succeq (A \circ B)^{-1}$.

(f) If $A \succ 0$, and $B \succeq 0$ with $r$ nonzero diagonal entries, then $\text{rank}(A \circ B) = r$.

(g) If $B \succ 0$, and $A \succeq 0$ with positive diagonal elements, then $A \circ B \succ 0$.

(h) If $A \succ 0$, then $A \circ A^{-1} \succeq I_n \succeq (A^{-1} \circ A)^{-1}$. Horn and Johnson [1991: section 5.4] discuss the properties of $A \circ A^{-1}$ and $A \circ (A^{-1})'$.

11.47. (Fejér's Theorem) Let $A$ be any $n \times n$ matrix. Then $A$ is Hermitian non-negative definite if and only if $\text{trace}(A \circ B) \geq 0$ for all Hermitian non-negative definite $n \times n$ matrices $B$.

11.48. (Eigenvalues) Let $A$ and $B$ be $n \times n$ Hermitian non-negative definite matrices.

(a) Let $b_{\text{max}}$ and $b_{\text{min}}$ be maximum and minimum entries of the diagonal elements of $B$. Then, for all $j$,

$$b_{\text{min}} \lambda_{\text{min}}(A) \leq \lambda_j(A \circ B) \leq b_{\text{max}} \lambda_{\text{max}}(A).$$

(b) $\lambda_{\text{min}}(A) \lambda_{\text{min}}(B) \leq \lambda_j(A \circ B) \leq \lambda_{\text{max}}(A) \lambda_{\text{max}}(B)$ for all $j$.

(c) Let $R = (\rho_{ij})$ be any $n \times n$ correlation matrix.

(i) Since $\rho_{ii} = 1$ for all $i$, it follows from (a) that

$$\lambda_{\text{min}}(A) \leq \lambda_j(A \circ R) \leq \lambda_{\text{max}}(A).$$

(ii) Setting $R = I_n$, we have $\lambda_{\text{min}}(A) \leq a_{jj} \leq \lambda_{\text{max}}(A)$.

(d) $\lambda_{\text{min}}(A \circ B) \geq \lambda_{\text{min}}(AB)$.

11.49. (Singular Values) Let $A$ and $B$ be $m \times n$ matrices, and let $\sigma_j(C)$ be the $j$th singular value of $C$, where the singular values are listed in decreasing order of magnitude. Then

$$\sum_{j=1}^{i} \sigma_j(A \circ B) \leq \sum_{j=1}^{i} \sigma_j(A) \sigma_j(B), \quad i = 1, 2, \ldots, n.$$

11.50. If $A$ and $B$ are real or complex $m \times n$ matrices, then

$$(AA^*) \circ (BB^*) \succeq (A \circ B)(A^* \circ B^*).$$
11.51. Let $A$ and $B$ be $n \times n$ Hermitian positive definite matrices, and let $C$ and $D$ be any $m \times n$ real or complex matrices. Then

$$(CA^{-1}C^*) \circ (DB^{-1}D^*) \succeq (C \circ D)(A \circ B)^{-1}(C \circ D)^*.$$  

**Proofs.** Section 11.7.

11.39. Here (a) and (b) are obvious, (c) and (d) are given by Schott [2005: 297], and (d) is given by Horn and Johnson [1991: 307].
11.40. Follows directly from the definition of “$\circ$”.
11.42. Let $C = A \circ B$. Then $(DCE)_{ij} = \sum_r \sum_s d_{ir}c_{rs}e_{sj}$, which can be expressed in the form $\sum_r \sum_s d_{ir}a_{rs}e_{sj} \cdot b_{rs} = [(DAE) \circ B]_{ij}$, and so on.
11.43. Follows from $a_{ij} \cdot 1 = a_{ij}$.
11.46g. Horn and Johnson [1991: 309] and Schott [2005: 300, real case].
11.8 RAO–KHATRI PRODUCT

Definition 11.13. Let $A = (a_1, a_2, \ldots, a_n)$ be a $p \times n$ and $B = (b_1, b_2, \ldots, b_n)$ be $m \times n$ matrices. Then the Rao–Khatri product, denoted by $A \odot B$, of $A$ and $B$ is the $mp \times n$ partitioned matrix

$$A \odot B = (a_1 \otimes b_1, a_2 \otimes b_2, \ldots, a_n \otimes b_n).$$

11.52. Let $A_{p \times n}$, $B_{m \times n}$, $C_{m \times p}$, and $D_{n \times m}$ be four matrices. Then

$$(C \otimes D)_{mn \times mp}(A \odot B)_{mp \times n} = (CA)_{m \times n} \odot (DB)_{n \times n}.$$  

11.53. Let $A$ and $B$ be non-negative definite $n \times n$ matrices of ranks $r$ and $s$, respectively. Let $A = R'R$, where $R$ is $r \times n$, and let $B = S'S$, where $S$ is $s \times n$ [cf. (10.10)]. Then

$$A \odot B = (R \odot S)'(R \odot S).$$

Proofs. Section 11.8.

Inequalities are used extensively in statistics and, because they relate to almost every chapter in this book, they are difficult to categorize. Those concerned with general inner products and norms are considered in Sections 2.2.1 and 4.6. Those involved with ranks are discussed in Chapter 3, while those for eigenvalues appear in Chapter 6. Some inequalities for non-negative definite matrices appear in Chapter 9, and those relating to majorization appear in Chapter 23. There are a large number of inequalities involving probability and random variables and a selection of these appear in Chapters 22 and 23. Optimization in Chapter 24 generates further inequalities. So what is in this chapter? I have collected here some of the more traditional inequalities such as Cauchy–Schwarz, Kantorovich, Hölder, Minkowski, and so on, and their extensions. At the end I have listed a few identities that can be useful in setting up inequalities.

12.1 CAUCHY–SCHWARZ INEQUALITIES

The inequalities given below are fairly basic ones. However, for further extensions and refinements, including those for complex numbers, the reader is referred to Dragomir [2004: chapters 1–3].
12.1.1 Real Vector Inequalities and Extensions

12.1. Let \( \mathbf{x} = (x_i) \) and \( \mathbf{y} = (y_i) \) be real \( n \)-dimensional vectors. In addition to the basic inequality in (a) below, we can obtain various extensions from (2.17) by using a different vector space and a different inner product.

(a) (Cauchy–Schwarz) \( (\mathbf{x}'\mathbf{y})^2 \leq (\mathbf{x}'\mathbf{x})(\mathbf{y}'\mathbf{y}) \),
with equality if and only if \( \mathbf{x} \propto \mathbf{y} \). Many different proofs of this result are available. For example, we can use Lagrange’s identity of (12.44a). Alternatively, we also have

\[
\mathbf{x}'\mathbf{x} - (\mathbf{x}'\mathbf{y})(\mathbf{y}'\mathbf{y})^{-1}(\mathbf{y}'\mathbf{x}) = \mathbf{x}'(\mathbf{I}_n - \mathbf{P}_y)\mathbf{x} \geq 0,
\]

since the projection matrix \( \mathbf{I}_n - \mathbf{P}_y = \mathbf{P}_{\mathbb{C}(y)^\perp} \) that projects orthogonally onto \( \mathbb{C}(y)^\perp \) is non-negative definite (cf. 2.49f).

(b) Let \( \mathbf{A} \) be non-negative definite and, using (10.10), let \( \mathbf{A} = \mathbf{B}'\mathbf{B} \).

(i) \( (\mathbf{x}'\mathbf{A}\mathbf{y})^2 \leq (\mathbf{x}'\mathbf{A}\mathbf{x})(\mathbf{y}'\mathbf{A}\mathbf{y}) \), with equality if and only if \( \mathbf{B}\mathbf{x} \propto \mathbf{B}\mathbf{y} \). A sufficient condition for equality is \( \mathbf{x} \propto \mathbf{y} \). Furthermore, if \( \mathbf{A} \) is positive definite, then

\[
\sup_{\mathbf{x} : \mathbf{x} \neq \mathbf{0}} \frac{(\mathbf{x}'\mathbf{A}\mathbf{y})^2}{\mathbf{x}'\mathbf{A}\mathbf{x}} = \mathbf{y}'\mathbf{A}\mathbf{y}.
\]

(ii) From (i) we can deduce \( |a_{ij}| \leq \max_i |a_{ii}| \).

(c) If \( \mathbf{A} \) is non-negative definite and \( \mathbf{y} \in \mathbb{C}(\mathbf{A}) \), then for any weak inverse \( \mathbf{A}^{-} \),

\[
(\mathbf{x}'\mathbf{y})^2 \leq (\mathbf{x}'\mathbf{A}\mathbf{x})(\mathbf{y}'\mathbf{A}^{-}\mathbf{y}),
\]

with equality if and only if \( \mathbf{y} \propto \mathbf{A}\mathbf{x} \).

(d) If \( \mathbf{A} \) is positive definite, then

\[
(\mathbf{x}'\mathbf{y})^2 \leq (\mathbf{x}'\mathbf{A}\mathbf{x})(\mathbf{y}'\mathbf{A}^{-1}\mathbf{y}),
\]

with equality if and only if \( \mathbf{x} \propto \mathbf{A}^{-1}\mathbf{y} \) or, equivalently, \( \mathbf{y} \propto \mathbf{A}\mathbf{x} \).

(e) If \( \mathbf{A} \) is positive definite, then from (d) we have

\[
(\mathbf{x}'\mathbf{x})^2 \leq (\mathbf{x}'\mathbf{A}\mathbf{x})(\mathbf{x}'\mathbf{A}^{-1}\mathbf{x}),
\]

with equality when \( \mathbf{x} \propto \mathbf{A}\mathbf{x} \), that is, when \( \mathbf{x} \) is an eigenvector of \( \mathbf{A} \).

(f) Let \( \alpha_i \geq 0 \) (\( i = 1, 2, \ldots, n \)) such that \( \sum_i \alpha_i = 1 \). Let \( z_1, z_2, \ldots, z_n \) be real numbers.

(i) Setting \( x_i = \sqrt{\alpha_i} \) and \( y_i = \sqrt{\alpha_i}z_i \) in (a) leads to

\[
(\sum_i \alpha_i z_i)^2 \leq \sum_i \alpha_i z_i^2,
\]

with equality if and only if \( z_1 = z_2 = \cdots = z_n \).
(ii) We can set $\alpha_i = 1/n$ to get

$$\left( \sum_{i=1}^{n} z_i \right)^2 \leq n \sum_{i=1}^{n} z_i^2,$$

with equality if and only if the $z_i$s are all equal.

(iii) If all the eigenvalues $\lambda_i$ of the $n \times n$ matrix $A$ are real, then, from (i) with $\alpha_i = n^{-1}$ and $z_i = \lambda_i$, we have

$$\left( \frac{1}{n} \text{trace } A \right)^2 \leq \frac{1}{n} \text{trace}(A^2),$$

with equality if and only if the eigenvalues are all equal.

(iv) If $A$ is symmetric and nonzero with rank $r$, then, from (ii) with $n = r$, we have $(\sum_{i=1}^{r} \lambda_i)^2 \leq r \sum_{i=1}^{r} \lambda_i^2$, where the $\lambda_i$ are the nonzero eigenvalues of $A$. Hence

$$\text{rank } A \geq \frac{\text{trace}(A)^2}{\text{trace}(A^2)}.$$

Equality occurs if and only if $A$ is proportional to a symmetric idempotent matrix.

(g) If $p_i \geq 0$ for all $i$, then, replacing $x_i$ by $\sqrt{p_i} x_i$ and $y_i$ by $\sqrt{p_i} y_i$ in (a), we have

$$\left( \sum_{i=1}^{n} p_i x_i y_i \right)^2 \leq \left( \sum_{i=1}^{n} p_i x_i^2 \right) \left( \sum_{i=1}^{n} p_i y_i^2 \right).$$

(h) Suppose $x_i > 0$ for all $i$ and $\mu = (\mu_i)$ is arbitrary. Then, replacing $x_i$ by $\sqrt{x_i} / \mu_i$ and $y_i$ by $1 / \sqrt{x_i}$ in (a)(i) and rearranging, we get

$$\left( \sum_{i=1}^{n} x_i^{-1} \right)^{-1} \leq \left( \sum_{i=1}^{n} x_i \mu_i^{-2} \right) \left( \sum_{i=1}^{n} \mu_i^{-1} \right)^{-2}.$$

If $E(x_i) = \mu_i$, then taking expected values shows that expected value of a harmonic mean does not exceed the harmonic mean of their expected values.

(i) (Constrained Version) Let $A$ be an $n \times n$ matrix, and let $y \in C(A)$. If $P_A$ represents the orthogonal projection onto $C(A)$, so that we have $P_A = A(A'A)^{-1}A$ (cf. 2.49f), then

$$(x'y)^2 \leq (x'P_Ax)(y'y).$$

Equality occurs when $y \propto P_Ax$.

(j) When $A$ is positive definite and $x'y = 0$, then

$$(x'Ay)^2 \leq \left( \frac{\lambda_1 - \lambda_n}{\lambda_1 + \lambda_n} \right) x'Ax \cdot y'Ay,$$

where $\lambda_1$ and $\lambda_n$ are the maximum and minimum (positive) eigenvalues of $A$. 

12.2. (Some Lower Bounds) The results above give us upper bounds for \((x'x)^2\) and \((x'y)^2\). We now consider some lower bounds. Further details and extensions are given by Dragomir [2004: chapters 4 and 5].

(a) (Kantorovich) Let \(A\) be an \(n \times n\) real positive definite (p.d.) matrix with maximum and minimum eigenvalues of \(\lambda_1\) and \(\lambda_n\), respectively. Let \(x\) and \(y\) be any nonzero vectors in \(\mathbb{R}^n\).

(i) \((x'x)^2 \geq \frac{4\lambda_1\lambda_n}{(\lambda_1 + \lambda_n)^2} (x'Ax)(x'A^{-1}x)\).

There is a unit vector \(x\) for which there is an equality. The result also holds for a Hermitian p.d. matrix with ' replaced by ". For a generalization see Pronzato et al. [2005].

(ii) If \(A = \text{diag}(a)\) (\(a > 0\)), then the ordered eigenvalues are the same as the ordered \(a_i\) for a diagonal matrix. Let \(a_{\max} = \max\{a_i\}\), and so on. Then, from (i), we obtain

\[
(x'x)^2 \geq \frac{4a_{\max}a_{\min}}{(a_{\max} + a_{\min})^2} \left( \sum_{i=1}^{n} a_i x_i^2 \right) \left( \sum_{i=1}^{n} a_i^{-1} x_i^2 \right).
\]

(iii) If \(x_i = 1\) for all \(i\) in (ii), we have

\[
n^2 \geq \frac{4a_{\max}a_{\min}}{(a_{\max} + a_{\min})^2} \left( \sum_{i=1}^{n} a_i \right) \left( \sum_{i=1}^{n} a_i^{-1} \right).
\]

(b) (Polya–Szegö) Let \(x\) and \(y\) have positive elements. Then

\[
(x'y)^2 \geq \frac{4x_{\min}x_{\max}y_{\min}y_{\max}}{(x_{\max}y_{\max} + x_{\min}y_{\min})^2} (x'x)(y'y).
\]

(c) (Greub and Rheinboldt) Let \(A\) and \(B\) be \(n \times n\) positive definite commuting matrices (\(AB = BA\)) with eigenvalues \(\lambda_1 \geq \cdots \geq \lambda_n > 0\) and \(\mu_1 \geq \cdots \geq \mu_n > 0\), respectively. Then \(AB\) is symmetric and

\[
(x'ABx)^2 \geq \frac{4\lambda_1\lambda_n\mu_1\mu_n}{(\lambda_1\mu_1 + \lambda_n\mu_n)^2} (x'A^2x)(x'B^2x).
\]

(d) If \(A\) is an \(n \times n\) nonsingular matrix with maximum and minimum singular values of \(\sigma_1\) and \(\sigma_n\), respectively, then

\[
\frac{(x'Ay)(y'A^{-1}x)}{(x'x)(y'y)} \leq \frac{(\sigma_1 + \sigma_n)^2}{4\sigma_1\sigma_n}.
\]

Rao [2005: 67] uses the above result to define antisingular values and vectors.

(e) Suppose \(x = (x_i) > 0\), \(y = (y_i) > 0\), and \(w = (w_i) \geq 0\). Let

\[
m = \min_i \left\{ \frac{x_i}{y_i} \right\} \quad \text{and} \quad M = \max_i \left\{ \frac{x_i}{y_i} \right\}.
\]

Then

\[
\frac{\sum_{i=1}^{n} w_i x_i^2 \sum_{i=1}^{n} w_i y_i^2}{(\sum_{i=1}^{n} w_i x_i y_i)^2} \leq \frac{(m + M)^2}{4mM}.
\]
Proofs. Section 12.1.1.

12.1a. Abadir and Magnus [2005: 7].
12.1b. Abadir and Magnus [2005: 323].
12.1c. Neudecker and Liu [1994: 351]. Use $y'Ay = y'AA^-1Ay$ in (b)(i) and set $z = Ay$.
12.1d. Replace $x$ by $A^{1/2}x$ and $y$ by $A^{-1/2}y$ in (a).
12.1f(iv). Abadir and Magnus [2005: 324].
12.1i. Use (b) with $A$ replaced by $P_A$. If $y \in C(A)$, then $y = P_Ay$.
12.1j. Drury et al. [2002: 97].

12.2e. Dragomir [2004: 91].

12.1.2 Complex Vector Inequalities

Many of the above inequalities can be generalized to the complex case. By the same token, the following results for complex vectors will hold for their real counterparts.

12.3. Let $x$ and $y$ be two complex vectors in $\mathbb{C}^n$, and let $A$ be a Hermitian non-negative definite $n \times n$ matrix.

(a) There are two versions of the Cauchy-Schwarz inequality.

(i) Using the inner product $\langle x, y \rangle = x^*y$, we have from (2.17) that

$$x^*x - (x^*y)(y^*y)^{-1}(y^*x) \geq 0.$$ 

Equality occurs when $x \propto y$.

(ii) Since $|ab| = |a||b|$, we have from (5.1b),

$$\left| \sum_{i=1}^{n} x_i y_i \right|^2 \leq \left( \sum_{i=1}^{n} |x_i| y_i \right)^2 \leq \sum_{i=1}^{n} |x_i|^2 \sum_{i=1}^{n} |y_i|^2.$$ 

Equality occurs when $x = cy$ for any complex scalar $c$.

(b) $|x^*y|^2 \leq (x^*x)(y^*y)$. Equality occurs when $x \propto y$. 
(c) \(|x^*Ay|^2 \leq (x^*Ax)(y^*Ay)\), with equality when \(x \propto y\).

(d) Let \(A\) be Hermitian positive definite.

(i) \(|x^*y|^2 \leq (x^*Ax)(y^*A^{-1}y)\). Equality occurs when \(y \propto Ax\).

(ii) \((x^*x)^2 \leq (x^*Ax)(x^*A^{-1}x)\), which implies \((x^*Ax)^{-1} \leq x^*A^{-1}x\) when \(x^*x = 1\). Equality occurs when \(x \propto Ax\), that is, when \(x\) is an eigenvector.

(e) (Wielandt) If \(A\) is Hermitian positive definite and \(x^*y = 0\), then

\[|x^*Ay|^2 \leq \left(\frac{\lambda_1 - \lambda_n}{\lambda_1 + \lambda_n}\right)^2 (x^*Ax)(y^*Ay).\]

Equality occurs when \(x = (x_1 + x_n)/\sqrt{2}\) and \(y = (x_1 - x_n)/\sqrt{2}\), where \(x_1\) and \(x_n\) are the eigenvectors corresponding to \(\lambda_1\) and \(\lambda_n\), respectively, the maximum and minimum eigenvalues of \(A\). Rao [2005: 63] applies the above result to sphericity tests in multivariate analysis. Along with references, he also gives a matrix generalization of the above result (Rao [2005: 62]).

Note that \(|\cdot|\) represents the modulus.

**12.4.** Let \(A\) and \(C\) be Hermitian positive definite \(n \times n\) and \(m \times m\) matrices, respectively, and let \(B\) be \(n \times m\). The following statements are equivalent:

(1) \((x^*Ax)(y^*Cy) \geq |x^*By|^2\) for all \(x \in \mathbb{C}^n\) and all \(y \in \mathbb{C}^m\).

(2) \(x^*Ax + y^*Cy \geq 2|x^*By|\) for all \(x \in \mathbb{C}^n\) and all \(y \in \mathbb{C}^m\).

(3) \(\rho(B^*A^{-1}BC^{-1}) \leq 1\), where \(\rho(\cdot)\) is the spectral radius.

(4) \(\begin{pmatrix} A & B \\ B^* & C \end{pmatrix} \succeq 0\) (i.e., non-negative definite).

**Proofs.** Section 12.1.2.

12.3. For (a) see Dragomir [2004: 2–3]; for (a)–(d) see Zhang [1999: 203] (and quoted by Rao and Rao [1998: 455]); and for (e), Horn and Johnson [1985] and Rao [2005: 61, real case].

12.4. Horn and Johnson [1985: 473].

**12.1.3 Real Matrix Inequalities**

In this section we give a number of matrix inequalities that might be regarded as extensions of the Cauchy–Schwarz inequality for vectors.

**12.5.** Let \(A\) and \(B\) be any real \(m \times n\) matrices.

(a) \((\text{trace } A'B)^2 \leq (\text{trace } A'A)(\text{trace } B'B)\), with equality if and only if one of the matrices is a multiple of the other.
This inequality can also be expressed in the form \( |\langle \mathbf{A}, \mathbf{B} \rangle| \leq \|\mathbf{A}\|_F \|\mathbf{B}\|_F \) (cf. (2.20) and Harville [1997: 62]), where \( \| \cdot \|_F \) is the Frobenius norm. For some generalizations see Rao and Rao [1998: 494–495].

(b) \( \text{trace}[(\mathbf{A}'\mathbf{B})^2] \leq \text{trace}[(\mathbf{A}'\mathbf{A})(\mathbf{B}'\mathbf{B})] \), with equality if and only if \( \mathbf{AB}' \) is symmetric. Furthermore, since \( \text{trace}(\mathbf{A}'\mathbf{B}) = \text{trace}(\mathbf{B}'\mathbf{A}) = \text{trace}(\mathbf{AB}') \), we have

\[
\text{trace}[(\mathbf{A}'\mathbf{B})^2] \leq \text{trace}[(\mathbf{A}\mathbf{A}')((\mathbf{B}\mathbf{B}')), \n\]

with equality if and only if \( \mathbf{A}'\mathbf{B} \) is symmetric.

Setting \( m = n \) and \( \mathbf{A} = \mathbf{I}_n \), we have

\[
\text{trace}(\mathbf{B}') \leq \text{trace}(\mathbf{B}'\mathbf{B}),
\]

with equality if and only if \( \mathbf{B} \) is symmetric.

(c) \( (\det \mathbf{A}'\mathbf{B})^2 \leq (\det \mathbf{A}'\mathbf{A})(\det \mathbf{B}'\mathbf{B}) \), with equality if and only if \( \mathbf{A}'\mathbf{A} \) or \( \mathbf{B}'\mathbf{B} \) are singular, or if \( \mathbf{B} = \mathbf{AR} \) for some nonsingular \( \mathbf{R} \).

(d) From (2.15a) we have \( \|\mathbf{A} + \mathbf{B}\|_F \leq \|\mathbf{A}\|_F + \|\mathbf{B}\|_F \), where \( \| \cdot \|_F \) is the Frobenius norm.

(e) \( \mathbf{A}'[\mathbf{I}_m - \mathbf{B}(\mathbf{B}'\mathbf{B})^{-1} \mathbf{B}']\mathbf{A} = \mathbf{A}'(\mathbf{I}_m - \mathbf{P}_{\mathbf{B}})\mathbf{A} \) is non-negative definite since \( (\mathbf{I}_m - \mathbf{P}_{\mathbf{B}}) \) is non-negative definite (cf. 2.49f). Hence, from (10.48b),

\[
\det(\mathbf{A}'\mathbf{A}) \geq \det[\mathbf{A}'\mathbf{B}(\mathbf{B}'\mathbf{B})^{-1} \mathbf{B}'\mathbf{A}].
\]

12.6. (Measures of Relative Efficiency in Regression) Consider the linear regression model of Section 20.7, namely \( \mathbf{y} = \mathbf{X}\mathbf{\beta} + \mathbf{\epsilon} \), where \( \mathbf{X} \) is \( n \times p \) of rank \( p \), \( \text{var}(\mathbf{\epsilon}) = \sigma^2 \mathbf{V} \), and \( \mathbf{V} \) is positive definite. We define the eigenvalues of \( \mathbf{V} \) to be \( \lambda_i = \lambda_i(\mathbf{V}) \) and we impose the usual order \( \lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n > 0 \). Then the variance matrix of the generalized (weighted) least squares estimate of \( \mathbf{\beta} \) is \( (\mathbf{X}'\mathbf{V}^{-1}\mathbf{X})^{-1} \) and that of the ordinary least squares estimator is \( (\mathbf{X}'\mathbf{X})^{-1}(\mathbf{X}'\mathbf{V}\mathbf{X})(\mathbf{X}'\mathbf{X})^{-1} \). Measures of the relative efficiency of the ordinary least squares estimate with respect to the generalized least squares estimate have been based on the roots of

\[
\det[(\mathbf{X}'\mathbf{X})^{-1}(\mathbf{X}'\mathbf{V}\mathbf{X})(\mathbf{X}'\mathbf{X})^{-1} - \theta(\mathbf{X}'\mathbf{V}^{-1}\mathbf{X})^{-1}] = 0.
\]

Four such measures \( E_i \) \( (i = 1, 2, 3, 4) \) taken from Rao and Rao [1998: 464] are given below.

(a) \( E_1 = \frac{\det(\mathbf{X}'\mathbf{V}\mathbf{X}) \det(\mathbf{X}'\mathbf{V}^{-1}\mathbf{X})}{[\det(\mathbf{X}'\mathbf{X})]^2} = \prod_{i=1}^{p} \theta_i \). If \( s = \min\{p, n - p\} \), then

\[
1 \leq E_1 \leq \prod_{i=1}^{s} \left( \frac{\lambda_i + \lambda_{n-i+1}}{4\lambda_i \lambda_{n-i+1}} \right)^2.
\]

(b) \( E_2 = \sum_{i=1}^{p} \theta_i \). If \( s = \min\{p, n - p\} \), \( t = 0 \) if \( s = p \), and \( t = 2p - n \) if \( s = n - p \), then

\[
p \leq \sum_{i=1}^{p} \theta_i \leq \sum_{i=1}^{s} \left( \frac{\lambda_i + \lambda_{n-i+1}}{4\lambda_i \lambda_{n-i+1}} \right)^2 + t.
\]
(c) \( E_3 = \text{trace}[(X'X)^{-1}(X'VX)(X'X)^{-1} - (X'V^{-1}X)^{-1}] \).

When \( X'X = I_n \),

\[
0 \leq E_3 \leq \frac{1}{4} \sum_{i=1}^{s} (\sqrt{\lambda_i} - \sqrt{\lambda_{n-i+1}})^2,
\]

where \( s = \min\{p, n - p\} \).

(d) \( E_4 = \text{trace}[PV^2P - (PVP)(PVP)] \), where \( P = X(X'X)^{-1}X' \) represents the orthogonal projection onto \( C(X) \). Then

\[
0 \leq E_4 \leq \frac{1}{4} \sum_{i=1}^{s} (\lambda_i - \lambda_{n-i+1})^2.
\]

12.7. (Matrix Kantorovich Inequality) Let \( A \) be a positive definite \( n \times n \) matrix, and let \( U \) be an \( n \times p \) matrix such that \( U'U = I_p \). If \( \lambda_1 = \lambda_{\text{max}}(A) \) and \( \lambda_n = \lambda_{\text{min}}(A) \), then

\[
U'AU \preceq \frac{(\lambda_1 + \lambda_n)^2}{4\lambda_1\lambda_n} (U'A^{-1}U)^{-1}.
\]

Interchanging \( A \) and \( A^{-1} \) so that \( \lambda_1^{-1} = \lambda_{\text{min}}(A^{-1}) \) and \( \lambda_n^{-1} = \lambda_{\text{max}}(A^{-1}) \), we have

\[
U'A^{-1}U \preceq \frac{(\lambda_1 + \lambda_n)^2}{4\lambda_1\lambda_n} (U'AU)^{-1}.
\]

Also

\[
(U'AU)^{-1} \preceq U'A^{-1}U.
\]

(Note that \( B \preceq C \) means that \( C - B \) is non-negative definite.) For further extensions see Baksalary and Puntanen [1991] and Drury et al. [2002].

12.8. (Further Matrix Kantorovich-Type Inequalities)

(a) Let \( A, B, \) and \( C \) be \( n \times n \) positive definite matrices, and let \( X \) be an \( n \times k \) matrix of rank \( k \). Then:

(i) \[
\sup_X \frac{\det(X'B^{-1}AB^{-1}X) \det(X'A^{-1}X)}{[\det(X'B^{-1}X)]^2} = \sum_{i=1}^{m} \frac{(\mu_i + \mu_{n-i+1})^2}{4\mu_i\mu_{n-i+1}},
\]

where \( m = \min\{k, n - k\} \) and \( \mu_1 \geq \cdots \geq \mu_n > 0 \) are the roots of \( \det(B - \mu A) = 0 \), that is, the eigenvalues of \( BA^{-1} \) (and of \( A^{-1}B \)).

(ii) \[
\sup_X \frac{\det(X'B^2X) \det(X'C^2X)}{[\det(X'BCX)]^2} = \sum_{i=1}^{m} \frac{(\mu_i + \mu_{n-i+1})^2}{4\mu_i\mu_{n-i+1}},
\]

where \( m = \min\{k, n - k\} \), \( BC = CB \), and the \( \mu_i \) are the eigenvalues of \( BC^{-1} \).
(b) Let $B$ be an $n \times n$ non-negative definite matrix of rank $b$, and let $A$ be $n \times r$ of rank $a$ ($a \leq \min\{b, r\}$) such that $C(A) \subseteq C(B)$. Furthermore, let $\lambda_1 \geq \cdots \geq \lambda_b > 0$ be the eigenvalues of $B$. Then, if $A^+$ and $B^+$ are Moore–Penrose inverses, we have:

\[(i) \quad A^+B^+(A^+)' \leq (\frac{\lambda_1 + \lambda_b}{4\lambda_1\lambda_b})^2 (A'B A)^+,\]

with equality if and only if $A = 0$, or $A'BA = \frac{1}{2}(\lambda_1 + \lambda_b)A'A$ and $A'B^+A = (\frac{\lambda_1 + \lambda_b}{2\lambda_1\lambda_b}) A'A$.

\[(ii) \quad A^+B(A^+)' - (A'B^+A)^+ \leq (\sqrt{\lambda_1} - \sqrt{\lambda_b})^2 (A'A)^+ ,\]

with equality if and only if $A = 0$, or $\lambda_1 = \lambda_b$, or $A'BA = (\lambda_1 - \lambda_b - \sqrt{\lambda_1\lambda_b})A'A$ and $A'B^+A = (\lambda_1\lambda_b)^{-1/2}A'A$.

The above, along with two further results, are quoted by Rao and Rao [1998: 496]. They also give a Kantorovich-type inequality for complex matrices. See also Liu [2002a] and Liu and Neudecker [1996].

**Proofs.** Section 12.1.3.


12.6c. Rao [1985]; see also Drury et al. [2002: section 3] for further details and related work.

12.6d. Bloomfield and Watson [1975].


12.8a(i). Lin [1984].

12.8a(ii). Khatri and Rao [1981]. This result follows from (i) by replacing $A^{-1}$ by $C^2$ and $B^{-1}$ by $BC$. Here $BC$ is symmetric and positive definite when $BC = CB$ as the eigenvalues of $B^{1/2}CB^{1/2}$ are positive.

12.1.4 Complex Matrix Inequalities

12.9. Let $X$ and $Y$ be $n \times p$ and $n \times q$ complex matrices, respectively. Then generalizing (12.5e), we have

\[X^*X - X^*Y(Y^*Y)^{-1}Y^*X = X^*(I_n - P_Y)X \succeq 0,\]

i.e., non-negative definite as the orthogonal projector $I_n - P_Y$ is Hermitian non-negative definite (cf. 2.49f). Equality occurs if and only if $C(X) \subseteq C(Y)$. A generalization of this result follows.
12.10. Let $A$ be an $n \times n$ Hermitian non-negative definite matrix with $P_A = A(A^*A)^{-1}A^*$, and let $U$ be an $n \times p$ matrix. Then

$$U^*A^+U \succeq U^*P_AU(U^*AU)^+U^*P_AU,$$

with equality if and only if $C(AU) = C(P_AU)$.

12.11. Let $A$ be an $n \times n$ Hermitian positive definite matrix, and let $X$ be $n \times p$ and $Y$ be $n \times q$ satisfying $X^*Y = 0$. Then

$$(X^*AY)(Y^*AY)^-(Y^*AX) \leq \left(\frac{\lambda_1 - \lambda_n}{\lambda_1 + \lambda_n}\right)^2 X^*AX,$$

where $(Y^*AY)^-$ is any weak inverse, with equality when

$$(u_1 + u_n) \propto (\lambda_1^{-1}P_{u_1} + \lambda_n^{-1}P_{u_n}).$$

Here $P = X(X^*X)^{-1}X^*$ is the orthogonal projector onto $C(X)$ and $\lambda_1$ and $\lambda_n$ are the largest and smallest eigenvalues, respectively, of $A$ with corresponding eigenvectors $u_1$ and $u_n$.

12.12. Let $A$ and $B$ be $n \times n$ real or complex matrices.

(a) $|\text{trace}(AB)|^2 \leq \text{trace}(A^*A)\text{trace}(B^*B)$.

(b) If $A$ and $B$ are Hermitian, then

$$\text{trace}([AB]^2) \leq \text{trace}(A^2B^2),$$

with equality if and only if $AB = BA$. For a generalization see (12.33d).

12.13. (Unitarily Invariant Norm) Let $\| \cdot \|_{ui}$ be any unitarily invariant norm defined on the vector space of $m \times n$ complex matrices (Section 4.6.3), and let $A$ and $B$ be $m \times n$ matrices.

(a) If $|A|$ represents the general square root of $A$ (i.e., $|A| = (A^*A)^{1/2}$), then:

(i) $\|A^*B\|_{ui}^p \leq \|(A^*A)^p\|_{ui} \|(B^*B)^p\|_{ui}$ for all $p > 0$.

(ii) Setting $p = \frac{1}{2}$ in (i) and using $\|A\|_{ui} = \|A\|_{ui}$ (cf. 4.86), we have

$$\|A^*B\|_{ui}^{1/2} \|A\|_{ui}^2 \|B\|_{ui}.$$

(iii) If $p = 1$ in (i), we have a Cauchy–Schwarz type of inequality

$$\|A^*B\|_{ui}^2 \leq \|A\|_{ui}^2 \|B\|_{ui}^2.$$

(b) (Hadamard Product) $\|A \circ B\|_{ui}^2 \leq \|AA^*\|_{ui} \|BB^*\|_{ui}$.

Proofs. Section 12.1.4.

12.10. Baksalary and Puntanen [1991: 104], who also give some special cases and variations on the result.

12.11. Wang and Ip [2000] (see also Drury [2002]).


12.13a. Horn and Johnson [1985: 212, exercises 6 and 7, hint for proof only].

12.13b. Horn and Johnson [1991: 212, exercise 8, hint for proof only].
12.2 Hölder’s Inequality and Extensions

Let \( a, b, \ldots, g \) be \( m \) real \( n \times 1 \) vectors of non-negative elements, and let \( \alpha_i > 0 \) \((i = 1, 2, \ldots, n)\) such that \( \sum_{i=1}^{m} \alpha_i = 1. \)


\[
\prod_{i=1}^{n} a_i^{\alpha_i} \prod_{i=1}^{n} b_i^{\alpha_i} + \cdots + \prod_{i=1}^{n} g_i^{\alpha_i} \leq \prod_{i=1}^{n} (a_i + b_i + \cdots + g_i)^{\alpha_i}.
\]

Equality occurs if and only if either every pair of vectors \( a, b, \) and so on, are proportional, or there is a \( k \) such that \( a_k = b_k = \cdots = g_k = 0. \) If \( A = (a, b, \ldots, g) \), then the conditions for equality are either rank \( A = 1 \) or \( A \) contains a row of zeros.

12.15. Interchanging the rows and columns of \( A \) in the previous result leads to the following.

(a) \[
\sum_{i=1}^{n} a_i^{\alpha_1} b_i^{\alpha_2} \cdots g_i^{\alpha_m} \leq (\sum_{i=1}^{n} a_i)^{\alpha_1} (\sum_{i=1}^{n} b_i)^{\alpha_2} \cdots (\sum_{i=1}^{n} g_i)^{\alpha_m},
\]

with equality if and only if rank \( A = 1 \) or \( A \) contains a column of zeros.

(b) Putting \( m = 2 \) in (a) leads to

\[
\sum_{i=1}^{n} a_i^{\alpha} b_i^{1-\alpha} \leq (\sum_{i=1}^{n} a_i)^{\alpha} (\sum_{i=1}^{n} b_i)^{1-\alpha} \quad (0 < \alpha < 1),
\]

with equality if and only if \( a = kb. \)

(c) (Hölder’s Inequality) Replacing \( a_i \) by \( a_i^{1/\alpha} \) and \( b_i \) by \( b_i^{1/(1-\alpha)} \) in (b) leads to

\[
\sum_{i=1}^{n} a_i b_i \leq (\sum_{i=1}^{n} a_i^{1/\alpha})^{\alpha} (\sum_{i=1}^{n} b_i^{1/(1-\alpha)})^{1-\alpha}
= (\sum_{i=1}^{n} a_i^r)^{1/r} (\sum_{i=1}^{n} b_i^s)^{1/s},
\]

where \( r (= 1/\alpha) > 1 \) and \( r^{-1} + s^{-1} = 1. \) Equality occurs if and only if \( a_i^r = kb_i^s \) for \( i = 1, 2, \ldots, n, \) or either \( a \) or \( b \) is 0. The inequality in (c) is reversed if \( r \neq 0, r < 1 \) (and \( s < 0). \) We can deduce the previous results from (c).

(d) If \( a \) and \( b \) are vectors of complex numbers, then replacing \( a_i \) by \( |a_i|, \) and so on, in (c), we have for \( r > 1 \) and \( r^{-1} + s^{-1} = 1, \)

\[
\sum_{i=1}^{n} |a_i b_i| \leq (\sum_{i=1}^{n} |a_i|^r)^{1/r} (\sum_{i=1}^{n} |b_i|^s)^{1/s}.
\]

Equality occurs if and only if

\[
|a_i|^r = k|b_i|^s
\]

for \( i = 1, 2, \ldots, n, \) and \( \arg(a_i b_i) \) is independent of \( i. \)
12.16. (Matrix Analogues) Let $A$ and $B$ any two $n \times n$ non-negative definite matrices, and let $0 < \alpha < 1$.

(a) (Magnus) \[ \text{trace}(A^\alpha B^{1-\alpha}) \leq (\text{trace } A)^\alpha (\text{trace } B)^{1-\alpha} \]
with equality if and only if $B = kA$ for some $k > 0$.

(b) \[ \text{trace}(A^\alpha B^{1-\alpha}) \leq \text{trace}[\alpha A + (1 - \alpha)B] \]
with equality if and only if $A = B$.

(c) \[ (\det A)^\alpha (\det B)^{1-\alpha} \leq \det(\alpha A + (1 - \alpha)B) \]
with equality if and only if $A = B$ or $\det(\alpha A + (1 - \alpha)B) = 0$. The result is obviously true if either $A$ or $B$ is singular, so it is more applicable to positive definite matrices. In this case it follows that $\phi(A) = \log \det A$ is concave on the space of positive definite matrices.

(d) Let $A_i$ be positive definite and $\alpha_i > 0$ for $(i = 1, 2, \ldots, k)$, where $\sum \alpha_i = 1$. Then
\[ (\det A_1)^{\alpha_1}(\det A_2)^{\alpha_2}\cdots(\det A_k)^{\alpha_k} \leq \det(\alpha_1 A_1 + \alpha_2 A_2 + \cdots + \alpha_k A_k), \]
with equality if and only if the $A_i$ are all equal.

Proofs. Section 12.2.


12.15c. For a direct proof see, for example, Marcus and Minc [1964: 108], Rao and Bhimasankaram [2000: 254], and Rao and Rao [1998: 457].

12.16a. Magnus and Neudecker [1999: 221].

12.16b. Magnus and Neudecker [1999: 222].


12.3 MINKOWSKI’S INEQUALITY AND EXTENSIONS

12.17. Let $X$ be an $m \times n$ real matrix whose elements are non-negative and not all zero. If $p > 1$, then
\[ \left(\sum_{i=1}^{m} \left(\sum_{j=1}^{n} x_{ij}\right)^p\right)^{1/p} \leq \sum_{j=1}^{n} \left(\sum_{i=1}^{m} x_{ij}^p\right)^{1/p}, \]
with equality if and only if rank $X = 1$. The inequality reverses if $p < 1$ ($p \neq 0$). If $p < 0$, then the $x_{ij}$ are assumed to be all positive. A number of special cases follow below.
MINKOWSKI’S INEQUALITY AND EXTENSIONS

(a) Putting \( n = 2, a_i = x_{i1}, \) and \( b_i = x_{i2}, \) we have

\[
\left[ \sum_{i=1}^{m} (a_i + b_i)^p \right]^{1/p} \leq \left( \sum_{i=1}^{m} a_i^p \right)^{1/p} + \left( \sum_{i=1}^{m} b_i^p \right)^{1/p} \quad (p > 1),
\]

with equality if and only if \( a_i = kb_i \) for \( i = 1, 2, \ldots, n. \)

(b) Putting \( m = 2, c_j = x_{1j}, \) and \( d_j = x_{2j}, \) we have

\[
\left[ \sum_{j=1}^{n} c_j^p \right]^{1/p} + \left[ \sum_{j=1}^{n} d_j^p \right]^{1/p} \leq \left( \sum_{j=1}^{n} c_j^p \right)^{1/p} + \left( \sum_{j=1}^{n} d_j^p \right)^{1/p} \quad (p > 1),
\]

with equality if and only if \( c_j = kd_j \) for \( j = 1, 2, \ldots, n. \)

(c) If \( \alpha_i \geq 0 \) (\( i = 1, 2, \ldots, m \)) such that \( \sum_{i=1}^{m} \alpha_i = 1, \) then replacing \( x_{ij} \) by \( \alpha_i^{1/p} x_{ij} \) leads to

\[
\left[ \sum_{i=1}^{m} \alpha_i \left( \sum_{j=1}^{n} x_{ij}^p \right) \right]^{1/p} \leq \left( \sum_{j=1}^{n} \left( \sum_{i=1}^{m} \alpha_i x_{ij}^p \right)^{1/p} \right) \quad (p > 1),
\]

with equality if and only if \( \text{rank} \mathbf{X} = 1. \) The inequality reverses for \( p < 1 \) \( (p \neq 0) \).

12.18. (Matrix Analogue) Let \( \mathbf{A} \) and \( \mathbf{B} \) any two \( n \times n \) Hermitian non-negative definite matrices.

(a) (Magnus) \( |\text{trace}(\mathbf{A} + \mathbf{B})|^{1/p} \leq |\text{trace} \mathbf{A}^p|^{1/p} + |\text{trace} \mathbf{B}^p|^{1/p} \quad (p > 1), \)

with equality if and only if \( \mathbf{A} = k \mathbf{B} \) for some \( k > 0. \)

(b) \( |\det(\mathbf{A} + \mathbf{B})|^{1/n} \geq |\det \mathbf{A}|^{1/n} + |\det \mathbf{B}|^{1/n}, \)

with equality if and only if \( \det(\mathbf{A} + \mathbf{B}) = 0 \) or \( \mathbf{A} = k \mathbf{B} \) for some \( k > 0. \)

(c) \( |\det(\alpha \mathbf{A} + (1 - \alpha) \mathbf{B})|^{1/n} \geq \alpha |\det \mathbf{A}|^{1/n} + (1 - \alpha) |\det \mathbf{B}|^{1/n}, \quad 0 \leq \alpha \leq 1. \)

Proofs. Section 12.3.


12.18c. Marcus and Minc [1964: 115].
12.4 WEIGHTED MEANS

Let \( x_1, x_2, \ldots, x_n \) be non-negative real numbers, and let \( \alpha_i > 0 \) \((i = 1, 2, \ldots, n)\) be such that \( \sum_{i=1}^n \alpha_i = 1 \). Define

\[
M_p(x) = \begin{cases} 
\prod_i x_i^{\alpha_i}, & p = 0, \\
\left( \sum_i \alpha_i x_i^p \right)^{1/p}, & p \neq 0.
\end{cases}
\]

If \( p < 0 \), we assume that the \( x_i \)'s are all positive. An important special case is \( \alpha_i = 1/n \) for all \( i \). For further details see Bullen [2003], Hardy et al. [1952: chapter II], and Magnus and Neudecker [1999: 227–231].

12.19. For every \( \lambda > 0 \), \( M_p(\lambda x) = \lambda M_p(x) \).

12.20. Equality occurs in each of the following two inequalities if and only if the \( x_i \)'s are all equal.

(a) \( M_0(x) \leq M_1(x) \), so that \( \prod_i x_i^{\alpha_i} \leq \sum_i \alpha_i x_i \).

Setting each \( \alpha_i = n^{-1} \), we see that the geometric mean is less than or equal to the arithmetic mean. Note the special case \( x^a y^{1-a} \leq ax + (1-a)y \).

(b) \( M_p(x) \leq M_q(x) \) for \( p < q \).

Setting each \( \alpha_i = n^{-1} \), \( p = -1 \), and \( q = 0 \), we see that the harmonic mean is less than or equal to the geometric mean.

(c) (Matrix Version) If \( A_i \) \((i = 1, 2, \ldots, n)\) are positive definite pairwise commuting matrices (i.e., \( A_i A_j = A_j A_i \) for all \( i, j, i \neq j \)), then

\[
\frac{1}{n} \sum_{i=1}^n A_i \succeq (A_1 \cdots A_n)^{1/n} \succeq \left( \sum_{i=1}^n A_i^{-1} \right)^{-1}.
\]

Equality occurs if and only if the \( A_i \) are all equal. (Here \( A \succeq B \) means that \( A - B \) is non-negative definite.)

12.21. (Limits)

(a) \( \lim_{p \to 0^+} M_p(x) = M_0(x) \).

(b) Let \( x_{\min} \) be the smallest \( x_i \) and \( x_{\max} \) the largest. Then

\[
\lim_{p \to -\infty} M_p(x) = x_{\max}, \quad \lim_{p \to -\infty} M_p(x) = x_{\min}, \quad \text{and} \quad x_{\min} \leq M_r(x) \leq x_{\max}.
\]

12.22. \( M_p(x) \) is a concave function of \( x \) for \( p \leq 1 \) and a convex function for \( p \geq 1 \). In particular,

\[
M_p(x) + M_p(y) \leq M_p(x + y) \quad (p < 1)
\]

\[
M_p(x) + M_p(y) \geq M_p(x + y) \quad (p > 1),
\]

with equality if and only if \( x \) and \( y \) are linearly dependent.

Also \( p \log M_p(x) \) is a convex function of \( p \).
Proofs. Section 12.4.

12.20b. Magnus and Neudecker [1999: 230]. These inequalities can also be deduced from likelihood ratio test inequalities (Stefanski [1996]).

12.5 QUASILINEARIZATION (REPRESENTATION) THEOREMS

The representation of a nonlinear function as an envelope of linear functions is called quasilinearization or representation. The method is useful in proving a number of inequalities.

12.23. Let $p > 1$, $q = p/(p - 1)$, and $a_i \geq 0$ for $i = 1, 2, \ldots, n$. Then

$$
\sum_{i=1}^{n} a_i x_i \leq \left( \sum_{i=1}^{n} a_i^p \right)^{1/p}
$$

for every set of non-negative $x_1, x_2, \ldots, x_n$ satisfying $\sum_i x_i^q = 1$. Equality occurs if and only if all the $a_i$ are zero or

$$
x_i^q = \frac{a_i^p}{\sum_{j=1}^{n} a_j^p}
$$

for $i = 1, 2, \ldots, n$.

Hence

$$
\max_{\mathcal{R}} \sum_{i=1}^{n} a_i x_i = \left( \sum_{i=1}^{n} a_i^p \right)^{1/p},
$$

where $\mathcal{R}$ is the region defined by $\sum_i x_i^q = 1, x_i \geq 0$ ($i = 1, 2, \ldots, n$).

12.24. (Matrix Versions) Let $A$ be a non-negative definite $n \times n$ matrix.

(a) If $p > 1$ and $q = p/(p - 1)$, then

$$
\text{trace}(AX) \leq (\text{trace } A^p)^{1/p}
$$

for every non-negative definite $n \times n$ matrix $X$ satisfying $\text{trace}(X^q) = 1$. Equality occurs if and only if $X^q = A^p/(\text{trace } A^p)$. Hence

$$
\max_{\mathcal{R}} \text{trace}(AX) = (\text{trace } A^p)^{1/p},
$$

where $\mathcal{R}$ is the region of all non-negative definite matrices $X$ of the same size satisfying $\text{trace } X^q = 1$. 

(b) If \( A \) is also positive definite, then for every positive definite \( n \times n \) matrix \( X \) satisfying \( \det X = 1 \) we have

\[
n^{-1} \text{trace}(AX) \geq (\det A)^{1/n},
\]

with equality if and only if \( X = (\det A)^{1/n} A^{-1} \).

If \( X = I_n \), then \( n^{-1} \text{trace}(A) \geq (\det A)^{1/n} \) with equality if and only if \( A = kI_n \) for some \( k \geq 0 \).

Therefore, given \( A \) positive definite, we have

\[
\min_{X} n^{-1} \text{trace}(AX) = (\det A)^{1/n},
\]

where the minimization is over the space of all positive definite matrices \( X \) such that \( \det X = 1 \).

(c) If \( A \) is a positive definite \( n \times n \) matrix and \( B \) is any \( m \times n \) matrix of rank \( m \), then

\[
\text{trace}(X'AX) \geq \text{trace}[(BA^{-1}B')^{-1}]
\]

for every \( n \times m \) matrix \( X \) satisfying \( BX = I_m \) with equality if and only if \( X = A^{-1}B'(BA^{-1}B')^{-1} \).

(d) Let \( A \) be an \( n \times n \) symmetric matrix with (not necessarily distinct) eigenvalues \( \lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n \). Then, for any \( n \times k \) matrix \( X \) such that \( X'X = I_k \) \((k \leq n)\), we obtain

\[
\text{trace}(X'AX) \leq \sum_{i=1}^{k} \lambda_i,
\]

with equality when the columns of \( X \) are orthonormal right eigenvectors corresponding to \( \lambda_1, \ldots, \lambda_k \), respectively.

**Proofs.** Section 12.5.

12.23. Magnus and Neudecker [1999: 218].


12.24c. Quoted by Magnus and Neudecker [1999: 237, exercise 10].


**12.6 SOME GEOMETRICAL PROPERTIES**

12.25. (Ellipsoids) Let \( a, y, \) and \( \theta \) be \( n \)-dimensional real vectors, and let \( L \) be a positive definite \( n \times n \) matrix. Then, for \( r > 0, \) \( \theta \) satisfies

\[
a'y - r(a'La)^{1/2} \leq a'\theta \leq a'y + r(a'La)^{1/2}
\]
for all \( a \) if and only if \((y - \theta)^T L^{-1} (y - \theta) \leq r^2\). Geometrically, this result states that a point \( y \) lies in an ellipsoid with center \( \theta \) if and only if it lies between every pair of parallel tangent planes. This result was originally proved geometrically by Scheffé [1953]. When \( L = I_n \), the ellipsoid becomes a sphere, and Hsu [1996: 231–233] gives a simple proof of this case.

12.26. (Rectangles) Let \( a, c (c \geq 0) \), and \( z \) be \( n \)-dimensional real vectors, then

\[
\max_{1 \leq i \leq n} |z_i| \leq c_i \quad \text{if and only if} \quad |a'z| \leq \sum_{i=1}^{n} c_i |a_i| \quad \text{for all} \quad a.
\]

This result is useful for the construction of simultaneous confidence intervals (Hsu [1996: 233]).

Proofs. Section 12.6.


12.7 MISCELLANEOUS INEQUALITIES

12.7.1 Determinants

12.27. (Hadamard) Let \( A = (a_{ij}) \) be a non-negative definite \( n \times n \) Hermitian matrix. Then

\[
\det A \leq a_{11} a_{22} \cdots a_{nn},
\]

with equality if and only if some \( a_{ii} = 0 \) or \( A \) is diagonal.

12.28. (Hadamard) If \( A = (a_{ij}) \) is any \( n \times n \) complex matrix, then

\[
|\det A| \leq \prod_{i=1}^{n} (\sum_{j=1}^{n} |a_{ij}|^2)^{1/2} \quad \text{and}
\]

\[
|\det A| \leq \prod_{j=1}^{n} (\sum_{i=1}^{n} |a_{ij}|^2)^{1/2},
\]

with equality if and only if \( AA^* \) is diagonal or \( A \) has a zero row; alternatively, if \( A^*A \) is diagonal or \( A \) has a zero column.

12.29. Let \( A \) and \( B \) be Hermitian non-negative definite \( n \times n \) matrices. Then:

(a) \( \det(A+B) \geq \det A + \det B \), with equality if and only if \( n = 1 \) or \( \det(A+B) = 0 \).

(b) If \( A - B \) is non-negative definite, then \( \det A \geq \det B \) with equality if and only if \( A \) and \( B \) are nonsingular (i.e., positive definite) and \( A = B \), or if \( A \) and \( B \) are both singular.
12.30. If \( A \) and \( B \) are \( n \times n \) real or complex matrices, then

\[
\det(I_n + AA^*) \det(I_n + BB^*) \geq |\det(A + B)|^2 + |(\det(I_n - AB^*)|^2, 
\]
with equality if and only if \( n = 1, \) or \( A + B = 0, \) or \( AB^* = I_n. \)

12.31. If \( X \) is \( m \times n \) and \( Y \) is \( n \times p, \) both real or complex matrices, then from (12.9) we have that \( X^*X - X^*Y(Y^*Y)^{-1}Y^*X \) is non-negative definite. Hence, by (12.29b),

\[
\det(X^*X) \geq \det(X^*Y(Y^*Y)^{-1}Y^*X),
\]
with equality when \( C(X) \subseteq C(Y). \)

Proofs. Section 12.7.1.


12.28. This follows from the previous inequality (12.27) applied to \( AA^*, \) and so on. See also Basilevsky [1983: 100], Horn and Johnson [1985: 477-478], and Magnus and Neudecker [1999: 214, real case].


12.7.2 Trace

12.32. If \( A = (a_{ij}) \) is a non-negative definite matrix, then

\[
\text{trace}(A^p) \geq \sum_{i=1}^{n} a_{ii}^p \quad (p > 1),
\]

\[
\text{trace}(A^p) \leq \sum_{i=1}^{n} a_{ii}^p \quad (0 < p < 1),
\]
with equality if and only if \( A \) is diagonal.

12.33. Let \( A \) and \( B \) be \( n \times n \) non-negative definite matrices.

(a) \( 0 \leq \text{trace}(AB) \leq (\text{trace } A)(\text{trace } B). \)

(b) \( \sqrt{\text{trace}(AB)} \leq \frac{1}{2}(\text{trace } A + \text{trace } B), \) with equality if \( A = 0 \) and \( \text{trace } B = 0, \)

or if \( B = 0 \) and \( \text{trace } A = 0, \) but also if \( A = B = aa' \) for some \( a \neq 0. \)

(c) (Araki–Lieb–Thirring)

\[
\text{trace}[(B^{1/2}AB^{1/2})^{st}] \leq \text{trace}[(B^{t/2}A'B'^{t/2})^s],
\]

where \( s \) and \( t \) are positive real numbers with \( t \geq 1. \)

(d) (Lieb–Thirring) Let \( m \) and \( k \) be positive integers with \( m \geq k. \) Then

\[
\text{trace}[(A^kB^k)^m] \leq [\text{trace}(A^mB^m)]^k.
\]
In particular, 

\[ \text{trace}[(AB)^m] \leq \text{trace}(A^mB^m). \]

**Proofs.** Section 12.7.2.

12.32. Magnus and Neudecker [1999: 217].
12.33c. Quoted by Bhatia [1997: 258].
12.33d. Quoted by Bhatia [1997: 279].

**12.7.3 Quadratics**

12.34. (Bergstrom) If A and B are both positive definite, then

\[ x'(A + B)^{-1}x \leq \frac{(x' A^{-1}x)(x' B^{-1}x)}{x'(A^{-1} + B^{-1})x}. \]

12.35. Let A \( \geq 0 \) (i.e., has non-negative elements) be an \( n \times n \) matrix and let \( x \geq 0 \) be an \( n \times 1 \) vector. Then, for any positive integer \( k \),

\[ (x' A^k x)(x' x)^{k-1} \geq (x' Ax)^k, \]

with equality if and only if \( x \) is an eigenvector of \( A \).

**Proofs.** Section 12.7.3.

12.34. Abadir and Magnus [2005: 323].
12.35. Mulholland and Smith [1959].

**12.7.4 Sums and Products**

12.36. (Triangle Inequality) For all \( a_i, b_i, \ldots, g_i \) \( (i = 1, 2, \ldots, n) \),

\[ \left( \sum_{i=1}^{n} (a_i + b_i + \cdots + g_i)^2 \right)^{1/2} \leq \left( \sum_{i=1}^{n} a_i^2 \right)^{1/2} + \left( \sum_{i=1}^{n} b_i^2 \right)^{1/2} + \cdots + \left( \sum_{i=1}^{n} g_i^2 \right)^{1/2}. \]

12.37. For all non-negative \( a_i, b_i, \ldots, g_i \) \( (i = 1, 2, \ldots, n) \),

\[ \sum_{i=1}^{n} (a_i + b_i + \cdots + g_i)^r \geq \sum_{i=1}^{n} a_i^r + \sum_{i=1}^{n} b_i^r + \cdots + \sum_{i=1}^{n} g_i^r, \quad r > 1, \]
\[ \sum_{i=1}^{n} (a_i + b_i + \cdots + g_i)^r \leq \sum_{i=1}^{n} a_i^r + \sum_{i=1}^{n} b_i^r + \cdots + \sum_{i=1}^{n} g_i^r, \quad 0 < r < 1, \]

with equality if and only if all the numbers but one of each set \( a_j, b_j, \ldots, g_j \) \( (j = 1, 2, \ldots, n) \) are zero.
12.38. (Ordered Numbers) Let \( a_1 \geq a_2 \geq \cdots \geq a_n \geq 0 \) and \( b_1 \geq b_2 \geq \cdots \geq b_n \geq 0 \). If
\[
\prod_{i=1}^{k} a_i \leq \prod_{i=1}^{k} b_i, \quad k = 1, 2, \ldots, n,
\]
then
\[
\sum_{i=1}^{k} a_i \leq \sum_{i=1}^{k} b_i, \quad k = 1, 2, \ldots, n.
\]

12.39. (Information Inequalities) Let \( \mathbf{a} = (a_1, a_2, \ldots, a_n)' \) and \( \mathbf{b} = (b_1, b_2, \ldots, b_n)' \) be two vectors.

(a) Suppose \( \mathbf{a} > 0 \) and \( \mathbf{b} > 0 \) (i.e., have positive elements) such that \( \sum_{i} a_i \geq \sum_{i} b_i \).

Then
\[
\sum_{i=1}^{n} a_i \log \frac{b_i}{a_i} \leq 0,
\]
with equality being attained if and only if \( a_i = b_i \) for all \( i \). Also, if \( a_i < 1 \) and \( b_i \leq 1 \) for all \( i \), then
\[
2 \sum_{i=1}^{n} a_i \log \frac{a_i}{b_i} \leq \sum_{i=1}^{n} a_i (a_i - b_i)^2.
\]

(b) Suppose \( \mathbf{a} \geq 0 \) and \( \mathbf{b} \geq 0 \) (i.e., have non-negative elements) such that \( \sum_{i} a_i = \sum_{i} b_i > 0 \), then
\[
\prod_{i=1}^{n} a_i^{a_i} \geq \prod_{i=1}^{n} b_i^{b_i},
\]
with equality if and only if \( \mathbf{a} = \mathbf{b} \).

12.40. (Jensen) Let \( x_i \geq 0 \) (\( i = 1, 2, \ldots, n \)), then
\[
(\sum_{i=1}^{n} x_i^r)^{1/r} \geq (\sum_{i=1}^{n} x_i^s)^{1/s}, \quad 0 < r < s,
\]
with equality if and only if all the \( x_i \) are zero except one. Also
\[
\lim_{r \to \infty} (\sum_{i=1}^{n} x_i^r)^{1/r} = \max_{i} x_i.
\]

12.41. If \( \lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n > 0 \), then
\[
\max_{i,j} \left[ \frac{(\lambda_i + \lambda_j)^2}{4\lambda_i \lambda_j} \right] = \frac{(\lambda_1 + \lambda_n)^2}{4\lambda_1 \lambda_n}.
\]

12.42. If \( x_i \geq 0 \) for \( i = 1, 2, \ldots, n \), then
\[
\prod_{i=1}^{n} (1 + x_i) \geq (1 + (x_1 x_2 \cdots x_n)^{1/n})^n,
\]
with equality if and only if \( x_1 = x_2 = \cdots = x_n \).
12.43. Suppose $x_1 \geq x_2 \geq \cdots \geq x_n > 0$ and $y_i / x_i$ is decreasing in $i$. Let $\alpha_i \geq 0$ for $i = 1, 2, \ldots, n$ such that $\sum_{i=1}^{n} \alpha_i = 1$, and define

$$g(r) = \begin{cases} 
\left( \sum_{i=1}^{n} \alpha_i x_i^r / \sum_{i=1}^{n} \alpha_i y_i^r \right)^{1/r}, & \text{if } r \neq 0, \\
\prod_{i=1}^{n} x_i^{\alpha_i} / \prod_{i=1}^{n} y_i^{\alpha_i}, & \text{if } r = 0.
\end{cases}$$

Then $g(r)$ increases as $r$ increases.

**Proofs.** Section 12.7.4.

12.36. Follows from (12.17).

12.37. Hardy et al. [1952: 32].


12.40. Hardy et al. [1952: 28].


12.43. Marshall and Olkin [1979: 131].

12.8 SOME IDENTITIES

12.44. Let $a = (a_i)$ and $b = (b_i)$.

(a) (Lagrange Identity)

(i) (Real Vectors) $(a'a)(b'b) - (a'b)^2 = \frac{1}{2} \sum_i \sum_j (a_i b_j - a_j b_i)^2$.

(ii) (Complex Vectors)

$\sum_i |a_i|^2 \sum_i |b_i|^2 - |\sum_i a_i b_i|^2 = \frac{1}{2} \sum_i \sum_j |\overline{a}_i b_j - \overline{a}_j b_i|^2$.

(b) (Abel’s Identity)

$$a'b = \sum_{i=1}^{n-1} \left( a_i - a_{i+1} \right) \sum_{j=1}^{i} b_j + a_n \sum_{j=1}^{n} b_j.$$

12.45. If $a$, $b$, and $c$ are $n \times 1$ vectors then

$$\sum_i a_i \sum_j a_j b_j c_j - \sum_i a_i \sum_j a_j c_j = \frac{1}{2} \sum_i \sum_j a_i a_j (b_i - b_j)(c_i - c_j).$$

12.46. If $A$ is symmetric and nonsingular, we have from (24.26a)

$$x'Ax - 2b'x = (x - A^{-1}b)'A(x - A^{-1}b) - b'A^{-1}b.$$
12.47. Suppose that $A$ and $B$ are $n \times n$ symmetric matrices, and $A + B$ is non-singular. Let $a$, $b$, and $x$ be $n \times 1$ vectors. Then

$$(x - a)'A(x - a) + (x - b)'B(x - b) = (x - c)'(A + B)(x - c) + (a - b)'A(A + B)^{-1}B(a - b),$$

where $c = (A + B)^{-1}(Aa + Bb)$.

12.48. Suppose $A$ and $B$ positive definite matrices, and let $a$, $b$, and $x$ be $n \times 1$ vectors. Define

$$C^{-1} = A^{-1} + B^{-1} \quad \text{and} \quad D = A + B.$$ 

Then

$$(x - a)'A^{-1}(x - a) + (x - b)'B^{-1}(x - b) = (x - c)'C^{-1}(x - c) + (a - b)'D^{-1}(a - b),$$

where $c = C(A^{-1}a + B^{-1}b)$.

**Proofs.** Section 12.8.

12.44a. Dragomir [2004: 3].


12.46. Use $x = x - A^{-1}b + A^{-1}b$.

12.47. Multiply out and use (15.4c).

12.48. Abadir and Magnus [2005: 217]. Follows from (12.47) by replacing $A$ by $A^{-1}$ and $B$ by $B^{-1}$ and using $A^{-1}(A^{-1} + B^{-1})^{-1}B^{-1} = (A + B)^{-1}$ (cf. 15.4c).
In this chapter we investigate the solution of various linear equations with a vector or matrix of unknown variables. Nonlinear matrix equations are not considered in this book except in (13.24) and (13.25), and the reader is referred to Horn and Johnson [1991: Section 6.4] for some background on this topic.

13.1 UNKNOWN VECTOR

13.1.1 Consistency

Definition 13.1. In this section we consider the problem of solving the equation $A_{m \times n}x_{n \times 1} = b_{m \times 1}$ for $x$ when $\text{rank } A = r$ ($r \leq \min(m, n)$) and $b \neq 0$. The equation is said to be consistent if there exists at least one solution. Otherwise, the equation is said to be inconsistent. Clearly we must have $b \in \mathcal{C}(A)$ for consistency. Note that this section is a special case of Section 13.2, which considers the equation $AXB = C$.

13.1. Using the above notation, the following are equivalent.

(a) The equation $Ax = b$ is consistent.

(b) $\text{rank}(A, b) = \text{rank } A$.

(c) $AA^-b = b$, where $A^-$ is any weak inverse of $A$. 

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13.2. From (16.33) we can find nonsingular $P$ and $Q$ such that

$$PAQ = \begin{pmatrix} I_r & 0 \\ 0 & 0 \end{pmatrix}.$$ 

Then the equation $Ax = b$ is consistent if and only if the last $m - r$ elements of $Pb$ are zero.

13.3. The equation $Ax = b$ has a unique solution if and only if $A$ has full column rank (i.e., $n = r$). When $A$ has full column rank, it has a left inverse $L$ such that $LA = I_n$. Then $\hat{x} = Lb$ is the solution. In particular, we can choose $L = (A'A)^{-1}A'$.


13.1.2 Solutions

13.4. All possible solutions of the consistent equation $Ax = b$ can be generated from

$$\hat{x} = A^{-}b + (I_n - A^{-}A)z$$

for any specific weak inverse $A^{-}$ by using all possible values of the arbitrary $n \times 1$ vector $z$ (including $z = 0$). Thus every solution of $Ax = b$ can be expressed in the above form for some $z$.

13.5. All possible solutions of the consistent equation $Ax = b$ can be generated from $\hat{x} = A^{-}b$ by using all possible weak inverses $A^{-}$ of $A$.

13.6. If $\hat{x}_1, \hat{x}_2, \ldots, \hat{x}_t$ are any $t$ solutions of the consistent equation $Ax = b$, then $\sum_{i=1}^{t} a_i \hat{x}_i$ is a solution if and only if $\sum_{i=1}^{t} a_i = 1$.

13.7. If $A$ is $m \times n$ of rank $r$, the consistent equation $Ax = b$ has exactly $n - r + 1$ linearly independent solutions.

(a) One possible set of such solutions is $A^{-}b$ along with the set

$$\hat{x}_i = A^{-}b + (I_n - A^{-}A)z_i, \quad i = 1, 2, \ldots, n - r,$$

where the $z_i$ are arbitrary, but chosen so that the $(I_n - A^{-}A)z_i$ are all linearly independent.

(b) Every solution can be expressed as a linear combination of the linearly independent solutions.

13.8. The value of $a'\hat{x}$ is the same for all solutions $\hat{x}$ to $Ax = b$ if and only if $a' = a'A^{-}A$. There are only $r$ linearly independent vectors $a_i$ satisfying $a'_i = a'_i A^{-}A$. 
13.9. (Methods of Solution for Consistent Equations) These methods generally involve some factorization of $A$.

(a) (Singular Value Decomposition) Suppose $A$ is $m \times n$ with singular value decomposition $A = PQ\Sigma Q'$, where $P$ and $Q$ are orthogonal $m \times m$ and $n \times n$ matrices, respectively, with columns $p_i$ and $q_i$, and $\Sigma$ is an $m \times n$ diagonal matrix with positive or zero diagonal elements $\sigma_i$, the singular values of $A$. Then $Ax = b$ implies that $\Sigma Q'x = P'b$, or $\Sigma y = c$. This simplified form can be used to determine the nature of the solutions of the original equations (Schott [2005: 242]).

If $A$ is nonsingular and $n \times n$, and $P = (p_1, p_2, \ldots, p_n)$, then

$$x = A^{-1}b = Q\Sigma^{-1}P'b = \sum_{i=1}^{n} \frac{P_i'b}{\sigma_i}q_i,$$

so that if $\sigma_n$, the smallest singular value of $A$, is small, a small change in $A$ or $b$ can induce a relatively large change in $x$ (Golub and Van Loan [1996: 80]).

(b) (LU Factorization) We can use the factorization $A = LU$, where $L$ is a lower-triangular matrix with unit diagonal elements and $U$ is an upper-triangular matrix (cf. Section 16.4). Since $Ax = LUx = Ly = b$, we simply solve $Ly = b$ for $y$ and $Ux = y$ for $x$. The process used for carrying out the calculations is called Gaussian elimination with the related ideas of pivoting and sweeping. It can also be applied to $m \times n$ matrices (Golub and Van Loan [1996: chapter 3] and Rao and Bhimasankaram [2000: section 5.6]). The method can be used for solving normal equations that arise in least squares estimation for linear regression (Seber and Lee [2003: section 11.2]).

Proofs. Section 13.1.2.


13.1.3 Homogeneous Equations

13.10. We consider solutions of $Ax = 0$, where $A$ is $m \times n$ of rank $r$.

(a) The solutions form the null space $N(A)$ of $A$ of dimension $n - r$. Any orthonormal basis for $N(A)$ will give a set of $n - r$ orthogonal solutions.

(b) A nonzero solution exists if and only if det $A = 0$.

(c) All the solutions to $Ax = 0$ are of the form $x_0 = (I_n - A^-A)z$ for arbitrary $z$ and any weak inverse $A^-$ of $A$. For $z_i \neq 0$, there exist $q - r$ linearly independent such solutions $(I_n - A^-A)z_i$.

Proofs. Section 13.1.3.

13.10. Searle [1982: section 9.7].
13.1.4 Restricted Equations

13.11. Given $A$ is $m \times n$, we wish to solve the consistent equation $Ax = b$ with the restriction that $x \in V$, a vector subspace of $\mathbb{R}^n$. Here $V$ could represent the column space or null space of a matrix.

(a) If $P_V$ is the orthogonal projection onto $V$, then $I_n - P_V$ is the orthogonal projection onto $V^\perp$. We are now interested in the solution of

$$
\begin{pmatrix}
Ax \\
(I - P_V)x
\end{pmatrix}
= 
\begin{pmatrix}
b \\
0
\end{pmatrix}.
$$

(b) The restricted equation is consistent if and only if the equation $AP_Vz = b$ is consistent. If this is the case and $z_0$ is a solution of the latter equation, then $x_0$ is a solution of the restricted equation if and only if $x_0 = P_Vz_0$.

(c) If the restricted equations are consistent, then a general solution is

$$
\{x_0 : x_0 = P_V(AP_V)^{-}b + P_V[I - (AP_V)^{-}AP_V]y,
$$

where $y$ is an arbitrary $n \times 1$ vector and $(AP_V)^{-}$ is any weak inverse of $AP_V$.

Proofs. Section 13.1.4.


13.2 UNKNOWN MATRIX

We are interested in solving the equation $A_{m \times n}X_{n \times p}B_{p \times q} = C_{m \times q}$. When the appropriate matrices are square, special cases follow by setting $A = I$ or $B = I$, and using $I^{-} = I$ in the result below. We note that if $x = \text{vec } X$ and $c = \text{vec } C$, then, by 11.16b),

$$(B' \otimes A)x = \text{vec } (AXB) = \text{vec } C = c,$$

which reduces the problem to the case considered in the previous section. More generally, consider the system

$$
\sum_{i=1}^{r} A_i X B_i + \sum_{j=1}^{s} L_j X' M_j = C,
$$

where the $A_i$ are $m \times n$, the $B_i$ are $p \times q$, the $L_j$ are $m \times p$, and the $M_j$ are $n \times q$. This can be reexpressed in the form (cf. 11.18b(ii))

$$
\left\{ \sum_{i=1}^{r} (B'_i \otimes A_i) + \sum_{j=1}^{s} (M'_j \otimes L_j) \right\} I_{(p, n)} \right\} x = c.
$$
13.2.1 Consistency

13.12. The equation $AXB = C$ is said to be *consistent* if it has at least one solution for $X$.

(a) A necessary and sufficient condition for $AXB = C$ to be consistent is that $AA^{-}CB^{-}B = C$ for any particular pair of weak inverses $A^{-}$ and $B^{-}$.

(b) $AXB = C$ is consistent if and only if $C(C) \subseteq C(A)$ and $C(C') \subseteq C(B')$.

(c) If the equation $AXB = C$ is consistent, then the following are general solutions for $X$ with $X_0 = A^{-}CB^{-}$.

(i) $X_0 + W - A^{-}AWBB^{-}$ for conformable arbitrary $W$.

(ii) $X_0 + (I - A^{-}A)U + V(I - BB^{-})$ for conformable arbitrary $U$ and $V$. This result can also be expressed in the form $A^{-}CB^{-} + Z_0$, where $Z_0$ is a solution of $AZB = 0$.

(iii) $X_0 + A^{-}AR(I - BB^{-}) + (I - A^{-}A)SBB^{-} + (I - A^{-}A)T(I - BB^{-})$, for conformable arbitrary $R$, $S$, and $T$.

(d) A number of special cases follow from the above results—for example, the general solution of $AX = 0$ is $X = (I - A^{-}A)U$, where $U$ is arbitrary.

Proofs. Section 13.2.1.


13.12c. Harville [1997: section 11.12]. In each case we simply check that the solution satisfies $AXB = C$ using (a) for $X_0$. For the second part of (ii), we simply show that $AZ_0B = 0$ using $AA^{-}A = A$, and so on.

13.2.2 Some Special Cases

13.13. Setting $B = I$ in (13.12) above, we see that the following conditions are equivalent.

(1) The equations $AX = C$ are consistent (i.e., have a solution).

(2) $C(C) \subseteq C(A)$.

(3) $AA^{-}C = C$ for any particular weak inverse $A^{-}$ (cf. 13.12a).

(4) $k'C = 0$ for every row vector $k'$ such that $k'A = 0$. Harville [1997: 73] calls the equations *compatible* if they have this property.

The equations are also consistent if the rows of $A$ are linearly independent.

13.14. Let $A$ be an $n \times n$ matrix, which is possibly complex, of rank $n - 1$. Let $u$ and $v$ be any eigenvectors of $A$ associated with the eigenvalue zero (not necessarily simple) such that $Au = 0$ and $v^*A = 0'$. Then the general solution of $AX = 0$ is $X = uz^*$, where $z$ is arbitrary. Similarly, the general solution of $XA = 0$ is $X = wv^*$, where $w$ is arbitrary. Finally, the general solution of the equations $AX = 0$ and $XA = 0$ is $X = cuv^*$, where $c$ is an arbitrary constant.
13.15. Let $X$ be an unknown $n \times p$ matrix. For any $m \times n$ matrix $A$ and any $m \times p$ matrix $C$, the equations $A'AX = A'C$ are consistent since from (2.35) $C(A') = C(A'A)$. These equations arise in multivariate least squares estimation.

13.16. If the following matrices are conformable and $C(C) \subset C(L')$, then the equations

\[
\begin{pmatrix}
A' & L \\
L' & 0
\end{pmatrix}
\begin{pmatrix}
X \\
Y
\end{pmatrix} =
\begin{pmatrix}
A'B \\
C
\end{pmatrix}
\]

are consistent for the unknowns $X$ and $Y$. This result is used for restricted least squares theory.

13.17. Suppose $X$ is an unknown $m \times n$ matrix.

(a) If “$\otimes$” is the Kronecker product, then, using (11.16a), the equation $A_{m \times m}X + XB_{n \times n} = C_{m \times n}$ can be expressed in the form

\[(I_n \otimes A + B' \otimes I_m)vec X = vec C,
\]

or $Fx = c$, say, where $F$ is called the Kronecker sum. Some properties of $F$ are given by Horn and Johnson [1991: section 4.4]. The equation has a unique solution if and only if $A$ and $-B$ have no eigenvalues in common.

(b) We also have from (a),

\[(SAS^{-1})SXT + SXT(T^{-1}BT) = SCT,
\]

which may be rewritten as $A_1X_1 + X_1B_1 = C_1$. With suitable similarity transformations, the transformed equation may be easier to handle; the original solution is then readily recovered (Horn and Johnson [1991: 256]).

(c) A related equation is Lyapunov's equation

\[XA + A^*X = H,
\]

where $A$, $X$, and $H$ are all $n \times n$, and $H$ is Hermitian. This equation arises in the study of matrix stability and is discussed in detail by Horn and Johnson [1991: chapter 4]. The equation

\[XA + A^*X = C
\]

has a unique solution for any $n \times n$ matrix $C$ if and only if $\lambda$ and $-\bar{\lambda}$ are not both eigenvalues of $A$.

13.18. If $X$ and $A$ are $n \times n$, and the eigenvalues of $A$ are $\lambda_i$, then the equation

\[AX - XA = aX
\]

has a nontrivial solution if and only if $a = \lambda_i - \lambda_j$.

13.19. Suppose $A$ is $m \times m$, $X$ is $m \times n$, and $B$ is $n \times n$. If $A$ and $B$ have no eigenvalues in common, then $AX - XB = 0$ has a unique solution $X = 0$. A nonzero solution exists if there are eigenvalues in common.
13.20. \( \mathbf{AX} + \mathbf{YB} = \mathbf{C} \) if and only if \((\mathbf{I} \otimes \mathbf{A}) \mathbf{vec} \mathbf{X} + (\mathbf{B}' \otimes \mathbf{I}) \mathbf{vec} \mathbf{Y} = \mathbf{vec} \mathbf{C} \), where \( \otimes \) is the Kronecker product.

13.21. The equation \( \mathbf{AX} - \mathbf{YB} = \mathbf{C} \) has a solution for \( \mathbf{X} \) and \( \mathbf{Y} \) if and only if
\[
\text{rank}\left( \begin{pmatrix} \mathbf{A} & \mathbf{C} \\ 0 & \mathbf{B} \end{pmatrix} \right) = \text{rank}\left( \begin{pmatrix} \mathbf{A} & 0 \\ 0 & \mathbf{B} \end{pmatrix} \right).
\]

13.22. The matrix equation
\[
\begin{pmatrix} \mathbf{A} & \mathbf{B} \\ \mathbf{B}' & 0 \end{pmatrix} \begin{pmatrix} \mathbf{X}_1' \\ \mathbf{X}_2' \end{pmatrix} = \begin{pmatrix} \mathbf{G}_1' \\ \mathbf{G}_2' \end{pmatrix},
\]
in \( \mathbf{X}_1 \) and \( \mathbf{X}_2 \), where \( \mathbf{A}, \mathbf{B}, \mathbf{G}_1, \) and \( \mathbf{G}_2 \) are given matrices of appropriate orders and \( \mathbf{A} \) is non-negative definite, has a solution if and only if
\[
\mathcal{C} (\mathbf{G}_1') \subset \mathcal{C} (\mathbf{A}, \mathbf{B}) \quad \text{and} \quad \mathcal{C} (\mathbf{G}_2') \subset \mathcal{C} (\mathbf{B}'),
\]
in which case the general solution is
\[
\begin{align*}
\mathbf{X}_1 &= G_1 (\mathbf{N}^+ - \mathbf{N}^+ \mathbf{B} \mathbf{C}^+ \mathbf{B}' \mathbf{N}^+) + G_2 \mathbf{C}^+ \mathbf{B}' \mathbf{N}^+ + Q_1 (\mathbf{I} - \mathbf{N} \mathbf{N}^+) \quad \text{and} \\
\mathbf{X}_2 &= G_1 \mathbf{N}^+ \mathbf{B} \mathbf{C}^+ + G_2 (\mathbf{I} - \mathbf{C}^+) + Q_2 (\mathbf{I} - \mathbf{B}^+ \mathbf{B}),
\end{align*}
\]
where \( \mathbf{N} = \mathbf{A} + \mathbf{B} \mathbf{B}' \), \( \mathbf{C} = \mathbf{B}' \mathbf{N}^+, \) and \( \mathbf{Q}_1 \) and \( \mathbf{Q}_2 \) are arbitrary matrices of appropriate orders. (Note that \( \mathbf{N}, \mathbf{N}^+, \mathbf{N} \mathbf{N}^+, \mathbf{B}^+ \mathbf{B}, \mathbf{C}, \) and \( \mathbf{C}^+ \) are all symmetric.) Special cases are:

(a) If \( \mathcal{C} (\mathbf{B}') \subset \mathcal{C} (\mathbf{A}) \), then we can take \( \mathbf{N} = \mathbf{A} \).

(b) If \( \mathbf{G}_1 = \mathbf{0} \), then the original equations have a solution if and only if \( \mathcal{C} (\mathbf{G}_2') \subset \mathcal{C} (\mathbf{B}') \), in which case the general solution for \( \mathbf{X}_1 \) is
\[
\mathbf{X}_1 = G_2 (\mathbf{B}' \mathbf{N}^+ \mathbf{B})^+ \mathbf{B}' \mathbf{N}^+ + Q (\mathbf{I} - \mathbf{N} \mathbf{N}^+),
\]
where \( \mathbf{N} = \mathbf{A} + \mathbf{B} \mathbf{B}' \) and \( \mathbf{Q} \) is arbitrary of appropriate order. If, in addition, \( \mathcal{C} (\mathbf{B}) \subset \mathcal{C} (\mathbf{A}) \), then the general solution can be written as
\[
\mathbf{X}_1 = G_2 (\mathbf{B}' \mathbf{A}^+ \mathbf{B})^+ \mathbf{B}' \mathbf{A}^+ + Q (\mathbf{I} - \mathbf{A} \mathbf{A}^+).
\]

13.23. The equations \( \mathbf{AX} = \mathbf{C} \) and \( \mathbf{XB} = \mathbf{D} \) have a common solution if and only if each equation separately has a solution and \( \mathbf{AD} = \mathbf{CB} \), in which case, the general expression for a common solution is
\[
\mathbf{X} = \mathbf{A}^{-} \mathbf{C} + \mathbf{D} \mathbf{B}^{-} - \mathbf{A}^{-} \mathbf{A} \mathbf{D} \mathbf{B}^{-} + (\mathbf{I} - \mathbf{A}^{-} \mathbf{A}) \mathbf{Z} (\mathbf{I} - \mathbf{B} \mathbf{B}^{-})
\]
\[
= \mathbf{X}_0 + (\mathbf{I} - \mathbf{A}^{-} \mathbf{A}) \mathbf{Z} (\mathbf{I} - \mathbf{B} \mathbf{B}^{-}),
\]
where \( \mathbf{X}_0 \) is a common solution and \( \mathbf{Z} \) is arbitrary.

13.24. If \( \mathbf{B} \) is \( m \times n \) and \( \mathbf{X} \) is \( n \times m \), then the general solution \( \mathbf{X} \) of \( \mathbf{XBX} = \mathbf{X} \) is
\[
\mathbf{X} = \mathcal{C} (\mathbf{DBC})_{12} \mathbf{D},
\]
where \( (\cdot)_{12} \) is the reflexive inverse, and \( n \times p \) \( \mathbf{C} \) and \( q \times m \) \( \mathbf{D} \) are arbitrary matrices. The solution has the same rank as \( \mathbf{DBC} \).
13.25. If $B$ is $m \times n$ and $X$ is $n \times m$, then the general solution of $XBX = 0$ is $X = YC$, where $p$ as well as the $p \times m$ matrix $C$ are arbitrary, and $Y$ is an arbitrary solution of $CBY = 0$. If $X$ also has to satisfy $WBX = 0$, then $Y$ is now an arbitrary solution of

$$
\begin{pmatrix}
C \\
W
\end{pmatrix}BY = 0.
$$

13.26. The equations $A_1XB_1 = C_1$ and $A_2XB_2 = C_2$ have a common solution if and only if each equation is consistent and

$$
\min_{A_2XB_2=C_2} \text{rank}(C_1 - A_1XB_1) = 0,
$$

which is equivalent to

$$
\text{rank}
\begin{pmatrix}
C_1 & 0 & A_1 \\
0 & -C_2 & A_2 \\
B_1 & B_2 & 0
\end{pmatrix}
= \text{rank}(A_1) + \text{rank}(B_1, B_2).
$$

A proof and further details relating to this problem are given by Tian [2002: 197]

13.27. (Two Unknowns) We wish to consider the solution of the matrix equation $AXB + CYD = M$ for $X$ and $Y$. Since $\text{vec}(AXB) = (B' \otimes A)\text{vec}X$, we can rewrite the matrix equation in the form

$$
(B' \otimes A, D' \otimes C)(\begin{pmatrix}
\text{vec}X \\
\text{vec}Y
\end{pmatrix}) = \text{vec}M,
$$

which is solvable if and only if (cf. 13.1c)

$$(B' \otimes A, D' \otimes C)(B' \otimes A, D' \otimes C)^{-} \text{vec}M = \text{vec}M.
$$

In this case, from (13.4), the general solution is

$$
\begin{pmatrix}
\text{vec}X \\
\text{vec}Y
\end{pmatrix} = (B' \otimes A, D' \otimes C)^{-}\text{vec}M + [I - (B' \otimes A, D' \otimes C)^{-}(B' \otimes A, D' \otimes C)]\mathbf{v},
$$

where $\mathbf{v}$ is an arbitrary vector. Using his extremal ranks method, Tian [2006b] gives necessary and sufficient rank conditions for solutions $X$ and $Y$ to exist and also provides methods for finding solutions.

Proofs. Section 13.2.2.


13.18. Graham [1981: 40].


\[ XBXB = XB, \ BXBX = BX, \ BXBXB = XB, \text{ and } XBXBX = XB. \]
PARTITIONED MATRICES

Partitioned matrices arise frequently in statistics, especially in proofs. For some partitions and their relationship with ranks, the reader should consult Section 3.6. This chapter is closely linked to the next chapter on patterned matrices.

14.1 SCHUR COMPLEMENT

Definition 14.1. Let

\[ A = \begin{pmatrix} E & F \\ G & H \end{pmatrix}, \]

where \( A \) is possibly rectangular. If \( E \) is square and nonsingular, then

\[ S = H - GE^{-1}F = (A/E) \]

is called the Schur complement of \( E \) in \( A \). If \( H \) is nonsingular (instead of, or in addition to, \( E \)), then

\[ T = E - FH^{-1}G = (A/H) \]

is the Schur complement of \( H \) in \( A \).

Schur complements occur in various places in this book, sometimes using a different notation. Because of the wide applicability of Schur complements, we have collected some of the results together here in one place using the present notation, which is the one used in three key references, namely Ouellette [1981], Puntanen
and Styan, [2005b], and Styan [1985]. These writers show how the Schur complement can be used to prove a number of matrix results that are typically proved by other methods. They also show how Schur complements arise naturally in statistics, especially in multivariate analysis and in linear models.

14.1. (Determinants) If \( A \) is nonsingular, we have that (see also 14.17)

\[
\det A = \begin{cases} 
\det E \cdot \det(A/E), & \text{if } E \text{ is nonsingular,} \\
\det H \cdot \det(A/H), & \text{if } H \text{ is nonsingular.}
\end{cases}
\]

Therefore if \( A \) and \( E \) are nonsingular, then so is \( A/E \). The same applies to \( A \) and \( H \).

14.2. (Ranks) From (3.40a(vi) and (3.40(vii)) we have:

(a) If \( E \) is nonsingular, \( \text{rank } A = \text{rank } E + \text{rank}(A/E) \).

(b) If \( H \) is nonsingular, \( \text{rank } A = \text{rank } H + \text{rank}(A/H) \).

14.3. (Inverses) If \( A \), \( E \), and \( H \) are all nonsingular, then:

(a) \( (A/H)^{-1} = E^{-1} + E^{-1}F(A/E)^{-1}GE^{-1} \).

(b) \( (A/E)^{-1} = H^{-1} + H^{-1}G(A/H)^{-1}FH^{-1} \).

14.4. (Inertia) We recall that the inertia \( \text{In}(A) \) of a symmetric matrix \( A \) is given by the triple \((r_+, r_-, r_0)\), where \( r_+ \) is the number of positive eigenvalues, \( r_- \) is the number of negative eigenvalues, and \( r_0 \) is the number of zero eigenvalues. Then, if \( A \) is symmetric and \( E \) is nonsingular,

\[
\text{In}(A) = \text{In}(E) + \text{In}(A/E).
\]

Ouellette [1981: 207–210] extends the above result to the case when \((A/E)\) is also partitioned.

14.5. (Non-negative Definite Matrices) Suppose \( A \) is symmetric and \( E \) is positive definite.

(a) \( A \) is non-negative definite if and only if \((A/E)\) is non-negative definite.

(b) \( A \) is positive definite if and only if \((A/E)\) is positive definite.

14.6. (Subpartition) Suppose that

\[
A = \begin{pmatrix}
E & F \\
\vdots & \ddots & \ddots \\
G & \vdots & H
\end{pmatrix} = \begin{pmatrix}
K & L & F_1 \\
M & N & F_2 \\
\vdots & \ddots & \ddots \\
G_1 & G_2 & H
\end{pmatrix},
\]

where \( E \) and \( K \) are nonsingular. Then \((E/K)\) is a nonsingular leading principal submatrix of \((A/K)\), and

\[
(A/E) = ((A/K)/(E/K)).
\]
14.7. (Sum) Let

\[ A = \begin{pmatrix} E & F \\ F' & H \end{pmatrix} \quad \text{and} \quad B = \begin{pmatrix} K & L \\ L' & N \end{pmatrix} \]

be symmetric \((m + n) \times (m + n)\) matrices, where \(E\) and \(K\) are \(m \times m\). Suppose that \(A\) and \(B\) are non-negative definite (n.n.d.) and \(E\) and \(K\) are positive definite.

(a) \(F' E^{-1} F + L' K^{-1} L - (F + L)' (E + K)^{-1} (F + L)\) is n.n.d. with the same rank as \(F - E K^{-1} L\).

(b) \(((A + B)/(E + K)) - (A/E) - (B/K)\) is n.n.d.

(c) \(\det[(A + B)/(E + K)] = \frac{\det(A + B)}{\det(E + K)} \geq \frac{\det A}{\det E} + \frac{\det B}{\det K}.\)

**Definition 14.2.** (Generalized Schur Complement) Referring to Definition 14.1, if \(E\) is rectangular, or square and singular, then we replace \(E^{-1}\) by any weak inverse \(E^{-}\) and call \((A/E)\) the generalized Schur complement of \(E\) in \(A\). We have a similar definition for \((A/H)\).

We shall use the following notation below:

\[ S = (A/E) = H - GE^{-}F \quad \text{and} \quad T = (A/H) = E = FH^{-}G. \]

14.8. (General Properties of the Generalized Schur Complement)

(a) If \(A\) and \(E\) are both square and either \(\mathcal{C}(F) \subseteq \mathcal{C}(E)\) or \(\mathcal{C}(G') \subseteq \mathcal{C}(E')\), then \(S\) is invariant for all weak inverses \(E^{-}\) and

\[ \det A = \det E \cdot \det S. \]

(b) If \(A\) and \(H\) are both square and either \(\mathcal{C}(G) \subseteq \mathcal{C}(H)\) or \(\mathcal{C}(F') \subseteq \mathcal{C}(H')\), then \(T\) is invariant for all weak inverses \(H^{-}\) and

\[ \det A = \det H \cdot \det T. \]

(c) If \(A\) is non-negative definite and \(E\) and \(H\) are both square (i.e., \(G = F'\)), then \(\mathcal{C}(F) \subseteq \mathcal{C}(E)\) and \(\mathcal{C}(F') \subseteq \mathcal{C}(H)\); also (a) and (b) hold.

14.9. Suppose \(A\) is non-negative definite and \(E\) and \(H\) are both square, then:

(a) \(S\) and \(T\) are invariant with respect to the weak inverses \(E^{-}\) and \(H^{-}\).

(b) (Rank)

(i) \(\text{rank } A = \text{rank } E + \text{rank}(A/E)\).

(ii) \(\text{rank } A = \text{rank } H + \text{rank}(A/H)\).

(c) (Inertia)

(i) \(\text{In}(A) = \text{In}(E) + \text{In}(A/E)\).

(ii) \(\text{In}(A) = \text{In}(H) + \text{In}(A/H)\).
(d) If \( \nu(A) \) refers to the nullity of \( A \), then:

(i) \( \nu(A) = \nu(E) + \nu[(A/E)] \).

(ii) \( \nu(A) = \nu(H) + \nu[(A/H)] \).

**Proofs.** Section 14.1.


14.3. Abadir and Magnus [2005: 107]. See also (15.3c).


14.8c. Follows from (a) and (b) and (14.26g).

14.9a–d. Puntanen and Styan [2005b: section 6.0.4]; for (a) see Ouellette [1981: 242] and Styan [1985: 45]; for (b) see Styan [1985: 45] and (4.40a(iii)); for (c) see Ouellette [1981: 238, theorem 4.7]; and (d) follows from (b) and the fact that the rank plus the nullity of a matrix is equal to the number of columns.

### 14.2 INVERSES

The notation used so far for Schur complements is sometimes not so helpful for the more general results in this section, as it is not easy to see the patterns. I now introduce a subscript notation as well, as both are used in the literature. Some of the above results will appear again under a different guise. The results on inverses in this section are established by simply checking that \( AA^{-1} = I \). The other results are verified by multiplying out the matrices concerned and using (14.11).

14.10. Let

\[
A = \begin{pmatrix}
A_{11} & A_{12} \\
A_{21} & A_{22}
\end{pmatrix},
\]

where \( A, A_{11}, \) and \( A_{22} \) are all real or complex matrices that are not necessarily square.

(a) If \( A_{11} \) is nonsingular and \( A_{22,1} = A_{22} - A_{21} A_{11}^{-1} A_{12} (= A/A_{11}) \), then

(i) \( A = \begin{pmatrix}
I & 0 \\
A_{21} A_{11}^{-1} & I
\end{pmatrix} \begin{pmatrix}
A_{11} & 0 \\
0 & A_{22,1}
\end{pmatrix} \begin{pmatrix}
I & A_{11}^{-1} A_{12} \\
0 & I
\end{pmatrix}.\)

This is sometimes called the *Aitken block-diagonalization formula*. When
A is non-negative definite, the above result still holds with $A_{21} = A'_{12}$ and $A_{11}^{-1}$ replaced by $A_{11}^{-}$ throughout.

(ii) $\begin{pmatrix} A_{11}^{-1} & 0 \\ -A_{21}A_{11}^{-1} & I \end{pmatrix} A = \begin{pmatrix} I & A_{11}^{-1}A_{12} \\ 0 & A_{22}^{-1} \end{pmatrix}$.

(iii) If $A^{-1}$ exists, then

$$A^{-1} = \begin{pmatrix} I & -A_{11}^{-1}A_{12} \\ 0 & I \end{pmatrix} \begin{pmatrix} A_{11}^{-1} & 0 \\ -A_{22}^{-1}A_{21}A_{11}^{-1} & A_{22}^{-1} \end{pmatrix}.$$

(iv) If $A^{-1}$ exists, then

$$A^{-1} = \begin{pmatrix} A_{11}^{-1} & 0 \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} -A_{11}^{-1}A_{12} \\ I \end{pmatrix} A_{22}^{-1}(-A_{21}A_{11}^{-1}, I).$$

(v) If $A$ and $A_{11}$ have rank $r$ and $A_{11}$ is $r \times r$, then $A_{22}^{-1} = 0$.

(b) If $A_{22}$ is nonsingular and $A_{11,2} = A_{11} - A_{12}A_{22}^{-1}A_{21} = (A/A_{22})$, then

(i) $A = \begin{pmatrix} I & A_{12}A_{22}^{-1} \\ 0 & I \end{pmatrix} \begin{pmatrix} A_{11,2} & 0 \\ 0 & A_{22} \end{pmatrix} \begin{pmatrix} I & 0 \\ A_{22}^{-1}A_{21} & I \end{pmatrix}$.

When $A$ is non-negative definite, the above result still holds with $A_{21} = A'_{12}$ and $A_{22}^{-1}$ replaced by $A_{22}^{-}$ throughout.

(ii) $A \begin{pmatrix} I & 0 \\ -A_{22}^{-1}A_{21} & A_{22}^{-1} \end{pmatrix} = \begin{pmatrix} A_{11,2} & A_{12}A_{22}^{-1} \\ 0 & I \end{pmatrix}$.

(iii) If $A^{-1}$ exists, then

$$A^{-1} = \begin{pmatrix} I & 0 \\ -A_{22}^{-1}A_{21} & I \end{pmatrix} \begin{pmatrix} A_{11,2}^{-1} & -A_{11,2}A_{12}A_{22}^{-1} \\ 0 & A_{22}^{-1} \end{pmatrix}.$$

(iv) If $A^{-1}$ exists, then

$$A^{-1} = \begin{pmatrix} 0 & 0 \\ 0 & A_{22}^{-1} \end{pmatrix} \begin{pmatrix} I \\ -A_{22}^{-1}A_{21} \end{pmatrix} A_{11,2}^{-1}(I, -A_{12}A_{22}^{-1}).$$

(v) If $A$ and $A_{22}$ have rank $r$ and $A_{22}$ is $r \times r$, then $A_{11,2} = 0$.

14.11. Suppose $A$ is partitioned as above and is nonsingular.

(a) If $A_{11}$ is nonsingular and $A_{22,1} = A_{22} - A_{21}A_{11}^{-1}A_{12}$, then

$$A^{-1} = \begin{pmatrix} A_{11}^{-1} + A_{11}^{-1}A_{12}A_{22}^{-1}A_{21}A_{11}^{-1} - A_{11}^{-1}A_{12}A_{22}^{-1}A_{22,1} & A_{11}^{-1}A_{12}A_{22}^{-1}A_{21}A_{11}^{-1} \\ -A_{22,1}A_{11}^{-1}A_{21}A_{12}A_{22}^{-1} & A_{22,1}^{-1} \end{pmatrix}.$$

(b) If $A_{22}$ is nonsingular and $A_{11,2} = A_{11} - A_{12}A_{22}^{-1}A_{21}$, then

$$A^{-1} = \begin{pmatrix} A_{11,2}^{-1} - A_{11,2}A_{12}A_{22}^{-1} & -A_{11,2}A_{12}A_{22}^{-1}A_{21}A_{11,2}A_{12}A_{22}^{-1} \\ -A_{22}^{-1}A_{21}A_{11,2}A_{12}A_{22}^{-1} & A_{22}^{-1} + A_{22}^{-1}A_{21}A_{11,2}A_{12}A_{22}^{-1} \end{pmatrix}.$$
(c) If $A_{11}$ and $A_{22}$ are both nonsingular, then we have the following.

(i) $A_{22}^{-1} = A_{22}^{-1} + A_{22}^{-1} A_{21} A_{11}^{-1} A_{12} A_{22}^{-1}$.

(ii) Interchanging 1 and 2 above,

$$A_{11}^{-1} = A_{11}^{-1} + A_{11}^{-1} A_{12} A_{22}^{-1} A_{21} A_{11}^{-1}.$$ 

When $A_{11}$ and $A_{22}$ are both nonsingular, the two representations of $A^{-1}$ given by (a) and (b) above are identical, by the uniqueness of the inverse, even though the off-diagonal blocks may not look equal. Thus, for example, it can be shown that

(iii) $A_{22}^{-1} A_{21} A_{11}^{-1} = A_{22}^{-1} A_{21} A_{11}^{-1}$.

For this reason the reader will find various versions of $A^{-1}$ in the literature. (e.g., compare Graybill [1983: 184] and Muirhead [1982: 580] with Anderson [2003: 638] and Zhang [1999: 184, where $A$ is positive definite). When $A$ is symmetric or Hermitian we have $A_{22}^{-1} = A_{22}^{-1}$.

Some special cases follow.

14.12. If $A_{11}$ and $A_{22}$ are nonsingular, then the following inverses below exist (by 14.18) below, and

$$\left( \begin{array}{cc} A_{11} & 0 \\ A_{21} & A_{22} \end{array} \right)^{-1} = \left( \begin{array}{cc} A_{11}^{-1} & 0 \\ -A_{22}^{-1} A_{21} A_{11}^{-1} & A_{22}^{-1} \end{array} \right).$$

Similarly,

$$\left( \begin{array}{cc} A_{11} & A_{12} \\ 0 & A_{22} \end{array} \right)^{-1} = \left( \begin{array}{cc} A_{11}^{-1} & -A_{11}^{-1} A_{12} A_{22}^{-1} \\ 0 & A_{22}^{-1} \end{array} \right).$$

We get special cases if we set $A_{11}$ and/or $A_{22}$ equal to identity matrices.

Non-singular block-triangular matrices with more than two blocks can be inverted by applying the above method iteratively (cf. Harville [1997: 94]).

14.13. Suppose $A$ and $D$ are nonsingular.

(a) If $\alpha = d - c'A^{-1}b \neq 0$, we have from (14.10a(iv))

$$\left( \begin{array}{cc} A & b \\ c' & d \end{array} \right)^{-1} = \left( \begin{array}{cc} A^{-1} & 0 \\ 0' & 0 \end{array} \right) + \frac{1}{\alpha} \left( A^{-1} b \right) \left( c'A^{-1}, -1 \right).$$

(b) If $\beta = a - b'D^{-1}c \neq 0$, we have from (14.10b(iv))

$$\left( \begin{array}{cc} a & b' \\ c & D \end{array} \right)^{-1} = \left( \begin{array}{cc} 0 & 0' \\ 0 & D^{-1} \end{array} \right) + \frac{1}{\beta} \left( D^{-1} c \right) \left( -1, b'D^{-1} \right).$$

14.14. Let $(A, B)$ be an $n \times (k + m)$ matrix of full column rank, where $A$ is $n \times k$. Define

$$Z = (A, B)'(A, B) = \left( \begin{array}{cc} A'A & A'B \\ B'A & B'B \end{array} \right).$$
Let $M_C = I_n - C(C'C)^{-1}C$ for $C = A, B$, and define $E = B'M_AB$ and $F = A'M_BA$. Then, from (14.11a,b),
\[
Z^{-1} = \begin{pmatrix}
(A'A)^{-1} + (A'A)^{-1}A'BE^{-1}B'A(A'A)^{-1} & -(A'A)^{-1}A'BE^{-1} \\
E^{-1}B'A(A'A)^{-1}
\end{pmatrix}
\]
\[
= \begin{pmatrix}
F^{-1} & -F^{-1}A'B(B'B)^{-1} \\
-(B'B)^{-1}B'AF^{-1} & (B'B)^{-1} + (B'B)^{-1}B'AF^{-1}A'B(B'B)^{-1}
\end{pmatrix}
\]

14.15. Given conformable matrices and the existence of the appropriate inverses, we have
\[
\begin{pmatrix}
A & B & C \\
B' & D & 0 \\
C' & 0 & E
\end{pmatrix}^{-1}
\]
\[
= \begin{pmatrix}
Q^{-1} & -Q^{-1}BD^{-1} & -Q^{-1}CE^{-1} \\
-D^{-1}B'Q^{-1} & D^{-1} + D^{-1}B'Q^{-1}BD^{-1} & D^{-1}B'Q^{-1}CE^{-1} \\
-E^{-1}C'Q^{-1} & E^{-1}C'Q^{-1}BD^{-1} & E^{-1} + E^{-1}C'Q^{-1}CE^{-1}
\end{pmatrix}
\]
where $Q = A - BD^{-1}B' - CE^{-1}C$.

14.16. (Powers) Suppose $A$ is $m \times m$ and $D$ is $n \times n$.

(a)
\[
\begin{pmatrix}
A & B \\
0 & D
\end{pmatrix}^k = \begin{pmatrix}
A^k & Q_k \\
0 & D^k
\end{pmatrix}, \quad k = 1, 2, \ldots,
\]
where $Q_k = \sum_{i=1}^{k} A^{k-i}BD^{i-1}$.

(b) If, in (a), $D = I_n$ and $I_m - A$ is nonsingular, then
\[
Q_k = (I_m - A)^{-1}(I_m - A^k)B.
\]

(c) If $A$ and $B$ are nonsingular,
\[
\begin{pmatrix}
A & B \\
0 & D
\end{pmatrix}^{-k} = \begin{pmatrix}
A^{-k} & R_k \\
0 & D^{-k}
\end{pmatrix},
\]
where $R_k = -\sum_{i=1}^{k} A^{-(k-i+1)}BD^{-i}$.

Proofs. Section 14.2.

14.10a(v) and b(v). Graybill [1983: 126–127].


14.15. Magnus and Neudecker [1999: 12].

14.3 DETERMINANTS

14.17. Suppose $A$ is partitioned as in (14.10).

(a) If $A_{11}$ is nonsingular,
\[ \det A = \det(A_{11}) \det(A_{22}). \]
If, in addition, $A$ is nonsingular, then so is $A_{22.1}$, the Schur complement of $A_{11}$.

(b) If $A_{22}$ is nonsingular,
\[ \det A = \det(A_{22}) \det(A_{11.2}). \]
If, in addition, $A$ is nonsingular, then so is $A_{11.2}$, the Schur complement of $A_{22}$.

(c) If $A_{11}^{-1}$ and $A_{22}^{-1}$ are any weak inverses of $A_{11}$ and $A_{22}$, then:
\begin{enumerate}
  \item [(i)] If $C(A_{21}) \subseteq C(A_{22})$ or $C(A_{12}') \subseteq C(A_{22}')$, we have
  \[ \det A = (\det A_{22}) \det(A_{11} - A_{12}A_{22}^{-1}A_{21}). \]
  \item [(ii)] If $C(A_{12}) \subseteq C(A_{11})$ or $C(A_{21}') \subseteq C(A_{11}')$, we have
  \[ \det A = (\det A_{11}) \det(A_{22} - A_{21}A_{11}^{-1}A_{12}). \]
\end{enumerate}

14.18. The following two results are often useful.

(a) If $A$ and $B$ are $m \times m$ and $n \times n$, respectively, then, for conformable matrices,
\[ \det \begin{pmatrix} A & 0 \\ E & B \end{pmatrix} = \det \begin{pmatrix} A & F \\ 0 & B \end{pmatrix} = \det A \cdot \det B. \]
We can set $A$ or $B$ equal to the identity matrix.

Note that the two matrices on the left are nonsingular if and only if both $A$ and $B$ are nonsingular.

(b) Using a similar notation to (a),
\[ \det \begin{pmatrix} 0 & F \\ E & B \end{pmatrix} = \det \begin{pmatrix} B & E \\ F & 0 \end{pmatrix} = (-1)^{mn} \det E \cdot \det F. \]

14.19. If $B$ and $C$ are $n \times n$ matrices, then
\[ \det \begin{pmatrix} 0 & B \\ -I_n & C \end{pmatrix} = \det B. \]

14.20. If $C = (A, B)$ is square, then from $\det(CC') = \det(C'C) = (C)^2$ we have
\[ \det(AA' + BB') = \det \begin{pmatrix} A'A & A'B \\ B'A & B'B \end{pmatrix}. \]
14.21. Let $A$ and $D$ be square matrices. Then:

(a) $\det \begin{pmatrix} A & b \\ c' & d \end{pmatrix} = d \det A - c'(\text{adj}A)b,$

or $\det A(d - c'A^{-1}b)$ if $A$ is nonsingular, where $\text{adj}A$ is the adjoint matrix of $A$.

(b) $\det \begin{pmatrix} a & b' \\ c & D \end{pmatrix} = \det D(a - b'D^{-1}c)$ if $D$ is nonsingular.

(c) From (a) we have $\det \begin{pmatrix} A & u \\ u' & -1 \end{pmatrix} = -\det(A + uu')$.

14.22. (Adjoint) Let 

$$A = \begin{pmatrix} E & F \\ G & H \end{pmatrix},$$

be an $n \times n$ matrix such that $E$ is $m \times m$. If

$$\text{adj}A = \begin{pmatrix} E_1 & F_1 \\ G_1 & H_1 \end{pmatrix},$$

where $E_1$ is $m \times m$, then:

(a) $\det H_1 = (\det A)^{n-m-1} \det E$ for $m = 0, 1, 2, \ldots, n - 1$.

(b) $\det E_1 = (\det A)^m \det H_1$ for $m = 0, 1, 2, \ldots, n - 1$.

14.23. If $AC = CA$, then

$$\det \begin{pmatrix} A & B \\ C & D \end{pmatrix} = \det(AD - CB).$$

If we set $A = I$, then the above is true.

14.24. If $A$ and $B$ are $n \times n$ matrices, then

$$\det \begin{pmatrix} A & B \\ B & A \end{pmatrix} = \det(A + B) \cdot \det(A - B).$$

14.25. The determinant of the matrix inversed in (14.15) is

$$\det D \cdot \det E \cdot \det(A - BD^{-1}B' - CE^{-1}C').$$

Proofs. Section 14.3.

14.17a. We take determinants in (14.10a(i)) and use the fact that the determinant of a triangular matrix is the product of its diagonal elements.

14.17b. Similar to (a), but using (14.10b(ii)).

14.17c. Schott [2005: 263]; see also (14.8a,b).


14.19. This follows from (14.18b) and the fact that \( n^2 + n = n(n + 1) \) is even. See also Searle [1982: 98].


14.4 POSITIVE AND NON-NEGATIVE DEFINITE MATRICES

Schur complements arise in this section using a different notation, and the results should be compared with those in Section 14.1. Note that \( \mathbf{A} \succeq \mathbf{B} \) means that \( \mathbf{A} - \mathbf{B} \) is non-negative definite.

14.26. Let

\[
\mathbf{A} = \begin{pmatrix}
\mathbf{A}_{11} & \mathbf{A}_{12} \\
\mathbf{A}_{21} & \mathbf{A}_{22}
\end{pmatrix}
\]

be a real symmetric matrix (i.e., \( \mathbf{A}_{12} = \mathbf{A}_{21}^\prime \), with \( \mathbf{A}_{11} \) and \( \mathbf{A}_{22} \) square matrices).

(a) \( \mathbf{A} \succ 0 \) (i.e., is positive definite or p.d.) if and only if \( \mathbf{A}_{11} \) and \( \mathbf{A}_{22} - \mathbf{A}_{21} \mathbf{A}^{-1}_{11} \mathbf{A}_{12} \) (or \( \mathbf{A} / \mathbf{A}_{11} \)) are p.d.

(b) \( \mathbf{A} \succ 0 \) if and only if \( \mathbf{A}_{22} \) and \( \mathbf{A}_{11} - \mathbf{A}_{12} \mathbf{A}_{22}^{-1} \mathbf{A}_{21} \) are p.d.

(c) If \( \mathbf{A} \succ 0 \), then

\[
\mathbf{A}_{22} \succeq \mathbf{A}_{22} - \mathbf{A}_{21} \mathbf{A}^{-1}_{11} \mathbf{A}_{12}.
\]

(d) If \( \mathbf{A} \succ 0 \) and \( \mathbf{A}^{11} \) is the leading principal submatrix of \( \mathbf{A}^{-1} \) with the same size as \( \mathbf{A}_{11} \), then

\[
\mathbf{A}^{11} - \mathbf{A}^{-1}_{11} \succeq 0.
\]

(e) (Fischer Inequality) If \( \mathbf{A} \succ 0 \), then

\[
\det \mathbf{A} \leq \det \mathbf{A}_{11} \cdot \det \mathbf{A}_{22},
\]

with equality if and only if both sides vanish or \( \mathbf{A}_{12} = 0 \).

(f) If \( \mathbf{A} \succeq 0 \) and the blocks \( \mathbf{A}_{11}, \mathbf{A}_{12}, \) and \( \mathbf{A}_{22} \) are square matrices of the same size, then

\[
|\det \mathbf{A}_{12}|^2 \leq \det \mathbf{A}_{11} \det \mathbf{A}_{22}.
\]

(g) If \( \mathbf{A} \succeq 0 \), then \( C(\mathbf{A}_{12}) \subseteq C(\mathbf{A}_{11}) \) and \( C(\mathbf{A}_{21}) \subseteq C(\mathbf{A}_{22}) \).

The above results will also hold if \( \mathbf{A} \) is Hermitian.
14.27. Let the real symmetric matrix $A$ be partitioned as in (14.10) above, where $A_{11} \succ 0$. Then for any square matrix $A_{22} \succeq 0$,

$$A \succeq 0 \text{ if and only if } A_{22} \succeq A_{21} A_{11}^{-1} A_{12}.$$ 

14.28. Let

$$A = 
\begin{pmatrix} 
A_{11} & A_{12} \\
A_{12}' & 0 
\end{pmatrix},$$

where $A_{11}$ is a non-negative definite $m \times m$ matrix and $A_{12}$ is $m \times n$. The symmetric $(m+n) \times (m+n)$ matrix $A$ is sometimes referred to as a bordered Gramian matrix.

(a) $A$ is nonsingular if and only if rank $A_{12} = n$ and $A_{11} + A_{12} A_{12}'$ is positive definite.

(b) If $A$ is nonsingular, and setting $A_{21} = A_{12}'$, then

$$A^{-1} = 
\begin{pmatrix} 
B_{11}^{-1} - B_{11}^{-1} A_{12} B_{22}^{-1} A_{21} B_{11}^{-1} & B_{11}^{-1} A_{12} B_{22}^{-1} \\
B_{22}^{-1} A_{21} B_{11}^{-1} & B_{22}^{-1}
\end{pmatrix},$$

where $B_{11} = A_{11} + A_{12} A_{21}$ and $B_{22} = A_{21} B_{11}^{-1} A_{12}$.

(c) If $B_{11}$ above is nonsingular, then

$$\det A = (-1)^n \det B_{11} \cdot \det B_{22}.$$ 

(d) If $A$ is nonsingular, then

$$\det A = (-1)^n \det A_{11} \cdot \det (A_{21} A_{11}^{-1} A_{12}).$$ 

14.29. Let $A$ be positive definite and let $B = \begin{pmatrix} A & b \\
b' & c \end{pmatrix}$, where $A$, $b$, and $c$ are real.

(a) $\det B = \det A(c - b'A^{-1}b) \leq c \det A$, with equality if and only if $b = 0$.

(b) $B$ is positive definite if and only if $\det B > 0$.

(c) If $c = b'A^{-1}b$, then $B$ is non-negative definite.

(d) $x'Ax - 2b'x \geq -b'A^{-1}b$.

14.30. Let $A$ and $B$ be real $n \times n$ matrices, and let

$$A = \begin{pmatrix} A_1 & a_1 \\
a_1' & a \end{pmatrix} \quad \text{and} \quad B = \begin{pmatrix} B_1 & b_1 \\
b_1' & b \end{pmatrix},$$

where $A_1$ and $B_1$ are positive definite. Then

$$a_1'A_1^{-1}a_1 + b_1'B_1^{-1}b_1 - (a_1 + b_1)'(A_1 + B_1)^{-1}(a_1 + b_1)$$

$$= (A_1^{-1}a_1 - B_1^{-1}b_1)'(A_1^{-1} + B_1^{-1})^{-1}(A_1^{-1}a_1 - B_1^{-1}b_1).$$

Anderson [2003: 419] gives an application to testing that several multivariate normal populations are identical.
14.31. Let $A$ and $B$ be $n \times n$ positive definite matrices. There exists a unique matrix $C$ such that
\[
\begin{align*}
    c_{ij} &= a_{ij}, \quad (i,j) \in \{1,2,\ldots,t\} \\
    c^{ij} &= b^{ij}, \quad (i,j) \notin \{1,2,\ldots,t\}
\end{align*}
\]
where $C^{-1} = c^{ij}$ and $B^{-1} = b^{ij}$. This result has an application to graphical models for determining patterns of independence.

Proofs. Section 14.4.


14.26b. Same as (a) with the subscripts 1 and 2 interchanged.


14.26d. Follows from (14.11a); see also Zhang [1999: 175, complex case].


14.26g. Sengupta and Jammalamadaka [2003: 45]; see also (14.8c).


14.5 EIGENVALUES

In this section we assume that the $n \times n$ matrix $A$ is partitioned as in (14.10) with $A_{ii}$ being $n_i \times n_i$, for $i = 1, 2$ ($n_1 + n_2 = n$). We also continue with the notation $\lambda_1(A) \geq \cdots \geq \lambda_n(A)$ for ordering the eigenvalues when they are real, which is the case for a symmetric matrix.

14.32. Suppose $A$ is non-negative definite. If $h$ and $i$ are integers between 1 and $n$ inclusive, then:
   
   (a) $\lambda_{h+i-1}(A) \leq \lambda_h(A_{11}) + \lambda_i(A_{22})$, if $h + i \leq n + 1$,
   
   (b) $\lambda_{h+i-n}(A) \geq \lambda_h(A_{11}) + \lambda_i(A_{22})$, if $h + i \geq n + 1$,

where $\lambda_h(A_{11}) = 0$ if $h > n_1$ and $\lambda_i(A_{22}) = 0$ if $i > n_2$. 

Suppose $A$ is non-negative definite and $i_1, i_2, \ldots, i_k$ are distinct integers between 1 and $n$, inclusive. Then for $k = 1, 2, \ldots, n$,

$$
\sum_{j=1}^{k} [\lambda_{ij}(A_{11}) + \lambda_{n-k+j}(A_{22})] \leq \sum_{j=1}^{k} \lambda_{ij}(A) \\
\leq \sum_{j=1}^{k} [\lambda_{ij}(A_{11}) + \lambda_{ij}(A_{22})],
$$

where $\lambda_{ij}(A_{11}) = 0$ if $j > n_1$ and $\lambda_{ij}(A_{22}) = 0$ if $j > n_2$.

Suppose $A$ is symmetric and $\lambda_{n_1}(A_{11}) > \lambda_1(A_{22})$.

(a) For $j = 1, 2, \ldots, n_1$,

$$
0 \leq \lambda_j(A) - \lambda_j(A_{11}) \leq \frac{\lambda_1(A_{12}A_{12}')}{\lambda_j(A_{11}) - \lambda_1(A_{22})},
$$

and for $j = 1, 2, \ldots, n_2$,

$$
0 \leq \lambda_{n_2-j+1}(A_{22}) - \lambda_{n-j+1}(A) \leq \frac{\lambda_1(A_{12}A_{12}')}{\lambda_{n_1}(A_{11}) - \lambda_{n_2-j+1}(A_{22})}.
$$

Tighter bounds are given by Dümbgen [1995]. The above bounds are useful in obtaining the asymptotic distribution of the eigenvalues of a random symmetric matrix (Eaton and Tyler [1991]).

(b) For $k = 1, 2, \ldots, n_1$,

$$
0 \leq \sum_{j=1}^{k} [\lambda_j(A) - \lambda_j(A_{11})] \leq \frac{\sum_{j=1}^{k} \lambda_j(A_{12}A_{12}')}{\lambda_k(A_{11}) - \lambda_1(A_{22})}.
$$

Suppose $A$ is positive definite, and let $B_1 = A_{11} - A_{12}A_{22}^{-1}A_{21}$, $B_2 = A_{22} - A_{21}A_{11}^{-1}A_{12}$, and $C = -B_1^{-1}A_{12}A_{22}^{-1}$, where $A_{12} = A_{21}'$. Then if $\lambda_1(B_1) < \lambda_{n_2}(B_2)$,

$$
0 \leq \sum_{j=1}^{k} [\lambda_{n_1-j+1}(B_1) - \lambda_{n-j+1}(A)] \leq \frac{\lambda_{n_1-k+1}(B_1)}{\lambda_{n_1-k+1}(B_1) - \lambda_{n_2}(B_2)} \sum_{j=1}^{k} \lambda_j(CC'),
$$

for $k = 1, 2, \ldots, n_1$.

Proofs. Section 14.5.


14.6 GENERALIZED INVERSES

14.6.1 Weak Inverses

14.36. Let \( A = (A_{11}, A_{12}) \), where \( A_{11} \) is nonsingular. Then

\[
A^- = \left( \frac{A_{11}^{-1} - A_{11}^{-1} A_{12} Y}{Y} \right)
\]

is a weak inverse of \( A \) for arbitrary \( Y \).

14.37. Let \( A = \begin{pmatrix} A_{11} \\ A_{21} \end{pmatrix} \), where \( A_{11} \) is nonsingular. Then

\[
A^- = (A_{11}^{-1} - X A_{21} A_{11}^{-1}, X)
\]

is a weak inverse of \( A \) for arbitrary \( X \).

14.38. Let \( A \) be \( m \times n \).

(a) \( (A^-_B) \) is a weak inverse of \( (A, B) \) if and only if \( A A^- B = 0 \) and \( B B^- A = 0 \).

(b) \( (A^-_A, C^-) \) is a weak inverse of \( (A_C) \) if and only if \( C A^- A = 0 \) and \( A C^- C = 0 \).

For conditions on the ranks for the above weak inverses to hold, see Tian [2005b].

14.39. Let

\[
A = \begin{pmatrix} A_1^{(p \times n)} \\ A_2^{(q \times n)} \end{pmatrix} \quad \text{and} \quad G = \begin{pmatrix} G_1^{(n \times p)} \\ G_2^{(n \times q)} \end{pmatrix},
\]

with \( p + q = m \). Then \( \mathcal{C}(A_1') \cap \mathcal{C}(A_2') = 0 \) and \( G \) is a weak inverse of \( A \) if and only if

\[
A_1 G_1 A_1 = A_1, \quad A_2 G_1 A_1 = 0, \quad A_2 G_2 A_2 = A_2, \quad \text{and} \quad A_1 G_2 A_2 = 0.
\]

If \( \text{rank } A_1 = p \), the first two equations above become \( A_1 G_1 = I_p \) and \( A_2 G_1 = 0 \).

14.40. Let

\[
A = \begin{pmatrix} A_1^{(m \times p)} \\ A_2^{(m \times q)} \end{pmatrix} \quad \text{and} \quad G = \begin{pmatrix} G_1^{(p \times m)} \\ G_2^{(q \times m)} \end{pmatrix},
\]

with \( p + q = n \). Then \( \mathcal{C}(A_1) \cap \mathcal{C}(A_2) = 0 \) and \( G \) is a weak inverse of \( A \) if and only if

\[
A_1 G_1 A_1 = A_1, \quad A_1 G_1 A_2 = 0, \quad A_2 G_2 A_2 = A_2, \quad \text{and} \quad A_2 G_2 A_1 = 0.
\]

If \( \text{rank } A_1 = p \), the first two equations above become \( G_1 A_1 = I_p \) and \( G_1 A_2 = 0 \).

14.41. Let \( A \) be partitioned in the form of (14.10).

(a) If \( \mathcal{C}(A_{12}) \subseteq \mathcal{C}(A_{11}), C(A_{21}) \subseteq \mathcal{C}(A_{11}'), A_{11}' \) is a particular weak inverse of \( A_{11} \), and \( A_{22-1} = A_{22} - A_{21} A_{11}' A_{12} \), we have

\[
A^- = \begin{pmatrix} A_{11}' + A_{11}' A_{12} A_{22-1} A_{21} A_{11}' - A_{11}' A_{12} A_{22-1} & -A_{11}' A_{12} A_{22-1} \\
-A_{22-1} A_{21} A_{11}' & A_{22-1} \end{pmatrix}.
\]
(b) If \( C(A_{21}) \sqsubseteq C(A_{22}) \), \( C(A'_{12}) \sqsubseteq C(A'_{22}) \), \( A_{22} \) is a particular weak inverse of \( A_{22} \), and \( A_{11.2} = A_{11} - A_{12}A_{22}A_{21} \), we have

\[
A^- = \begin{pmatrix}
A_{11.2}^{-1} & -A_{11.2}^{-1}A_{12}A_{22}^{-1} \\
-A_{22}A_{21}A_{11.2}^{-1} & A_{22}^{-1} + A_{22}^{-1}A_{21}A_{11.2}^{-1}A_{12}A_{22}^{-1}
\end{pmatrix}.
\]

Necessary and sufficient conditions are given in (14.44) below using a different notation. Some rank conditions for the above to hold are given by Tian and Takane [2005].

14.42. Let \( A \) be an \( n \times n \) non-negative definite matrix partitioned as in (14.10), where \( A_{11} \) is \( p \times p \). Suppose that the \( n \times n \) matrix \( G \) is a weak inverse of \( A \) and is partitioned in exactly the same way as \( A \). If each of the first \( p \) rows of \( A \) is nonzero and is not a linear combination of the remaining rows of \( A \), then

\[
G_{11} = (A_{11} - A_{12}A_{22}A_{21})^{-1}
\]

for any weak inverse \( A_{22}^- \) of \( A_{22} \). Also \( G_{11} \) is unique.

14.43. Let

\[
A = \begin{pmatrix} V & X \\ X' & 0 \end{pmatrix} \quad \text{and} \quad G = \begin{pmatrix} G_{11} & G_{12} \\ G_{21} & G_{22} \end{pmatrix},
\]

where \( V \) is an \( n \times n \) non-negative definite matrix, \( X \) is \( n \times p \), and \( G_{11} \) is \( n \times n \).

(a) If \( G \) is a weak inverse of \( A \), we have the following.

(i) \( G_{12} \) is weak inverse of of \( X' \).

(ii) \( G_{21} \) is weak inverse of of \( X \).

(iii) \( VG_{12}X' = XG_{21}V = -XG_{22}X' \).

(iv) \( VG_{11}X = 0, X'G_{11}V = 0, \) and \( X'G_{11}X = 0 \).

(v) \( V = VG_{11}V - XG_{22}X' \).

(vi) \( VG_{11}V, VG_{12}X', XG_{21}V, \) and \( XG_{22}X' \) are symmetric and invariant to the choice of the weak inverse \( G \).

(b) If \( U \) is any \( p \times p \) matrix such that \( C(X) \sqsubseteq C(V + UX'X') \), and \( W \) is any weak inverse of \( V + UX'X' \), then

\[
\begin{pmatrix}
W - WX(X'WX)^{-1}X'W & WX(X'WX)^{-1}X'W \\
(X'WX)^{-1}X'W & -(X'WX)^{-1} + U
\end{pmatrix}
\]

is a weak inverse of \( A \).

14.44. Let

\[
A = \begin{pmatrix} E & F \\ G & H \end{pmatrix}.
\]

(a) Let \( \hat{E} \) be a particular weak inverse of \( E \) and \( S = H - G\hat{E}F \), the generalized Schur complement. Then

\[
B = \begin{pmatrix}
\hat{E} + \hat{E}FS^{-1}G\hat{E} & -\hat{E}FS^{-1} \\
-S^{-1}G\hat{E} & S^{-1}
\end{pmatrix},
\]
is a weak inverse of $A$ for a particular weak inverse $S^-$ if and only if rank is additive on the Schur complement (i.e., $\text{rank } A = \text{rank } E + \text{rank } S$), and then $B$ is a weak inverse of $A$ for any weak inverse $S^-$. Sufficient conditions are $C(F) \subseteq C(E)$ and $C(G') \subseteq C(E')$, as in (14.41a).

(b) Let $\tilde{H}$ be a particular weak inverse of $H$ and $T = E - F\tilde{H}G$, the generalized Schur complement. Then

$$C = \begin{pmatrix} T^- & -T^-F\tilde{H} \\ -\tilde{H}GT^- & \tilde{H} + \tilde{H}GT^-F\tilde{H} \end{pmatrix},$$

is a weak inverse of $A$ for a particular weak inverse $T^-$ if and only if rank is additive on the Schur complement (i.e., $\text{rank } A = \text{rank } H + \text{rank } T$), and then $C$ is a weak inverse of $A$ for any weak inverse $T^-$. Sufficient conditions are $C(G) \subseteq C(H)$ and $C(F') \subseteq C(H')$, as in (14.41b).

We can obtain (b) from (a) by simply interchanging $E$ and $H$, $F$ and $G$, and $S$ and $T$.

**Proofs.** Section 14.6.1.


### 14.6.2 Moore–Penrose Inverses

We consider just a few special cases below. For further results relating to partitioned matrices see Baksalary and Styan [2002] and Groß [2000]. The Moore–Penrose inverse of $(A, B)$ is considered in detail by Campbell and Meyer [1979: 58–59] and Schott [2005: 192–195]. A number of general rank conditions for Moore–Penrose inverses to exist are given by Tian [2004].

14.45. Let $A$ and $B$ be defined as in (14.44) above.

(a) $B = A^+$ if and only if $\tilde{E} = E^+$, $S^- = S^+$,

$$\text{rank } \begin{pmatrix} E \\ G \end{pmatrix} = \text{rank } (E, F) = \text{rank } E \quad \text{and} \quad \text{rank } \begin{pmatrix} F \\ H \end{pmatrix} = \text{rank } (G, H) = \text{rank } S.$$
(b) Since $A^+$ is unique, we get the same result if we do the interchanges described at the end of (14.44). This leads to the following result.

If $S = H - GE^+F$ and $T = E - FH^+G$, then

$$A^+ = \begin{pmatrix} T^+ & -E^+FS^+ \\ -H^+GT^+ & S^+ \end{pmatrix},$$

if and only if

$$\text{rank} \begin{pmatrix} E \\ G \end{pmatrix} = \text{rank}(E, F) = \text{rank} E = \text{rank} T$$

and

$$\text{rank} \begin{pmatrix} F \\ H \end{pmatrix} = \text{rank}(G, H) = \text{rank} H = \text{rank} S.$$
14.7 MISCELLANEOUS PARTITIONS

We close this chapter with a few partitions that may provide some ideas in algebraic manipulations.

14.48. \( A + B = (A, B) \begin{pmatrix} I \\ I \end{pmatrix} = (I, I) \begin{pmatrix} A \\ B \end{pmatrix} \).

14.49. \( \begin{pmatrix} I & -A \\ 0 & I \end{pmatrix} \begin{pmatrix} 0 & AB \\ BC & B \end{pmatrix} \begin{pmatrix} I & 0 \\ -C & I \end{pmatrix} = \begin{pmatrix} -ABC & 0 \\ 0 & B \end{pmatrix} \).

We can set \( B = I \).

14.50. \( \begin{pmatrix} I & A \\ 0 & I \end{pmatrix} \begin{pmatrix} A & 0 \\ -I & B \end{pmatrix} = \begin{pmatrix} 0 & AB \\ -I & B \end{pmatrix} \).
15.1 INVERSES

Matrices that have a particular pattern occur frequently in statistics. Such matrices are typically used as intermediary steps in proofs and in perturbation techniques, when one is interested in the effect of making a small structural change to a matrix. Patterned matrices also occur in experimental designs and in certain variance matrices of random vectors. A related chapter is Chapter 14.

15.1. (Some Identities) There are a number of identities that are useful and which can be used to prove the results in this section. It is assumed that all inverses exist.

(a) (i) \( VA^{-1}(A - UD^{-1}V) = (D - VA^{-1}U)D^{-1}V, \)
    or taking the inverse of both sides,
    (ii) \( D^{-1}V(A - UD^{-1}V)^{-1} = (D - VA^{-1}U)VA^{-1}. \)

(b) Setting \( A = I, \ D = -I, \) and interchanging \( U \) and \( V \) in (a)(ii), we have that
    \[ U(I +Vu)^{-1} = (I + UV)^{-1}U. \]

(c) If \( I + U \) is nonsingular,
    \[ (I + U)^{-1} = I - (I + U)^{-1}U = I - U(I + U)^{-1}. \]

(d) \( U'A^{-1}U(I + U'A^{-1}U)^{-1} = I - (I + U'A^{-1}U)^{-1}. \)
(e) If \( A \) and \( B \) are \( n \times n \) complex matrices, then

\[
I_n + AA^* = (A + B)(I_n + B^*B)^{-1}(A + B)^* \\
+ (I_n - AB^*)(I_n + BB^*)^{-1}(I_n - AB^*)^*.
\]

Note that the right-hand side does not depend on \( B \).

(f) \((\alpha I_n - A)^{-1} - (\beta I_n - A)^{-1} = (\beta - \alpha)(\beta I_n - A)^{-1}(\alpha I_n - A)^{-1}\).

15.2. If \( A \) is nonsingular and the other matrices are conformable square or rectangular matrices (e.g., \( A \) is \( n \times n \), \( U \) is \( n \times p \), \( B \) is \( p \times q \), and \( V \) is \( q \times n \)), then we have the following inverses from Henderson and Searle [1981b: 57-58].

(a)

\[
(A + UBV)^{-1} = A^{-1} - (I + A^{-1}UBV)^{-1}A^{-1}UBV A^{-1} \\
= A^{-1} - A^{-1}(I + UBV A^{-1})^{-1}UBVA^{-1} \\
= A^{-1} - A^{-1}U(I + BVA^{-1}U)^{-1}BVA^{-1} \\
= A^{-1} - A^{-1}UB(I + VA^{-1}UB)^{-1}VA^{-1} \\
= A^{-1} - A^{-1}UBV(I + A^{-1}UBV)^{-1}A^{-1} \\
= A^{-1} - A^{-1}UBVA^{-1}(I + UBV A^{-1})^{-1}
\]

All results follow from the first by repeatedly applying (15.1b).

If the left-hand side exists, then the inverses on the right-hand side exist. This is because each inverse on the right-hand side is the inverse of the sum of \( I \) and a cyclic permutation of \( A^{-1}UBV \), and it exists because its determinant is nonzero. For example,

\[
det(I + A^{-1}UBV) = det(A^{-1}) det(A + UBV) \neq 0.
\]

We can then obtain the other determinants using

\[
det(I + CD) = det(I + DC)
\]

from (4.33) and (15.10b)

(b) A number of special cases are readily available by setting \( B = I \) and/or \( V = I \), and replacing matrices by vectors. For example, Steerneman and van Perlo-tten Kleij [2005] consider a matrix of the form \( V = A - XY^* \), where \( V \) is a nonsingular complex matrix and \( X \) and \( Y \) are \( n \times p \) complex matrices. They consider various special cases, and give eigenvalues and eigenvectors of the real matrix \( D - xy' \), where \( D \) is diagonal matrix (cf. 15.6).

We can also set \( V = U' \) in (a), in which case we get \((A + UBU')^{-1}\) that arises, for example, as a dispersion matrix for many mixed models in the analysis of variance. The following are special cases of (a).

(i) (Sherman–Morrison)

\[
(A + buv')^{-1} = A^{-1} - bA^{-1}uv'A^{-1}/(1 + bv'A^{-1}u).
\]
This is used as an "updating" formula discussed further in (15.11). The situation when $A$ or the modified matrix is singular is investigated by Baksalary and Baksalary [2004c] (see also Section 15.5.2).

(ii) $x'(A + xx')^{-1}x = \frac{x'Ax}{1 + x'A^{-1}x}$.

(iii) $(A + UBU')^{-1} = A^{-1} - A^{-1}UB(I + UA^{-1}UB)^{-1}U'A^{-1}$.

For a good historical discussion and further results see Henderson and Searle [1981b]. They also give some statistical applications of these identities such as inverting the variance matrix for a multinomial vector, inverting a matrix with the pattern of an intraclass correlation matrix, and obtaining the generalized least squares estimates for a variance component model.

15.3. Another set of results can be derived by assuming that $B$ is also nonsingular. From the fourth equation of (15.2a) we have:

(a) (i) $(A + UBV)^{-1} = A^{-1} - A^{-1}UB(B + VU^{-1}UB)^{-1}VU^{-1}BVA^{-1}$.

(ii) $(A + UBV)^{-1} = A^{-1} - A^{-1}U(B^{-1} + VA^{-1}U)^{-1}VA^{-1}$.

(iii) Setting $B = I$, we have the so-called Sherman-Morrison-Woodbury formula

$$(A + UV)^{-1} = A^{-1} - A^{-1}U(I + VA^{-1}U)^{-1}VA^{-1}. $$

This result also holds with $A$ Hermitian.

(iv) Setting $A$ and $B$ equal to identity matrices in (i) or (ii), we have

$$(I + UV)^{-1} = I - U(I + VU)^{-1}V.$$ 

(b) Setting $V = U'$ in (a)(ii) gives us

(i) $(A + UBU')^{-1} = A^{-1} - A^{-1}U(B^{-1} + U'A^{-1}U)^{-1}U'A^{-1}$.

(ii) If $C = (U'A^{-1}U)^{-1}$ exists, then using (15.4b) with $B$ and $C$ instead of $A$ and $B$, we have

$$(A + UBU')^{-1} = A^{-1} - A^{-1}UB(B + C)^{-1}CU'A^{-1} = A^{-1} - A^{-1}U(B + C - C)(B + C)^{-1}CU'A^{-1} = A^{-1} - A^{-1}UCU'A^{-1} + A^{-1}UC(B + C)^{-1} \times CU'A^{-1},$$

(iii) In particular,

$$(A + B)^{-1} = A^{-1} - A^{-1}(A^{-1} + B^{-1})^{-1}A^{-1}. $$

We can also interchange $A$ and $B$ and can replace $A$ by $A^{-1}$ and $B$ by $B^{-1}$.

We note that in (b) (and (a)) we can replace $B$ by $-B$. 
(c) Setting $B = -D^{-1}$ in (a)(ii) leads to a number of results like the following:

(i) $(A - UD^{-1}V)^{-1} = A^{-1} + A^{-1}U(D - VA^{-1}U)^{-1}VA^{-1}$.

Note that the left-hand side of the above is the inverse of a Schur complement. As a special case we have

(ii) $(I - UV)^{-1} = I + U(I - VU)^{-1}V$, as in (a)(iv) with a sign change.

15.4. Gentle [1998: 62] notes that in linear regression we often need inverses of various sums of matrices and gives the following additional identities for nonsingular $A$ and $B$.

(a) $(A + BB')^{-1}B = A^{-1}B(I + B'A^{-1}B)^{-1}$.

(b) $(A^{-1} + B^{-1})^{-1} = A(A + B)^{-1}B$.

(c) $A(A + B)^{-1}B = B(A + B)^{-1}A$.

(d) $A^{-1} + B^{-1} = A^{-1}(A + B)B^{-1}$

We can also add, for nonsingular $A + B$,

(e) $A - A(A + B)^{-1}A = B - B(A + B)^{-1}B$.

15.5. (Non-negative Definite Matrices)

(a) If $A$ is positive definite, then $A - bb'$ is positive definite if and only if $b' A^{-1} b < 1$.

(b) If $A$ is non-negative definite (n.n.d.), then $A - bb'$ is n.n.d. if and only if $b \in C(A)$ and $b'A- b \leq 1$.

15.6. If $A = \text{diag}(a_1, a_2, \ldots, a_n)$ is a nonsingular diagonal matrix and $C = A + \alpha uv'$, then we have the following.

(a) $C^{-1} = A^{-1} + \alpha \beta^{-1}fg'$, where $\beta = -(1 + \alpha \sum_{i=1}^{n} (u_i v_i / a_i) \neq 0)$, $f_i = u_i / a_i$, and $g_i = v_i / a_i$.

(b) $\det C = \left(1 + \alpha \sum_{i=1}^{n} \frac{u_i v_i}{a_i}\right) \prod_{i=1}^{n} a_i$.

(c) The characteristic equation of $C$ is given by

$$\det(C - \lambda I_n) = \left(1 + \alpha \sum_{i=1}^{n} \frac{u_i v_i}{a_i - \lambda}\right) \prod_{i=1}^{n} (a_i - \lambda) = 0.$$

For further details relating to the eigenvalues and eigenvectors of $C$ see Steerneman and van Perlo-ten Kleij [2005] and the references therein.

(d) If $a_1 = a_2 = \cdots = a_n = a$, then $C$ has $n - 1$ eigenvalues equal to $a$ and one eigenvalue equal to $a + \alpha \sum_{i=1}^{n} u_i v_i$. 
15.7. Let $p_i > 0$ for $i = 1, 2, \ldots, k-1$, where $\sum_{i=1}^{k-1} p_i < 1$, and let $p_k = 1 - \sum_{i=1}^{k-1} p_i$. Then the variance matrix for a nonsingular $(k-1)$-dimensional multinomial random variable is

$$ V = n \{ \text{diag}(p_1, p_2, \ldots, p_{k-1}) - pp' \}, $$

where $p' = (p_1, p_2, \ldots, p_{k-1})$. From (15.6a) with $n = k - 1$ and $\alpha = -1$, we have

$$ V^{-1} = n^{-1} \begin{pmatrix} (p_1^{-1} + p_k^{-1}) & p_k^{-1} & \cdots & p_k^{-1} \\ p_k^{-1} & (p_2^{-1} + p_k^{-1}) & \cdots & p_k^{-1} \\ \vdots & \vdots & \ddots & \vdots \\ p_k^{-1} & p_k^{-1} & \cdots & (p_{k-1}^{-1} + p_k^{-1}) \end{pmatrix}. $$

Proofs. Section 15.1.

15.1c. Use the identity $I = I + U - U$, multiply on the left by $(I + U)^{-1}$, and then multiply on the right.
15.1d. We take the inverse term on the right-hand side over to the left.
15.1e. Zhang [1999: 185].
15.1f. Multiply $(\beta I_n - A) - (\alpha I_n - A) = (\beta - \alpha)I_n$ on the left by $(\beta I_n - A)^{-1}$ and on the right by $(\alpha I_n - A)^{-1}$.
15.4a. We take the inverses of both sides.
15.4b. Take inverses of both sides.
15.4c. Interchange $A$ and $B$ in (b).
15.4d. Simply multiply out.
15.4e. This follows from $(A + B)(A + B)^{-1}C = C$ for $C = A, B$ and from (c).
15.5. Abadir and Magnus [2005: 227] and Rao and Bhimasankaram [2000: 345, see solution to exercise 15].
15.2 DETERMINANTS

15.8. If $A$ has rank 1, then from (3.4b) and (4.33),
\[ \det(I_n + xA) = 1 + x \text{trace}(A). \]

15.9. For general $A$, $\det(I + xA) = 1 + x \text{trace} A + O(x^2)$.

15.10. Suppose $C$ is $n \times m$, $D$ is $m \times n$, $u$ is $n \times 1$, $w$ is $n \times 1$, and $v$ is $m \times 1$, then we have the following results.

(a) $\det(I_n + CD) = \det \begin{pmatrix} I_n & C \\ -D & I_m \end{pmatrix}$.

(b) We have from (4.33), $\det(I_n \pm CD) = \det(I_m \pm DC)$.

(c) Setting $C = u'$ and $D = v'A$, we have from (b) and (15.8)
\[ \det(I_n \pm uv'A) = \det(1 \pm v'Au) = 1 \pm \text{trace}(v'Au) = 1 \pm v'Au. \]

(d) If $A$ is $n \times n$, $B$ is $m \times m$, and $A$ and $B$ are nonsingular, then
\[ \det(A + UBV) = \det(A) \det(I_m + VA^{-1}UB) = \det(A) \det(B^{-1} + VA^{-1}U) \det(B). \]

We have the following special cases.

(i) $\det(A \pm uu') = \det(A)(1 \pm u'A^{-1}u)$.

(ii) $u'A^{-1}u = 1 - (\det(A - uu')/\det(A))$.

(iii) $\det(A + \alpha uw') = \det(A)(1 + \alpha w'A^{-1}u) = \det(A) + \alpha w'(\text{adj}A)u$, where $\text{adj}A$ is the adjoint matrix of $A$.

Proofs. Section 15.2.

15.8. Abadir and Magnus [172–173].


15.10a–b. Muirhead [1982: 578].

15.10d. Harville [1997: 416].

15.3 PERTURBATIONS

**Definition 15.1.** Suppose we have a matrix $A$ involved in a system of equations and we wish to know what happens to the system if we change $A$ to $A + \delta A$. If the matrix $\delta A$ is of rank one (cf. (3.4b)), then it is called a rank one perturbation. Other kinds of perturbations may consist of adding or subtracting an observation to see what effect this has on any inference or diagnostics. Clearly, such perturbations have many uses in statistics, and although the theory underlying these is given above and elsewhere, it is helpful to collect some of the results used generally and
in linear regression together here. For a historical overview and some computational aspects see Hager [1989].

15.11. (General) Let \( A \) be an \( n \times n \) nonsingular matrix. We consider the effect on the inverse of \( A \) of three modifications using (15.2b(i)).

(a) (Add to an Element) If we add \( h \) to \( a_{ij} \), then \( A \) becomes \( A + hE_{ij} = A + he_i e_j' \), where \( e_i \) is the \( i \)th column of \( I_n \), and

\[
(A + he_i e_j')^{-1} = A^{-1} - \frac{hA^{-1}e_i e_j' A^{-1}}{1 + he_j' A^{-1} e_i}.
\]

(b) (Add to a Column) If \( f \) is added to the \( j \)th column of \( A \), then

\[
(A + fe_j')^{-1} = A^{-1} - \frac{A^{-1}fe_j' A^{-1}}{1 + e_j' A^{-1} f}.
\]

(c) (Add to a Row) If row \( g' \) is added to the \( i \)th row of \( A \), then

\[
(A + e_i g')^{-1} = A^{-1} + \frac{A^{-1}e_i g' A^{-1}}{1 + g' A^{-1} e_i}.
\]

(d) (Diagonal Increment) If the inverses exist, we have from (15.3a(ii)),

\[
(A + kI_n)^{-1} = A^{-1} - A^{-1}(k^{-1}I_n + A^{-1})^{-1}A.
\]

It is assumed that all the above denominators are nonzero.

15.12. (Sample Mean and Variance Matrix) Suppose we have a set of \( d \)-dimensional observations \( x_1, x_2, \ldots, x_n \), and we define

\[
W_n = \sum_{i=1}^{n} w_i \quad \tilde{x}_n = \sum_{i=1}^{n} w_i x_i / W_n, \quad \text{and} \quad S_n = \sum_{i=1}^{n} w_i (x_i - \tilde{x}_n)(x_i - \tilde{x}_n)',
\]

We want to know what happens to these quantities when we add an observation \( x_{n+1} \) or subtract \( x_n \). Setting \( d_{n+1} = x_{n+1} - \tilde{x}_n \) and \( f_n = x_n - \tilde{x}_n \), we have the following.

(a) (Add an Observation)

(i) \( \tilde{x}_{n+1} = \tilde{x}_n + \frac{w_{n+1}}{W_{n+1}} d_{n+1} \).

(ii) \( S_{n+1} = S_n + w_{n+1}(1 - \frac{w_{n+1}}{W_{n+1}}) d_{n+1} f_{n+1}' \).

(b) (Subtract an Observation)

(i) \( \tilde{x}_{n-1} = \tilde{x}_n - \frac{w_n}{W_{n-1}} f_n \).

(ii) \( S_{n-1} = S_n - w_n(1 - \frac{w_n}{W_{n-1}}) f_n f_n' \).

(c) (Equal Weights) With equal weights we have \( w_i = 1/n, W_n = 1 \), and so on.

Let \( \bar{x}_k = \sum_{i=1}^{k} x_i / k \) and \( S_k = \sum_{i=1}^{k} (x_i - \bar{x}_k)(x_i - \bar{x}_k)' / k \) for \( k = n-1, n, n+1 \). Then:
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(i) \( \overline{x}_{n+1} = \overline{x}_n + \frac{1}{n+1} d_{n+1} \) and \( \overline{x}_{n-1} = \overline{x}_n - \frac{1}{n-1} f_n \).

(ii) \( \frac{n+1}{n} S_{n+1} = S_n + \frac{1}{n+1} d_{n+1} d_{n+1}' \) and \( \frac{n-1}{n} S_{n-1} = S_n - \frac{1}{n-1} f_n f_n' \).

15.13. (Regression) Let \( X = (x_1, x_2, \ldots, x_n)' = (x^{(1)}, x^{(2)}, \ldots x^{(p)}) \) be an \( n \times p \) matrix of rank \( p \). We are interested what in happens to \( (X'X)^{-1} \) and related quantities when the rows and columns of \( X \) are modified.

(a) (Add or Delete a Row) Suppose that \( i \)th row \( x'_i \) is deleted giving us \( X(i) \) instead of \( X \), then \( X(i)'X(i) = X'X - x_ix_i' \). Let \( h_{ii} = x'_i(X'X)^{-1}x_i \).

(i) \( (X'X - x_ix_i')^{-1} = (X'X)^{-1} + \frac{(X'X)^{-1}x_i'x_i(X'X)^{-1}}{1 - h_{ii}} \).

(ii) \( \det(X'X - x_ix_i') = \det(X'X)(1 - h_{ii}) \) (from 15.10d(iii)).

(iii) If an extra row \( x' \) is added to \( X \), then one simply replaces \( x_i \) by \( x \) and changes all the signs in (i) and (ii) above.

(iv) Let \( \hat{\beta} = (X'X)^{-1}X'y \) and \( \hat{\beta}(i) = (X(i)'X(i))^{-1}X(i)'y(i) \), where \( y(i) \) is \( y \) without its \( i \)th element \( y_i \). Here \( \hat{\beta} \) and \( \hat{\beta}(i) \) are the respective least squares estimates of \( \beta \) under a regression model with full rank design matrix \( X \), and under the same model but with the \( i \)th case deleted, the so-called leaving-one-out model. Then

\[
\hat{\beta}(i) = \hat{\beta} - \frac{(X'X)^{-1}x_i(y_i - x'_i\hat{\beta})}{1 - h_{ii}}.
\]

This result forms the basis of a number of regression diagnostics (e.g., Seber and Lee [2003: section 10.6]).

(b) (Substitute One Row for Another) If we replace row \( x'_- \) by row \( x'_+ \), we can combine (a)(ii) and (iii) to get

\[
\det(X'X + x_+x'_+ - x_-x'_-) = \det(X'X) [(1 + x'_+(X'X)^{-1}x_+) \n - x'_-(X'X)^{-1}x_- (1 + x'_+(X'X)^{-1}x_+) \n + (x'_+(X'X)^{-1}x_-)^2],
\]

a result given by Gentle [1998: 171]. He indicates how this result is used in a stepwise method for maximizing \( \det(X'X) \), a problem that arises, for example, in optimal design theory (D-optimality, cf. Section 24.5).

(c) (Add or Delete a Column)

(i) If an extra column \( x \) is added to \( X \) giving \( X_1 = (X, x) \), then by (14.11),

\[
(X_1'X_1)^{-1} = \begin{pmatrix} X'X & X'x \\ x'X & x'x \end{pmatrix}^{-1} = \begin{pmatrix} (X'X)^{-1} + uu' & -uu' \\ -uu' & v \end{pmatrix},
\]

with \( u = (X'X)^{-1}X'x, v = [x'(I_n - P)x]^{-1}, \) and \( P = X(X'X)^{-1}X' \).
(ii) Suppose the last column \( x = x^{(p)} \) is deleted from \( X \) giving us \( X^{(p)} \) so that \( X = (X^{(p)}, x) \). Then

\[
X'X = \begin{pmatrix}
X^{(p)'X^{(p)}} & X^{(p)'x} \\
x'X^{(p)} & x'x
\end{pmatrix},
\]

and we can use (i) with \( X \) now playing the role of \( X_1 \) to pick out from \((X'X)^{-1}\) the values of \( u \) and \( v \) and obtain \((X^{(p)'X^{(p)}})^{-1}\) by subtraction.

(d) (Diagonal Increments) The expression \((X'X + kI_p)^{-1}\) occurs in the context of ridge regression and Bayes regression estimators, and can be expressed in terms of \((X'X)^{-1}\) using (15.11d) above.

The above expressions do not indicate how they are actually computed, as one avoids finding the inverse of a matrix directly. Computational details are given by Seber and Lee [2003: section 11.6; they involve using the sweep operator (Seber [1977: 351] or Seber and Lee [2003: 335]) and modifying the QR decomposition. One can also use a weighted least squares approach (Escobar and Moser [1993]). The above theory applies to the linear model \((y, X\beta, \sigma^2 I_n)\) (cf. Section 20.7), where \( X \) has full column rank. For updates relating to the more general model \((y, X\beta, \sigma^2 V)\), with \( X \) being less than full rank and \( V \) being possibly singular, the reader is referred to Sengupta and Jammalamadaka [2003: chapter 9], who also include changes produced in various other statistics.

15.14. (Interchanges in Design Models) Let \( A = X'PX \), where \( X \) is an \( n \times p \) matrix, \( P \) is an \( n \times n \) symmetric idempotent matrix, and \( A1_n = 0 \). Suppose we interchange two rows of \( X \) so that \( A \) becomes \( A_2 \). We can assume, without any loss of generality, that it is the first two rows. Let \( X \) and \( P \) be partitioned as follows:

\[
X = \begin{pmatrix} x'_1 \\ x'_2 \\ X_3 \end{pmatrix} \quad \text{and} \quad P = \begin{pmatrix} c_1 & c_2 & d'_1 \\ c_2 & c_3 & d'_2 \\ d_1 & d_2 & D_3 \end{pmatrix}.
\]

Then we find that

\[
A - A_2 = (c_1 - c_3)(x_1x'_1 - x_2x'_2) + B + B',
\]

where

\[
B = (x_1 - x_2)(d_1 - d_2)'X_3.
\]

Suppose that the spectral decomposition of the symmetric matrix \( A - A_2 \) is \( T\Lambda T' \), where \( \Lambda \) is a diagonal matrix whose diagonal elements are the eigenvalues of \( A - A_2 \), with corresponding eigenvectors given by the columns of the orthogonal matrix \( T \). Then, from (15.25),

\[
A_+ = (A - T\Lambda T')^+ = A^+ + A^+\Psi^+T'A^+,
\]

where \( \Psi = \Lambda^{-1} - T'A^+T \), provided \( C(T\Lambda T') \subset C(A) \). For further computational details and applications with regard to experimental designs with blocking structure, see John [2001]. This method of interchanging two rows is particularly useful in searching for the most efficient designs. It has been also applied to so-called \( \alpha \)-designs, where one is involved with block circulants and Hermitian matrices (Williams and John [2000]).
15.15. (Perturbed Identity Matrix) Let $T(\theta) = I_n - \theta e_i e_j'$ be an $n \times n$ matrix, where $\theta$ is a real scalar and $e_r$ is the $r$th column of $I_n$.

(a) If $i \neq j$, then $T^{-1}(\theta) = T(-\theta)$.

(b) Let $A = (a_{ij})$ be an $n \times n$ upper-triangular matrix. When $i < j$,

$$T^{-1}(\theta)AT(\theta) = A + \theta(e_i e_j'A - A e_i e_j') = A + \theta P,$$

where

$$P = \begin{pmatrix} 0 & Q \\ 0 & 0 \end{pmatrix}, \quad Q = \begin{pmatrix} -a_{1i} & 0 & \cdots & 0 \\ -a_{2i} & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ -a_{i-1,i} & 0 & \cdots & 0 \\ a_{jj} - a_{ii} & a_{j,i+1} & \cdots & a_{jn} \end{pmatrix},$$

and the submatrices in $P$ have $i$ and $n - i$ rows, and $j - 1$ and $n - j + 1$ columns, respectively.

(c) If $a_{ii} \neq a_{jj}$ and $\theta = a_{ij}/(a_{ii} - a_{jj})$, then $[T^{-1}(\theta)AT(\theta)]_{ij} = 0$ and the only elements in $A$ to be disturbed are in row $i$ to the right of $a_{jj}$ and in column $j$ above $a_{jj}$.

15.16. The effect of a perturbation on a finite irreducible discrete time Markov chain is examined by Hunter [2005] with reference to mean first passage times and the stationary distribution. He also gives references to the literature on the subject. In a random environment there could be small random perturbations to a transition matrix and an example of this is considered by Hoppensteadt et al. [1996].

Proofs. Section 15.3.


15.4 MATRICES WITH REPEATED ELEMENTS AND BLOCKS

15.17. If $A = \begin{pmatrix} aI_n & bI_n \\ cI_n & dI_n \end{pmatrix}$, then $\det A = (ad - bc)^n$.

15.18. Let $J_{m,n}$ be an $m \times n$ matrix of ones, i.e., $J_{m,n} = 1_m 1'_n$, and define $J_m$ to be $J_{m,m}$. We now consider a number of results that use these matrices.

(a) If $A = aI_n + bJ_n$ ($b \neq 0$), that is, we have $a + b$ on the diagonal and $b$ everywhere else, then:

(i) $\det A = a^{n-1}(a + nb)$.

(ii) $A^{-1} = \frac{1}{a} \left( I_n - \frac{b}{a + nb} J_n \right)$, ($a \neq 0, a \neq -nb$).
(iii) $\det(\lambda I_n - A) = (\lambda - a - nb)(\lambda - a)^{n-1}$, so that the eigenvalue $a + nb$ has algebraic multiplicity 1 and $a$ has multiplicity $n - 1$. The eigenvector $n^{-1/2}1_n$ corresponds to the eigenvalue $\lambda = a + nb$. A set of eigenvectors of $A$ are the rows of the Helmert matrix (8.10).

(iv) Sometimes we have $c$ on the diagonal and $b$ everywhere else. In this case we set $a = c - b$ in the above. For example, a common case is the correlation matrix that arises, for example, in a one-way random effects model, namely

$$R = (1 - \rho)I_n + \rho J_n.$$  

This has eigenvalues $(1 - \rho)$ and $1 + \rho(n - 1)$, so that $R$ is positive definite if the eigenvalues are positive, that is, when

$$-\frac{1}{n - 1} < \rho < 1.$$  

(b) If

$$A = \begin{pmatrix} mI_m & J_{m,m-1} & J_{m,m-1} \\ J'_{m,m-1} & mI_{m-1} & J_{m,m-1} \\ J'_{m,m-1} & J_{m-1,m} & mI_{m-1} \end{pmatrix},$$

then

$$mA^{-1} = \begin{pmatrix} I_m + \frac{2(m-1)}{m}J_m & -J_{m,m-1} & -J_{m,m-1} \\ -J'_{m,m-1} & I_{m-1} + J_{m-1} & 0 \\ -J'_{m,m-1} & 0 & I_{m-1} + J_{m-1} \end{pmatrix}.$$

This kind of pattern arises in Latin square designs.

(c) Consider the $(m + n) \times (m + n)$ matrix

$$A = \begin{pmatrix} a_1I_m & a_2J_{m,n} \\ a_2J'_{m,n} & a_3I_n \end{pmatrix},$$

where $a_1 \neq 0$ and $a_3 \neq 0$.

(i) If $d = a_1 a_3 - mna_2^2 \neq 0$,

$$A^{-1} = \begin{pmatrix} a_1^{-1}I_m + b_1J_m & b_2J_{m,n} \\ b_2J'_{m,n} & a_3^{-1}I_n + b_3J_n \end{pmatrix},$$

where $b_1 = na_2^2/(a_1d_1)$, $b_2 = -a_2/d$ and $b_3 = ma_2^2/(a_3d)$.

(ii) $\det A = a_1^{m-1}a_3^{n-1}d$.

(iii) The matrix $A$ above occurs in the form $X'X$, where $X$ is the so-called design matrix, in a 2-way ANOVA with equal numbers of observations per cell by setting $a_1 = n$, $a_3 = m$, and $a_2 = 1$. This matrix is singular as $d = 0$, and it is in fact non-negative definite. A generalized inverse is

$$A^- = \begin{pmatrix} I_m/n & 0 \\ 0 & C_{n/m} \end{pmatrix},$$

where $C_n$ is the centering matrix $(I_n - 1_n1'_n/n)$.
(iv) If we set $a_1 = a_3 = 1$, and $a_2 = \rho$, we get the so-called intraclass correlation matrix. The eigenvalues of $A$ are then 1 with algebraic multiplicity $m + n - 2$ and $1 \pm \rho \sqrt{mn}$, each with multiplicity 1. $A$ is then positive definite if and only if

$$-(mn)^{-1/2} < \rho < (mn)^{-1/2}.$$  

(d) Let

$$A = \begin{pmatrix}
    a_1 & a_2I_m' & a_3I_m' & \cdots & a_nI'_n \\
    a_2I_m & b_2I_m + c_2J_m & b_3I_m + c_3J_m & \cdots & b_nI_m + c_nJ_m \\
    a_3I_m & b_3I_m + c_3J_m & b_4I_m + c_4J_m & \cdots & b_nI_m + c_nJ_m \\
    \vdots & \vdots & \vdots & \ddots & \vdots \\
    a_nI_m & b_nI_m + c_nJ_m & d_nI_m + e_nJ_m & \cdots & y_nI_m + z_nJ_m
\end{pmatrix}.$$  

If the inverse of $A$ exists, then it has the same pattern as $A$. For example,

$$\begin{pmatrix}
    a & b_{1n-1}' \\
    b_{1n-1} & (c-d)I_{n-1} + dJ_{n-1}
\end{pmatrix}^{-1} = \begin{pmatrix}
    e & f_{1n-1}' \\
    f_{1n-1} & (g-h)I_{n-1} + hJ_{n-1}
\end{pmatrix},$$

where $e = \frac{1}{a}[1 + \lambda b^2(n-1)], f = -\lambda b, g = \frac{1}{c-d}[1 - \lambda (ad - b^2)], h = \frac{1}{c-d} \lambda (b^2 - ad)$, and $\lambda = \{a(c-d)+(n-1)(ad-b^2)\}^{-1}$. This example arises in Latin square models and response surfaces; Graybill [1983: 195–196] gives a numerical example.

15.19. Let $A$ and $B$ be $m \times m$ matrices, and let

$$C = \begin{pmatrix}
    A + B & B & \cdots & B & B \\
    B & A + B & \cdots & B & B \\
    \vdots & \vdots & \ddots & \vdots & \vdots \\
    B & B & \cdots & A + B & B
\end{pmatrix},$$

where $C$ has $n$ diagonal blocks.

(a) (i) $\det C = (\det A)^{n-1} \det(A + nB)$.

(ii) $C$ has eigenvalues $\lambda_i$ ($i = 1, 2, \ldots, m$) each of algebraic multiplicity 1 and eigenvalues $\mu_i$ ($i = 1, 2, \ldots, m$) each of multiplicity $n - 1$, where the $\lambda_i$ are the eigenvalues of $A + nB$ and the $\mu_i$ are the eigenvalues of $A$.

(b) Consider the special case $A + B = I_m$ and $B = J_m$.

(i) Using (15.18a(i))

$$\det C = \det(A + B - B)^{n-1} \det[A + B + (n-1)B]
= (1 - m)^{n-1}[1 + m(n-1)].$$

(ii) $C$ is nonsingular if and only if $m > 1$.

(iii) If $C^{-1}$ exists, it has the same block structure as $C$ with $I_m + aJ_m$ in each of the diagonal block positions and $bJ_m$ in all the off-diagonal block positions, where

$$a = \frac{m(n-1)(n-1)}{(n-1)m + 1} \quad \text{and} \quad b = \frac{-(m-1)}{(n-1)m + 1}(m-1).$$
15.20. Let

\[ A = \begin{pmatrix}
  a_1 b_1 & 0 & 0 & \cdots & 0 \\
a_2 b_1 & a_2 b_2 & 0 & \cdots & 0 \\
\vdots & \vdots & \ddots & \ddots & \vdots \\
a_n b_1 & a_n b_2 & a_n b_3 & \cdots & a_n b_n
\end{pmatrix}, \]

where all the \( a_i \) and \( b_i \) are nonzero. Then \( \det A = \prod_{i=1}^{n} (a_i b_i) \) and

\[ A^{-1} = \begin{pmatrix}
  (a_1 b_1)^{-1} & 0 & 0 & \cdots & 0 & 0 \\
-(a_1 b_2)^{-1} & (a_2 b_2)^{-1} & 0 & \cdots & 0 & 0 \\
0 & -(a_2 b_3)^{-1} & (a_3 b_3)^{-1} & \cdots & 0 & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\
0 & 0 & 0 & \cdots & (a_{n-1} b_{n-1})^{-1} & 0 \\
0 & 0 & 0 & \cdots & -(a_{n-1} b_n)^{-1} & (a_n b_n)^{-1}
\end{pmatrix}. \]

For other patterned matrices that are either tridiagonal or have a tridiagonal inverse see Section 8.11.

15.21. Let \( A = (a_{ij}) \) be any \( n \times n \) matrix. If \( B = (a_{ij} - a_i a_j/a_{..}) \), where \( a_i = \sum_j a_{ij}, a_j = \sum_i a_{ij}, \) and \( a_{..} = \sum_i \sum_j a_{ij} \), then

\[ B = A - A 1_n (1'_n A 1_n)^{-1} 1'_n A. \]

**Proofs.** Section 15.4.


15.18a. Graybill [1983: 191, 204, and a special case of 206, with \( a - b \) replaced by \( a \)].

15.18b. Roy and Sarhan [1956: 230].

15.18c(i)–(ii). Graybill [1983: 193, 205] and Roy and Sarhan [1956].

15.18c(iii). Ouellette [1981: 284].

15.18c(iv). Ouellette [1981: 285].

15.18d. Roy and Sarhan [1956: 230].

15.19a(i). Graybill [1983: 231, with \( A - B \) replaced by \( A \)].

15.19a(ii). Simply replace \( A \) by \( A - \lambda I_m \) in (a).


15.21. Given the vector \( n \times 1 \) vector \( x = (x_i) \), we have \( \sum_i x_i = 1'_n x \). We use this for the rows and columns of \( A \).
15.5 GENERALIZED INVERSES

15.5.1 Weak Inverses

15.22. Suppose that \( C(UBV) \subset C(A) \) (or equivalently \( AA^{-1}UBV = UBV \)) and \( C([UBV]'') \subset C(A') \) (or equivalently \( UBVA^{-1}A = UBV \)), then we have the following weak inverses of \( (A + UBV) \).

\[
\begin{align*}
G_1 &= A^+ - A^+(A^+ + A^+UBVA^-)A^+UBVA^- , \\
G_2 &= A^+ - A^+U(U + UBVA^-U)UBVA^- , \\
G_3 &= A^+ - A^+UB(B + BVA^-UB)^-BVA^- , \\
G_4 &= A^+ - A^+UBV(V + VA^-UBV)^-VA^- , \\
\end{align*}
\]

The above sufficient conditions are satisfied if \( A \) is nonsingular.

15.23. Let \( X \) be an \( n \times p \) matrix of rank \( r \), and let \( H \) be a \( q \times p \) matrix of rank \( p - r \) such that \( C(X') \cap C(H') = 0 \).

(a) \( \begin{pmatrix} X \\ H \end{pmatrix} \) has rank \( p \) so that \( A = X'X + H'H \) is nonsingular.

(b) \( A^{-1} \) is a weak inverse of \( X'X \).

(c) \( \begin{pmatrix} X'X & H' \\ H & 0 \end{pmatrix} \) is nonsingular if \( q = p - r \), and its inverse is then a weak inverse of the matrix \( X'X \).

The above results arise in studying identifiability constraints in analysis of variance models.

15.24. Let \( A \) be \( m \times n \), and let \( x \) and \( y \) be \( m \times 1 \) and \( n \times 1 \) vectors, respectively. If either \( x \in C(A) \) or \( y \in C(A') \), then, for any weak inverse \( A^- \) of \( A \),

\[
(A + xy')^- = A^- - \frac{A^-xy'A^-}{1 + y'A^-x},
\]

provided \( 1 + y'A^-x \neq 0 \).

Proofs. Section 15.5.1.


15.24. Quoted in Rao and Rao [1998: 281]. Setting \( C = A + xy' \), we can show, after some algebra, that \( CC^-C = C \). We make use of the fact that \( AA^- \) projects onto \( C(A) \). In particular, if \( x = Ay \), then \( AA^-x = AA^-Ay = Ay = x \).
15.5.2 Moore–Penrose Inverses

15.25. If $B$ is nonsingular,

$$(A + UBU')^+ = A^+ - A^+U(B^{-1} + U'A^+U)^+U'A^+,$$

if and only if $C(UBU') \subseteq C(A)$, or equivalently $A^+UBU' = UBU'$. The result also holds if $A$ is Hermitian (Williams and John [2000: 697]).

15.26. Let $A$ be an $n \times n$ nonsingular matrix, and let $c$ and $d$ be $n \times 1$ vectors. Then $A + cd'$ is singular if and only if $1 + d'A^{-1}c = 0$ and, if this is the case, then

$$(A + cd')^+ = (I_n - yy^+)A^{-1}(I_n - xx^+),$$

where $x = A^{-1}d$, $y = A^{-1}c$, and $x^+ = (x'x)^{-1}x'$ etc.

15.27. Let $A$ be an $n \times n$ symmetric matrix, and suppose that $c$ and $d$ are $n \times 1$ vectors in $C(A)$. If $1 + d'A^+c \neq 0$, then

$$(A + cd')^+ = A^+ - \frac{A^+cd'A^+}{1 + d'A^+c}. $$

15.28. Let $A$ be an $m \times n$ complex matrix, $c \in \mathbb{C}^m$, $d \in \mathbb{C}^n$, and $\beta = 1 + d^*A^+c$. Define $k = A^+c$, $h' = d^*A^+$, $u = (I_m - AA^+)c$, and $v' = d^*(I_n - A^+A)$. Then:

(a) $\text{rank}(A + cd^*) = \text{rank} \begin{pmatrix} A & u \\ d^* & -\beta \end{pmatrix} - 1.$
(b) $(A + cd^*)^+ = A^+ - ku^+ - (hv^+)' + \beta v'^+u'^+.$

Note that $x^+ = x^*/(x^*x)$.

15.29. If $A$ is block diagonal, then $A^+$ is also block diagonal. For example,

$$A = \begin{pmatrix} A_1 & 0 & 0 \\ 0 & A_2 & 0 \\ 0 & 0 & 0 \end{pmatrix} \quad \text{if and only if} \quad A^+ = \begin{pmatrix} A_1^+ & 0 & 0 \\ 0 & A_2^+ & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

15.30. (Multinomial Distribution) Consider the variance matrix $\Sigma = (\sigma_{ij})$ of an $n$-dimensional (singular) multinomial distribution. Here $\sigma_{ii} = np_i(1 - p_i)$ and $\sigma_{ij} = -np_ip_j$ ($i \neq j$), where $0 < p_i < 1$ for all $i$ and $p_1 + p_2 + \cdots + p_n = 1$. If $D_p = \text{diag}(p_1, p_2, \ldots, p_n)$, then $\Sigma = n(D_p - pp')$ is singular and

$$\Sigma^+ = n^{-1}(I_n - n^{-1}1_n1_n')D_p^{-1}(I_n - n^{-1}1_n1_n').$$

15.31. Let

$$B = \begin{pmatrix} V & C^* \\ C & 0 \end{pmatrix},$$

where $V$ is $n \times n$ Hermitian non-negative definite and $C$ is $r \times n$. Then

$$B^+ = \begin{pmatrix} 0 & C^+ \\ C^{++} & -C^{++}VC^+ \end{pmatrix} + \begin{pmatrix} I_n \\ -C^{++}V \end{pmatrix} Q(I_n, -V^+C),$$

where $E = I_n - C^+C$ and $Q = (EVE)^+$. 

Proofs. Section 15.5.2.

15.25. John [2001: 1175].


15.27. Quoted by Schott [2005: 217, exercise 5.32]. Can be proved in a manner similar to that of (15.24).

15.28. Campbell and Meyer [1979: 47–48]. They also list several special cases in which one or more of $u$, $v$, and $\beta$ are zero. They also give Moore–Penrose inverses of $\begin{pmatrix} A & c \\ d^* & \alpha \end{pmatrix}$.

15.30. Follows from (15.26) above, along with $D_p^{-1}p = 1_n$.

15.31. Campbell and Meyer [1979: 64].
CHAPTER 16

FACTORORIZATION OF MATRICES

The factorization of a matrix $A$ can be expressed two ways; either as a reduction $XAY = C$ or as a factorization $A = URV$. In many cases these are equivalent because of the presence of nonsingular matrices—for example, $A = X^{-1}CY^{-1}$ if $X$ and $Y$ are nonsingular. Authors tend to have different preferences for which form they use. Useful summaries of some of the factorizations are given by Abadir and Magnus [2005: 158], Horn and Johnson [1985: 157], and Rao and Rao [1998: 190–193].

16.1 SIMILARITY REDUCTIONS

As eigenvalues are used in this section, we remind the reader of Definition 6.1. In what follows, we assume that an $n \times n$ matrix has eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_n$ with $|\lambda_1| \geq |\lambda_2| \geq \cdots \geq |\lambda_n| \geq 0$ and has distinct eigenvalues $\mu_1, \mu_2, \ldots, \mu_s$, similarly ordered, with algebraic and geometric multiplicities $m(\mu_j)$ and $g(\mu_j)$, respectively.

Definition 16.1. Let $A$ and $B$ be $n \times n$ matrices over $\mathcal{F}$. We say that $A$ is similar to $B$ if there exists a nonsingular matrix $K$ over $\mathcal{F}$ such that $K^{-1}AK = B$.

16.1. Let $A$ be an $n \times n$ real or complex matrix.

(a) $A$ is similar to its transpose.

(b) $A^*A$ is similar to $AA^*$. 

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(c) $\overline{A}A$ is similar to $A\overline{A}$.

(d) $A$ is similar to a symmetric matrix.

(e) $A$ is similar to a complex triangular matrix (either upper or lower) whose diagonal elements are the eigenvalues of $A$.

16.2. Let $A$ and $B$ be real $n \times n$ matrices. If $R$ is a complex nonsingular matrix such that $R^{-1}AR = B$, then there exists a real nonsingular matrix $S$ such that $S^{-1}AS = B$.

16.3. Let $A$ be an upper-triangular matrix with distinct diagonal elements $\text{diag}(A)$. Then there exists a unit upper-triangular matrix $R$ (i.e., with ones on the diagonal) such that $R^{-1}AR = \text{diag}(A)$.

**Definition 16.2.** Let $J_m(\lambda)$ be an $m \times m$ matrix of the form

$$
J_m(\lambda) = \begin{pmatrix}
\lambda & 1 & 0 & \cdots & 0 & 0 \\
0 & \lambda & 1 & \cdots & 0 & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\
0 & 0 & 0 & \cdots & \lambda & 1 \\
0 & 0 & 0 & \cdots & 0 & \lambda
\end{pmatrix},
$$

where $J_1(\lambda) = \lambda$. Then $J_m(\lambda)$ is said to be a Jordan block matrix. We find it convenient to include the case $m = 1$.

16.4. Every Jordan block $J_m(\lambda)$ ($m > 1$) is not diagonalizable because it has only one linearly independent eigenvector $x = (x_1, 0, \ldots, 0)'$, where $x_1$ is arbitrary (cf. Definition 16.3 above (16.10)). This follows from the fact the diagonal elements of the upper-triangular matrix $J_m(\lambda)$ are its eigenvalues, so that it has one eigenvalue $\lambda$ repeated $m$ times, and $x$ satisfies $J_m(\lambda)x = \lambda x$.

16.5. Every Jordan block is permutation similar to its transpose since $J_m(\lambda)' = \Pi J_m(\lambda)\Pi$, where $\Pi = (e_m, e_{m-1}, \ldots, e_1)$ is the backward identity permutation matrix, where $(e_1, e_2, \ldots, e_m) = I_m$.

16.6. Let $x = (x_i)$ be an $m \times 1$ vector. The Jordan block $J = J_m(0)$ has the following properties.

(a) $Jx = (x_2, x_3, \ldots, x_m, 0)'$, representing a forward shift.

(b) $J'x = (0, x_1, x_2, \ldots, x_{m-1})'$, representing a backward shift.

(c) $(I_m - J')x = (x_1, x_2 - x_1, x_3 - x_2, \ldots, x_m - x_{m-1})'$, representing a difference operator.

(d) $(I_m - J')^{-1}x = (x_1, x_1 + x_2, x_1 + x_2 + x_3, \ldots, x_1 + x_2 + \cdots + x_m)'$, which can be called a partial sum operator.

16.7. (Jordan Canonical Form) If $A$ is a real or complex $n \times n$ matrix, then there exists a nonsingular matrix $R$ such that

$$
R^{-1}AR = \begin{pmatrix}
J_{n_1}(\lambda_1) & 0 & \cdots & 0 \\
0 & J_{n_2}(\lambda_2) & \cdots & 0 \\
\vdots & \vdots & \ddots & \vdots \\
0 & 0 & \cdots & J_{n_k}(\lambda_k)
\end{pmatrix} = J_O,
$$

where $J_{n_i}(\lambda_i)$ are the Jordan blocks of $A$. This is called the Jordan Canonical Form of $A$. 

$J_O$ is a direct sum of Jordan blocks corresponding to the eigenvalues of $A$. The Jordan Canonical Form is unique up to the order of the Jordan blocks.
where \( \sum_{i=1}^{k} n_i = n \) and the \( \lambda_i \) are the (not necessarily distinct) eigenvalues of \( A \); that is, \( A \) is similar to \( J_0 \). The matrix \( J_0 \) is said to be in \textit{Jordan canonical form}, which is unique apart from the order of the blocks. One application of the Jordan canonical form is in the analysis of a system of ordinary differential equations with constant coefficients (Horn and Johnson [1985: 132-133]). The topic of \textit{Jordan chains} is considered by Abadir and Magnus [2005: section 7.6].

If \( \mu_1, \mu_2, \ldots, \mu_s \) are the distinct \( \lambda_i \), then we have the following.

(a) The number \( k \) of Jordan blocks (including multiple occurrences of the same blocks) is the number of linearly independent eigenvectors of \( J_0 \).

(b) The matrix \( J_0 \) is diagonalizable (cf. Definition 16.3 above (16.10)) if and only if \( k = n \).

(c) The number of Jordan blocks corresponding to \( \mu_j \) is the geometric multiplicity \( g(\mu_j) \). The sum of the orders (sizes) of all the Jordan blocks corresponding to \( \mu_j \) is the algebraic multiplicity \( m(\mu_j) \).

(d) \( J_0 \) is not completely determined in general by a knowledge of the eigenvalues and their algebraic and geometric multiplicities. We must also know the sizes of the Jordan blocks corresponding to each \( \lambda_i \).

(e) The minimal polynomial of \( J_0 \) (and therefore of \( A \), as similar matrices have the same minimal polynomial, cf. (6.12)) is

\[
f(\mu) = \prod_{j=1}^{s} (\mu - \mu_j)^{r_j},
\]

where \( r_j \) is the order of the largest Jordan block of \( J_0 \) corresponding to \( \mu_j \).

(f) The sizes of the Jordan blocks corresponding to a given \( \mu_j \) are determined by a knowledge of the ranks of certain powers.

(g) If \( A \) is a real matrix with only real eigenvalues, then the similarity matrix \( R \) can be taken to be real.

(h) It is convenient to standardize the order of the Jordan blocks as follows. For each \( \mu_j \) we have \( g(\mu_j) \) blocks that we order in decreasing size, and we order these \( s \) groups of blocks according to our convention \( |\mu_1| > \cdots > |\mu_s| \); \( J_0 \) is then unique.

16.8. If \( A \) and \( B \) are \( n \times n \) similar matrices, then they have the same Jordan canonical form.

16.9. Let \( A \) be an \( n \times n \) upper-triangular matrix with zeros on the main diagonal (sometimes called a \textit{strictly upper-triangular matrix}).

(a) There exists a nonsingular \( n \times n \) matrix \( S \) and integers \( n_1, n_2, \ldots, n_m \) with \( n_1 \geq n_2 \geq \cdots \geq n_m \) and \( n_1 + n_2 + \cdots + n_m = n \) such that

\[
S^{-1}AS = \begin{pmatrix}
J_{n_1}(0) & 0 & \cdots & 0 \\
0 & J_{n_2}(0) & \cdots & 0 \\
& \ddots & \ddots & \ddots \\
0 & 0 & \cdots & J_{n_m}(0)
\end{pmatrix}.
\]
(b) If $A$ is nilpotent with nilpotency index $k$, then $m = \dim \mathcal{N}(A)$, the size of the largest block is $k \times k$, and each block is nilpotent.

**Definition 16.3.** If $A$ is similar to a diagonal matrix, then $A$ is said to be diagonalizable. Other terms used are diagonable, simple, semi-simple or nondefective. Note that $A$ can be real or complex.

16.10. $A$ is diagonalizable if and only if one, and hence all, of the following equivalent conditions are satisfied (cf. Definition 6.1):

1. $m(\mu_j) = g(\mu_j)$ for each $j$; that is, the eigenvalues of $A$ are all regular.
2. $g(\mu_1) + g(\mu_2) + \cdots + g(\mu_s) = n$, that is the sum of the eigenspaces of $A$ is $\mathbb{C}^n$.
3. $\text{rank}(A - \mu_jI_n) = n - m(\mu_j)$ for $j = 1, 2, \ldots, s$. The equivalence with (1) follows from (6.1b)
4. $A$ possesses $n$ linearly independent right (respectively left) eigenvectors.

16.11. If $A$ has $n$ distinct eigenvalues, then they are simple and therefore regular, so that by (16.10(1)) above $A$ is diagonalizable.

16.12. A matrix $A$ is diagonalizable if and only if $h(A) = 0$, where

$$h(x) = (x - \mu_1)(x - \mu_2)\cdots(x - \mu_s),$$

and the $\mu_j$ are the distinct eigenvalues of $A$. If $h(A) = 0$, then $h(\lambda) = q(\lambda)$, the minimal polynomial.

16.13. It follows from (16.12) above that an idempotent matrix $A$ is diagonalizable since $h(A) = 0$, where

$$h(x) = x(x - 1),$$

and the eigenvalues of $A$ are $\lambda = 0, 1$.

16.14. (Product) Suppose $A$ and $B$ are $n \times n$ Hermitian matrices with $A$ positive-definite. Then $AB$ has real eigenvalues and is diagonalizable. Also, $AB$ has the same number of positive, negative, and zero eigenvalues as $B$. Furthermore, any diagonalizable matrix with real eigenvalues is the product of a positive definite Hermitian matrix and a Hermitian matrix.

16.15. (Approximation) Let $A = (a_{ij})$ be an $n \times n$ matrix. For every $\epsilon > 0$, there exists a matrix $A(\epsilon) = (a_{ij}(\epsilon))$ with distinct eigenvalues (and is therefore diagonalizable) such that

$$\sum_{i=1}^{n} \sum_{j=1}^{n} |a_{ij} - a_{ij}(\epsilon)|^2 < \epsilon.$$

16.16. Let $A$ be $n \times n$ and $B$ be $m \times m$ matrices, and let

$$C = \begin{pmatrix} A & 0 \\ 0 & B \end{pmatrix}.$$ 

Then $C$ is diagonalizable if and only if $A$ and $B$ are both diagonalizable.
16.17. (Spectral Decomposition) Suppose $A$ is diagonalizable of rank $r$.

(a) There exist linearly independent right eigenvectors $x_1, x_2, \ldots, x_n$ and linearly independent left eigenvectors $y'_1, y'_2, \ldots, y'_n$ such that $y'_ix_j = \delta_{ij}$, where $\delta_{ij} = 1$ when $i = j$ and 0 otherwise. Also

$$A = \sum_{i=1}^{n} \lambda_i x_i y'_i$$

$$= \sum_{i=1}^{n} \lambda_i F_i$$

$$= \sum_{i=1}^{r} \lambda_i F_i$$

for nonzero $\lambda_i$, where the rank one $F_i$ are not unique unless all the eigenvalues are distinct. Here the $F_i$ are idempotent, mutually orthogonal, and $\sum_{i=1}^{n} F_i = I_n$. If $R = (x_1, x_2, \ldots, x_n)$ and $S = (y_1, y_2, \ldots, y_n)'$, then $A = RSA$, where $SR = I_n$ implies that $S = R^{-1}$. Note that as the rank is unchanged when multiplying by a nonsingular matrix, rank $A = \text{rank} A$, and rank $A$ is the number of nonzero eigenvalues of $A$.

(b) (Unique Decomposition)

(i) We can also write

$$A = \sum_{j=1}^{s} \mu_j E_j,$$

where $E_j$ represents the sum of the $F_i$ corresponding to the same eigenvalue and the $\mu_j$ are the distinct eigenvalues (including zero). The $E_j$, called the spectral set, are unique, idempotent, and mutually orthogonal (i.e., $E_j E_k = \delta_{jk} E_j$) and satisfy $\sum_{j=1}^{s} E_j = I_n$.

(ii) Also, for $k = 1, 2, \ldots$,

$$A^k = \sum_{j=1}^{s} \mu_j^k E_j.$$

(c) If $A$ is nonsingular, then

$$A^{-1} = \sum_{j=1}^{s} \mu_j^{-1} E_j.$$

If $A$ is singular, then

$$A^+ = \sum_{j} \mu_j^{-1} E_j,$$

where the summation is over the nonzero eigenvalues, and $A^+$ is the Moore–Penrose inverse of $A$. This is proved directly from the definition of $A^+$.

For a spectral decomposition of an arbitrary matrix see Rao and Mitra [1971: 38].
16.18. Suppose $A$ is an $n \times n$ diagonalizable matrix with distinct eigenvalues $\lambda_i$. Then the Vandermonde matrix (cf. Section 8.12.1)

$$
B = \begin{pmatrix}
1 & 1 & \cdots & 1 \\
\lambda_1 & \lambda_2 & \cdots & \lambda_n \\
\lambda_1^2 & \lambda_2^2 & \cdots & \lambda_n^2 \\
& & \ddots & \vdots \\
\lambda_1^{n-1} & \lambda_2^{n-1} & \cdots & \lambda_n^{n-1}
\end{pmatrix}
$$

is nonsingular with inverse $B^{-1} = (\beta_{ij})$, say. From the previous result (16.17b), with $s = n$ and $E_j = F_j$, we have

$$
\begin{pmatrix}
I_n \\
A \\
\vdots \\
A^{n-1}
\end{pmatrix} = (B \otimes I_n) \begin{pmatrix}
F_1 \\
F_2 \\
\vdots \\
F_n
\end{pmatrix},
$$

where "\( \otimes \)" is the Kronecker product. Now $B \otimes I_n$ can be expressed symbolically as $b_{ij}I_n$ so that using $(B \otimes I_n)^{-1} = B^{-1} \otimes I_n$ and defining $A^0 = I_n$ we have

$$
F_i = \sum_{j=1}^{n} \beta_{ij} A^{j-1}.
$$

Substituting in $A^k$ from (16.17b(ii)) gives us

$$
A^k = \sum_{i=1}^{n} \sum_{j=1}^{n} \lambda_i^k \beta_{ij} A^{j-1}, \quad k = 1, 2, \ldots,
$$

16.19. If $A$ is real symmetric (respectively Hermitian) $n \times n$ matrix with distinct eigenvalues $\mu_j$ ($j = 1, 2, \ldots, s$), then $m(\mu_j) = g(\mu_j)$ for $j = 1, 2, \ldots, s$. Hence, by (16.10(1)) above, all real symmetric (respectively Hermitian) matrices are diagonalizable.

Proofs. Section 16.1.


16.3. Abadir and Magnus [2006: 186].

16.5. Horn and Johnson [1985: 134].

16.7. For proofs, references, and comments see Abadir and Magnus [2005: section 7.5], Horn and Johnson [1985: section 3.1], Meyer [2000a: sections 7.7 and 7.8], and Rao and Bhimasankaram [2000: section 8.6].

16.8. The result follows from the uniqueness of the Jordan canonical form.


16.11. Horn and Johnson [1985: 48].


16.15. Horn and Johnson [1985: 89].


16.2 REDUCTION BY ELEMENTARY TRANSFORMATIONS

16.2.1 Types of Transformation

Definition 16.4. An elementary row transformation of an \( m \times n \) matrix \( A \) over \( F \) is one of the following operations:

1. Multiply row \( i \) by a scalar \( c \) in \( F \). This achieved by left-multiplying \( A \) by the identity matrix \( I_m \) with its \( i \)th diagonal element replaced by \( c \). The latter has determinant \( c \).

2. Add row \( j \) to row \( i \). This is achieved by left-multiplying by the matrix \( I_m + E_{ij} \), where \( E_{ij} \) has 1 in the \( (i,j) \)th position and zeros elsewhere. This transformation has determinant 1.

3. Interchange the \( i \)th and \( j \)th rows. This is achieved by left-multiplying by the permutation matrix \( \Pi_{ij} \), where \( \Pi_{ij} \) is \( I_m \) with its \( i \)th and \( j \)th rows interchanged. (Technically the third transformation can be carried out using a sequence of the previous two transformations, but that route is less convenient.)

These operations can also be extended to submatrices of partitioned matrices (cf. Zhang 1999: 30]).
16.20. Note the following:
   
   (a) $\Pi_{ij}$ is symmetric and orthogonal so that $\Pi_{ij}^{-1} = \Pi_{ij}$.
   
   (b) $E_{ij}^2 = 0$ and $(I_m + cE_{ij})^{-1} = I_m - cE_{ij}$.

**Definition 16.5.** An elementary (row) transformation matrix $M$ is defined to be one of the above three types of matrices, referred to as types (1), (2), and (3). For further details see, for example, Abadir and Magnus [2005: section 6.1]

   Elementary column transformations can be carried out by right-multiplying $A$ by an elementary transformation matrix (but using $E_{ij}$ instead of $E_{ij}$).

16.21. The inverse of an elementary transformation matrix is also an elementary transformation matrix. Also, as such matrices are all nonsingular, a product of such matrices is nonsingular. Therefore multiplying $A$ by such a matrix does not change the rank of $A$ (cf. 3.14a).

16.2.2 Equivalence Relation

**Definition 16.6.** Let $A$ and $B$ be $m \times n$ real or complex matrices. If $B$ is obtained from $A$ by elementary row or column transformations matrices, then $A$ is said to be equivalent to $B$, and we write $A \sim B$.

16.22. Any one of the following statements implies the other two.

   (1) $A \sim B$.
   
   (2) $B = RAS$ for some non-singular matrices $R$ and $S$.
   
   (3) rank $A = \text{rank } B$ (cf. 3.14a).

**Definition 16.7.** From (16.22(2)) above we see that: (i) $A \sim A$ (reflexive), (ii) if $A \sim B$, then $B \sim A$ (symmetric), and (iii) if $A \sim B$ and $B \sim C$, then $A \sim C$ (transitive). Any relation that satisfies these three conditions is called an SRT relation. Thus the equivalence relation “∼” is an SRT relation.

Other SRT relations for square matrices are summarised as follows:

   (1) If $B = R^{-1}AR$ for nonsingular $R$, then $B$ is said to be similar to $A$. This is discussed in Section 16.1 above.
   
   (2) If $B = R'AR$ for nonsingular $R$, then $B$ is said to be congruent to $A$. Its main application is for real matrices. If $A$ and $B$ are complex matrices such that $B = R^*AR$, then $B$ is said to be Hermitian congruent to $A$.
   
   (3) If $B = U^*AU$, where $U$ is unitary, then $B$ is said to be unitarily similar to $A$. If, for real matrices, $B = T'AT$, where $T$ is orthogonal, we say that $B$ is orthogonally similar to $A$.

16.2.3 Echelon Form

**Definition 16.8.** Using elementary row transformations, a real or complex $m \times n$ matrix $A$ can be reduced to a matrix $B$ with the following properties:

   (1) If a row contains at least one nonzero entry, then the first nonzero entry is 1.
(2) The zero rows, if any, come last.

(3) In any two consecutive nonzero rows, the leading 1 in the lower row occurs further to the right than the leading 1 in the upper row.

A matrix in the above form is said to be in *(row)* echelon form. For example,

\[ B_1 = \begin{pmatrix} 0 & 1 & * & * & * \\ 0 & 0 & 0 & 1 & * \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix} , \]

where the elements denoted * are arbitrary. If we now subtract multiples of the second and third rows from the first, we obtain

\[ B_2 = \begin{pmatrix} 0 & 1 & 0 & 0 & * \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix} . \]

This matrix has the additional property:

(4) Each column that contains a leading 1 has zeros elsewhere.

A matrix with the above four properties is said to be in reduced *(row)* echelon form. We shall omit the word “row” in using the above definitions. Rao and Bhimasankaram [2000: 167-170] give a number of algorithms for carrying out various reductions. It should be noted that the terminology relating to echelon forms is not consistent in the literature.

We see that the first three rows of \( B_2 \) give a row basis for the original matrix \( A \), and the three columns each containing 1 form a column basis for \( A \).

16.23. Any matrix \( A \) can be reduced to a unique matrix in reduced echelon form by elementary row transformations.

16.24. The rank of a matrix in reduced echelon form is the number of nonzero rows. This is the same as the rank of the original matrix.

16.25. If \( A \) is a nonsingular matrix of order \( n \), then its reduced echelon form is \( I_n \). Hence there exist elementary transformation matrices \( M_k \), \( k = 1, 2, \ldots, K \), such that \( M_K M_{K-1} \cdots M_1 A = I_n \), i.e., \( MA = I_n \), where \( M \) is nonsingular. Also, taking \( A \) over to the right-hand side, \( M_K M_{K-1} \cdots M_1 I_n = A^{-1} \). Thus any sequence of elementary row transformations that transforms \( A \) to \( I_n \) transforms \( I_n \) to \( A^{-1} \).

16.26. For any two \( n \times p \) matrices \( A \) and \( B \), the following statements are equivalent.

(1) \( C(A') = C(B') \).

(2) The reduced echelon forms of \( A \) and \( B \) are the same.

(3) \( B \) can be obtained from \( A \) by a finite sequence of elementary row operations.

(4) \( B = KA \) for some nonsingular matrix \( K \).

**Proofs.** Section 16.2.3.


16.2.4 Hermite Form

**Definition 16.9.** A square matrix \( H \) is said to be in (upper) Hermite form if (a) it is upper-triangular, (b) its principal diagonal elements are all zeros or ones, (c) when a diagonal element is zero the entire row is zero, and (d) when a diagonal element is one, the rest of the elements in the column are all zeros. For example, a Hermite form for a \( 5 \times 5 \) matrix \( A \) could take the form

\[
H_A = \begin{pmatrix}
0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & + & 0 \\
0 & 0 & 1 & + & 0 \\
0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 \\
\end{pmatrix},
\]

where the starred elements are arbitrary. If \( H \) comes from \( A \) we shall write \( H_A \).

There is a close relationship between the reduced echelon form and the Hermite form of a matrix. For example, the reduced echelon form corresponding to \( H_A \) would be

\[
B = \begin{pmatrix}
0 & 1 & 0 & + & 0 \\
0 & 0 & 1 & + & 0 \\
0 & 0 & 0 & 0 & 1 \\
0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 \\
\end{pmatrix}.
\]

We see that \( H_A \) can be obtained from \( B \) by simply interchanging rows, i.e., by carrying out elementary row transformations. This is the case in general so that many of the results for reduced echelon forms apply to Hermite forms, as we shall see later.

16.27. \( H_A^2 = H_A \).

16.28. If \( A \) is a square matrix over \( F \), there exists a nonsingular matrix \( K \) such that \( KA = H_A \). The matrix \( K \) is a product of elementary row transformation matrices.

16.29. Two real \( n \times n \) matrices \( A \) and \( B \) have the same Hermite form if and only if \( C(A') = C(B') \). The following are consequences of this result.

(a) \( A'A, A-A \) and \( A \) have the same Hermite form.

(b) If \( B \) is nonsingular, then \( BA \) and \( A \) have the same Hermite form.

16.30. Let \( A \) be \( n \times n \). Since \( H_A^2 = H_A \) we have the following.

(a) \( AH_A = A \).

(b) The identity matrix \( I_n \) is the only \( n \times n \) matrix in Hermite form that is nonsingular. Thus if \( A \) is nonsingular, then \( H_A = I_n \).

16.31. (Rank)

(a) \( \text{rank } H_A = \text{rank } A \).

(b) The rank of a matrix in Hermite form is the number of non-null rows in it, or the number of diagonal elements equal to one. Thus reducing a matrix to
echelon form is a method of finding its rank. (For an algorithm see Rao and Bhimasankaram [2000: 181–182].)

(c) If the \(i_1, i_2, \ldots, i_k\) diagonal elements of \(H_A\) are each equal to one, and the remaining diagonal elements of \(H_A\) are equal to zero, then the \(i_1, i_2, \ldots, i_k\) columns of \(A\) are linearly independent.

16.32. (Idempotency)

(a) \(A\) is idempotent if and only if \(H_A\) is a weak inverse of \(A\).

(b) \(A\) is idempotent if and only if \(H_A A = H_A\).

**Definition 16.10.** An \(n \times n\) matrix \(H\) is said to be in \((upper)\) Hermite canonical form if it takes the form

\[
H = \begin{pmatrix} I_r & C \\ 0 & 0 \end{pmatrix}.
\]

By looking at the example given in Definition 16.9, we see that a Hermite form can be transformed into a Hermite canonical form by carrying out suitable row and column interchanges. This process can be carried further to transform \(C\) into the zero matrix, as we see in the next result.

16.33. (Reduction to Diagonal Form) Let \(A\) be an \(m \times n\) matrix of rank \(r\) defined over \(\mathcal{F}\).

(a) There exist nonsingular matrices \(F\) and \(G\) of sizes \(m \times m\) and \(n \times n\), respectively, such that

\[
FAG = \begin{pmatrix} I_r & 0 \\ 0 & 0 \end{pmatrix},
\]

so that \(A\) is equivalent to a diagonal matrix. Thus

\[
A = F^{-1} \begin{pmatrix} I_r & 0 \\ 0 & 0 \end{pmatrix} G^{-1} = R \begin{pmatrix} I_r & 0 \\ 0 & 0 \end{pmatrix} S,
\]

say. (Some bordering matrices are absent if \(A\) has full row or column rank.) The matrices \(F\) and \(G\) and their respective inverses \(R\) and \(S\) are all products of elementary transformation matrices.

(b) (Full Rank Factorization) From (a) we have

\[
A = (R_1, R_2) \begin{pmatrix} I_r & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} S_1 \\ S_2 \end{pmatrix} = R_1 S_1,
\]

where \(R_1\) is \(m \times r\) of rank \(r\) and \(S_1\) is \(r \times n\) of rank \(r\).

(c) (Singular Value Decomposition) If \(A\) is real (respectively complex), we can choose \(R\) with orthogonal columns and \(S\) with orthogonal rows. If we then incorporate the lengths of the columns of \(R\) and the rows of \(S\) into \(I_r\), we get what is effectively the singular value decomposition of \(A\), namely
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A = P \begin{pmatrix} D_r & 0 \\ 0 & 0 \end{pmatrix} Q,

where $P$ and $Q$ are orthogonal (respectively unitary) matrices and $D_r$ is a diagonal matrix with positive elements. This decomposition is discussed in more detail in Section 16.3. We note that

$$A = (P_1, P_2) \begin{pmatrix} D_r & 0 \\ 0 & 0 \end{pmatrix} (Q_1, Q_2) = (P_1 D_r^{1/2})(D_r^{1/2} Q_1) = P_2 Q_2.$$ 

Thus $A$ can be expressed in the form $P_2 Q_2$, where $P_2$ has orthogonal columns and $Q_2$ has orthogonal rows. We can choose $P_2$ (respectively $Q_2$) to have orthonormal columns (respectively rows).

Proofs. Section 16.2.4.

16.27. Quoted by Graybill [1983: 131].


16.3 SINGULAR VALUE DECOMPOSITION (SVD)

The singular value decomposition is regarded by many as one of the most useful factorizations for real or complex matrices. For example, the SVD has many applications in statistics such as SAS (single-spectrum analysis) in times series (cf. Golyandina et al. [2001: chapter 4]), matrix approximation in dimension reduction techniques, least squares approximation of a square matrix by a scalar multiple of an orthogonal or unitary matrix (Horn and Johnson [1985: 429], and procrustes analysis (Gower and Dijksterhuis [2004] and Seber [1984: section 5.6]). It is also a useful computational tool for calculating various quantities. In what follows, we interpret the transpose as conjugate transpose when dealing with complex matrices.

Definition 16.11. Any $m \times n$ real (respectively complex) matrix of rank $r$ ($r \leq p = \min\{m, n\}$) can be expressed in the form

$$A_{m \times n} = P_{m \times m} \Sigma_{m \times n} Q'_{n \times n},$$

where $P$ is an $m \times m$ orthogonal (respectively unitary) matrix, $Q$ is an $n \times n$ orthogonal (respectively unitary) matrix, and $\Sigma = (\sigma_{ij})$ is an $m \times n$ matrix with

$$\sigma_{11} \geq \sigma_{22} \cdots \geq \sigma_{rr} > 0 = \sigma_{r+1,r+1} = \cdots = \sigma_{pp}, \text{ and } \sigma_{ij} = 0 \text{ for all } i, j, i \neq j.$$
This factorization of $A$ is called the singular value decomposition. The $\sigma_i$, abbreviated to $\sigma_i(A)$ ($i = 1, 2, \ldots, p$), are called the singular values of $A$, which are defined to be the positive square roots of the ranked eigenvalues of $AA'$. These eigenvalues are non-negative as $AA'$ is non-negative definite (by 10.10).

The columns of $p_i$ of $P$ are the orthonormalized right eigenvectors associated with $AA'$, and the columns $q_i$ of $Q$ are the orthonormalized right eigenvectors associated with $A'A$. The first $r$ columns in each case correspond to the nonzero $\sigma_i$. Note that $Aq_i = \sigma_ip_i$ and $A'p_i = \sigma_iq_i$ ($i = 1, 2, \ldots, r$). The vectors $p_i$ and $q_i$ are also called the left and right singular vectors, respectively, associated with $\sigma_i$.

We note that $AA'$ and $A'A$ have $p$ common eigenvalues (cf. 6.54c), including some zeros when $r < p$. Any remaining eigenvalues of $AA'$ (if $m > n$) or $A'A$ (if $m < n$) are zero.


In practice, several versions of the SVD are given in the literature, which we give below.

(1) Let $\Delta_p = \text{diag}(\sigma_1, \sigma_2, \ldots, \sigma_p)$. If $p = n \leq m$, then

$$A = P \begin{pmatrix} \Delta_n \\ 0 \end{pmatrix} Q' = P_n \Delta_n Q',$$

where the $m \times n$ matrix $P_n$ consists of the first $n$ columns of $P$, and $\Delta_n$ and $Q$ are both $n \times n$. The zero matrix is omitted if $m = n$. If $p = m < n$, then

$$A = P(\Delta_m, 0)Q' = P \Delta_m Q_m',$$

where $Q_m$ consists of the first $m$ columns of $Q$. We note that $P_nP_n = I_n$ and $Q_mQ_m = I_m$. These two versions are often referred to as the thin singular value decompositions.

Is the decomposition unique? If $m \geq n$ (i.e., $p = n$), then $\Sigma$ will be unique as the eigenvalues of $A'A$ are unique. However, the eigenvectors making up $P_n$ and $Q$ will not be unique unless the eigenvalues are distinct and an appropriate sign convention is adopted for eigenvectors.

(2) If $P = (p_{ij})$ and $Q = (q_{ij})$, with respective columns $p_i$ and $q_i$, then

$$A = P \begin{pmatrix} \Delta_r \\ 0 \end{pmatrix} Q' = P_r \Delta_r Q'_r = \sum_{k=1}^r \sigma_k p_k q'_k,$$

and $a_{ij} = \sum_{k=1}^r \sigma_k p_{ik} q_{jk}$.

If $A$ is complex and $P$ and $Q$ are unitary matrices, then $A = \sum_{k=1}^r \sigma_k p_k q'_k$ and $a_{ij} = \sum_{k=1}^r \sigma_k p_{ik} q_{jk}$.

Note that $AA'P_r = P_r \Delta_r^2$ and $A'AQ_r = Q_r \Delta_r^2$. The correct procedure is to find $P_r$ and $\Delta_r^2$ from $AA'P_r = P_r \Delta_r^2$ and then define $Q_r = A'P_r \Delta_r^{-1}$. Alternatively, we can obtain $Q_r$ and $\Delta_r^2$ from $A'AQ_r = Q_r \Delta_r^2$ and then define $P_r = AQ_r \Delta_r^{-1}$ (Abadir and Magnus [2005: 226]).
16.34. Let $A$ be an $m \times n$ matrix. From the above we have the following useful information.

(a) The number of nonzero singular values is the rank of $A$. This provides a useful computational method for finding the rank of a matrix.

(b) The $r$ columns of $P_r$ and $Q_r$ are orthonormal bases for $\mathcal{C}(A)$ and $\mathcal{C}(A')$, respectively, while the remaining columns of $P$ and $Q$ span $\mathcal{N}(A')$ and $\mathcal{N}(A)$, respectively.

(c) $P_A = P_r P'_r$, the orthogonal projection onto $\mathcal{C}(A)$.

(d) $A$ and $(A^* A)^{1/2}$ have the same singular values.

(e) Two full-rank factorizations of $A$ (cf. 3.5) are $(P_r \Delta_r) (Q'_r)$ and $(P_r) (\Delta_r Q'_r)$.

Proofs. Section 16.3.

16.34a–b. Schott [2005: 140–141].

16.34c. Sengupta and Jammalamadaka [2003: 43].

16.34d. Follows from the fact that $(A^* A)^{1/2}((A^* A)^{1/2})^* = A^* A$ is Hermitian with eigenvalues $\sigma_i^2(A)$.

16.4 TRIANGULAR FACTORIZATIONS

16.35. ($LU$ and $LDU$ factorizations) Under certain conditions, a real or complex $m \times n$ matrix can be expressed in the form $A = L_1 U_1$, where $L_1$ is lower-triangular and $U_1$ is upper-triangular. If $m < n$, then $L_1$ is $m \times m$, while if $m > n$, $L_1$ is $m \times n$.

(a) A sufficient condition for such a factorization to exist is that for $k = 1, 2, \ldots, p$ ($p = \min\{m, n\}$), each $k \times k$ leading principal submatrix $A_k$ of $A$ is nonsingular.

(i) The usual factorisation is to have either the diagonal elements of $L_1$ all ones (and written as $\tilde{L}$), or the diagonal elements of $U_1$ all ones (and written as $\tilde{U}$) so that

$$A = \tilde{L} U = L \tilde{U}.$$ 

(ii) If we put the diagonal elements from both matrices into a single diagonal matrix $D$, then

$$A = \tilde{L} D \tilde{U}.$$ 

(b) If $m < n$, which is often the case, and $A_k$ is nonsingular for $k = 1, 2, \ldots, m$, then $A = L \tilde{U}$, where $L$ is $m \times m$ and nonsingular, $\tilde{U}$ is an $m \times n$ matrix such that the first $m$ columns form an upper-triangular matrix with unit diagonal elements, and $L$ and $\tilde{U}$ are unique.

(c) A typical application of the above theory is the solution of linear equations, for example $Bx = b$. If we set $A = (B, I_m, b)$ and then factorize $A$, we can...
obtain $B^{-1}$ as a bonus (Rao and Bhimasankaram [2000: 213]). If $B$ is square and nonsingular and $B = LU$, then we can solve $Ly = b$ for $y$ using forward substitution and solve $Ux = y$ for $x$ by back substitution. The process is usually referred to as Gaussian elimination.

(d) The matrix $M_k = I_n - \tau e_k e_k'$, where $\tau \in \mathbb{R}^n$ and $e_k$ has 1 for its $k$th element and zeros elsewhere, is a Gauss transformation if the first $k$ elements of $\tau$ are zero. If this is the case, and $\tau_i = x_i / x_k$ ($x_k \neq 0$) for $i = k + 1, \ldots, n$, then

$$M_k x = (x_1, x_2, \ldots, x_k, 0, \ldots, 0)'$$

16.36. (Square Matrix $LU$ Factorizations) Let $A$ be a real or complex $n \times n$ matrix and let $A_k$ be its leading $k \times k$ principal submatrix.

(a) Suppose $A$ has rank $r$. If $A_k$ is nonsingular for $k = 1, 2, \ldots, r$, then $A$ may be factored as $A = LU$, where $L$ and $U$ are $n \times n$. Furthermore, the factorization may be chosen so that either $L$ or $U$ is nonsingular. Both $L$ and $U$ can be chosen to be nonsingular if $A$ is nonsingular (i.e., $r = n$).

(b) There exist $n \times n$ permutation matrices $\Pi_1$ and $\Pi_2$ such that $A = \Pi_1 LU \Pi_2$. If $A$ is nonsingular, it may be written as

$$A = \Pi_1 LU.$$

(c) Suppose $A_k$ is nonsingular for $k = 1, 2, \ldots, n - 1$.

(i) $A$ can be expressed in the form $A = \tilde{L} \tilde{U} = \tilde{L} \tilde{U}$, where all the triangular matrices are unique.

(ii) Also, $A$ can also be expressed in the form $A = \tilde{L} D \tilde{U}$, where $D$ is diagonal and all the matrices are unique. (Note that it is possible for $A$ be singular.)

(iii) If $A$ is a real symmetric matrix, then we can also write $A = U' D_1 U$, where $U$ is real and the diagonal matrix $D_1$ has elements $\pm 1$.

(d) Suppose $A$ is nonsingular and $A = LU$. If $L = (l_{ij})$, then, since $\det A = \det L \cdot \det \tilde{U}$, we have $\det A = \prod_{i=1}^{n} l_{ii} \neq 0$, $\det A_k = \prod_{i=1}^{k} l_{ii} \neq 0$ for $k = 1, 2, \ldots, n - 1$, and $L$ and $\tilde{U}$ are unique, by (c).

(e) If $A$ is Hermitian with an $LDU$ factorization, then we can express it in the form $A = U' D_2 U$, where $D_2$ is a diagonal matrix.

16.37. (Schur Decomposition Theorems) We now consider a series of powerful theorems that can be used to provide shorter proofs for a wide range of other results (e.g., Abadir and Magnus [2005: section 7.4]).

Let $\lambda_1, \lambda_2, \ldots, \lambda_n$ be the eigenvalues of the $n \times n$ matrix $A$ in a prescribed order.

(a) If $A$ is a real or complex matrix, there exists a unitary matrix $Q$ such that $Q^* A Q = T$ is upper-triangular with diagonal elements the eigenvalues of $A$ in the same order. Neither $Q$ nor $T$ are unique.

(b) If $A$ is real with real eigenvalues, then $Q$ can be chosen to be real and orthogonal. The upper-triangular matrix is also real.
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(c) If \( A \) is real with \( k \) real eigenvalues \( \lambda_1, \lambda_2, \ldots, \lambda_k \) and complex eigenvalues \( x_j + iy_j \) for \( j > k \), there exists a real orthogonal \( T \) such that \( T'AT = R \), where \( R \) resembles an upper-triangular matrix, but with diagonal blocks of the form \( R_{11}, R_{22}, \ldots, R_{tt} \). Here \( R_{jj} = \lambda_j \), for \( j = 1, 2, \ldots, k \); and for \( j > k \)

\[
R_{jj} = \begin{pmatrix} x_j & b_j \\ -c_j & x_j \end{pmatrix}, \quad \sqrt{b_j c_j} = y_j,
\]

where \( b_j \geq c_j \) and \( b_j c_j > 0 \). The elements below these blocks are zero so that \( R \) is of upper Hessenberg form. Golub and Van Loan [1996: 341] refer to such a matrix as quasi-triangular and show how to compute it using QR iterations (cf. Section 16.5). For an application to probability theory see Edelman [1997].

16.38. (Cholesky Decomposition for Non-negative Definite Matrices) If \( A \) is an \( n \times n \) non-negative definite matrix, there exist \( n \times n \) upper-triangular matrices \( U \) and \( U_1 \) with non-negative diagonal elements such that

\[
A = U'U = U_1U_1'.
\]

If \( A \) is positive definite, the matrix \( U \) is unique if its diagonal elements are all positive (or all negative); the same applies to \( U_1 \). Some writers prefer to use lower-triangular matrices \( L = U' \) or \( L_1 = U_1' \). The result also holds for \( A \) Hermitian non-negative definite, that is, there exists an upper-triangular matrix \( U \) such that \( A = U^*U \). If \( A \) is positive definite, then \( U \) is unique if its diagonal elements are positive (Rao and Rao [1998: 173]). For some computational aspects when \( A \) is non-negative definite see Smith [2001].

16.39. A scaled version of the above when \( A \) is positive definite is also used. If \( D = \text{diag}(u_{11}, u_{22}, \ldots, u_{nn}) \), then \( D \) has an inverse. Let

\[
\tilde{U} = D^{-1}U = \begin{pmatrix} 1 & \tilde{u}_{12} & \tilde{u}_{13} & \cdots & \tilde{u}_{1n} \\ 0 & 1 & \tilde{u}_{23} & \cdots & \tilde{u}_{2n} \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & \cdots & \cdots & 1 \end{pmatrix},
\]

so that

\[
A = U'U = \tilde{U}'D^2\tilde{U} = \tilde{U}'DU = \tilde{L}\tilde{D}\tilde{L}',
\]

where \( D \) is a diagonal matrix with positive diagonal elements.

16.40. (Algorithm for the Cholesky Decomposition) If \( A \) is a positive definite \( n \times n \) matrix, and the diagonal elements of \( U \) are all positive, we have the following steps.

Step 1: Set

\[
u_{11} = a_{11}^{1/2},
\]

\[
u_{jj} = \frac{a_{jj}}{u_{11}} \quad (j = 2, 3, \ldots, n).
\]

Step 2: For \( i = 2, 3, \ldots, p - 1 \) set

\[
u_{ij} = 0 \quad (j = 1, 2, \ldots, i - 1),
\]
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\[ u_{ii} = \left( a_{ii} - \sum_{k=1}^{i-1} u_{ki}^2 \right)^{1/2}, \]

\[ u_{ij} = \frac{a_{ij} - \sum_{k=1}^{i-1} u_{ki}u_{kj}}{u_{ii}} \quad (j = i + 1, \ldots, n). \]

**Step 3:** Set

\[ u_{nn} = \left( a_{nn} - \sum_{k=1}^{n-1} u_{ki}^2 \right)^{1/2}. \]

The decomposition \( A = \tilde{U}'D\tilde{U} \) can be used to avoid the computation of square roots. This modification is called the *Banachiewicz factorization* or the *root-free Cholesky decomposition* (Gentle [1998: 93–94]).

16.41. (Matrix Inverse) If \( A = U'U \) is a positive definite \( n \times n \) matrix, we have \( A^{-1} = U^{-1}(U')^{-1} = TT' \), where \( T \) is upper-triangular. From \( UT = I_n \) we find that \( T \) is given by

\[ t_{ii} = u_{ii}^{-1} \quad (i = 1, 2, \ldots, n), \]

\[ t_{ij} = 0 \quad (i > j), \]

\[ t_{ij} = -\frac{\sum_{k=i+1}^{j} u_{ik}t_{kj}}{u_{ii}} \quad (j = i + 1, \ldots, n). \]

Then

\[ (A^{-1})_{rs} = \sum_{k=s}^{n} t_{rk}t_{ks}' \]

\[ = \sum_{k=s}^{n} t_{rk}t_{sk} \quad (s = r, r + 1, \ldots, n), \]

which is the product of the \( r \)th and \( s \)th rows of \( T \).

**Proofs.** Section 16.4.


16.5 ORTHOGONAL–TRIANGULAR REDUCTIONS

The so-called QR decomposition plays an important role in the analysis of regression models, particularly in statistical computing packages. In fact, many of the regression theorems can actually be derived via the QR decomposition (e.g., Ansley [1985], Eubank and Webster [1985], Mandel [1982], and Nelder [1985]).

**Definition 16.12.** Any $n \times p$ real matrix $A$ of rank $r$ can be expressed in the form $A = QR$, where $Q$ is an $n \times n$ orthogonal matrix and $R$ is an $n \times p$ upper-triangular matrix. This is called the QR decomposition. If $n \geq p$, then

$$QR = \begin{pmatrix} Q_p, Q_{n-p} \end{pmatrix} \begin{pmatrix} R_1 \\ 0 \end{pmatrix} = Q_p R_1,$$


If $n \leq p$, we replace $R$ by $(R_2, S)$, where $R_2$ is an $n \times n$ upper-triangular matrix. The above results and those below are also true for complex $A$ if $Q$ is now unitary and we replace $\cdot$ by $^{*}$ (cf. Rao and Rao [1998: 168]).

Note that $Q'A = R$, and the reduction of $A$ can be carried out using a variety of algorithms. For example, the orthogonal matrix $Q'$ could consist of a product of Householder reflections or Givens rotations, or one could use the Gram–Schmidt algorithm. For further details of the real case see Seber and Lee [2003: chapter 11].

16.42. We use the above notation in what follows, and we assume $n \geq p$.

(a) Suppose $r = p$.

(i) Since $R_1$ has full rank $p$, $A'A = R_1'Q_p'Q_p R_1 = R_1' R_1$ is positive definite, and $R_1'R_1$ is the Cholesky decomposition of $A'A$. Therefore, if the diagonal elements of $R_1$ are all positive (or all negative), then $R_1$ is unique and $Q_p = AR_1^{-1}$ is unique. Hence the decomposition $A = Q_p R_1$ is also unique. However, the matrix $Q_{n-p}$ is not unique because any permutation of its columns will still give $A = QR$. 
(ii) The Moore–Penrose inverse of $A$ is  
\[ A^+ = (R_1^{-1}, 0)Q' = R_1^{-1}Q_p. \]

(iii) If $A$ is $n \times n$ and nonsingular, then  
\[ \det A = \det Q \det R_1 = \prod_{i=1}^{n} r_{ii}, \]
where $R_1 = (r_{ij})$. This is a useful method of finding a determinant. One application in statistics is in optimal experimental designs. For example, the D-optimal criterion chooses the design matrix $X$ such that $\det(X'X)$ is maximized.

(b) Suppose $r < p$.

(i) We first note that $A'A = R_1'R_1$ as above, but now $A'A$ is non-negative definite. However, $R_1'R_1$ is still the Cholesky decomposition of $A'A$ and $R_1$ is unique if the diagonal entries are non-negative. An inductive proof for the case $n = p$ is given by Graybill [1983: 210].

(ii) We can permute the columns of $A$ by postmultiplying by a permutation matrix $\Pi$ so that the first $r$ columns of the permuted matrix $\tilde{A} = A\Pi$ are linearly independent. Then $\tilde{A} = Q\tilde{R}$, where  
\[ \tilde{R} = \begin{pmatrix} R_{11} & R_{12} \\ 0 & 0 \end{pmatrix}, \]
and $R_{11}$ is an $r \times r$ nonsingular upper-triangular matrix. Thus $\tilde{R}$ is upper-triangular, but with its bottom $n - r$ rows all zeros. Since $\Pi^{-1} = \Pi'$ we have  
\[ A = Q\tilde{R}\Pi' \]
\[ = Q\begin{pmatrix} R_{11} & R_{12} \\ 0 & 0 \end{pmatrix}\Pi' \]
\[ = Q_r(R_{11}, R_{12})\Pi', \]
where $Q_r$ consists of the first $r$ columns of $Q$. As $\Pi$ is not unique, $Q_r$ will not be unique.

(iii) A weak inverse of $A$ is given by  
\[ A^- = \Pi \begin{pmatrix} R_{11}^{-1} & 0 \\ 0 & 0 \end{pmatrix} Q', \]
as $AA^-A = A$.

(iv) Additional orthogonal transformations can be applied to $A = Q\tilde{R}\Pi'$ to get  
\[ A = Q \begin{pmatrix} R_0 & 0 \\ 0 & 0 \end{pmatrix} P', \]
where $P$ is orthogonal and $R_0$ is $r \times r$ and nonsingular. This is a convenient method of finding $r$. 
(v) From (iv),

\[ A^+ = P \begin{pmatrix} R_0^{-1} & 0 \\ 0 & 0 \end{pmatrix} Q'. \]

For further computational details see Gentle [1998: 95–102] and Golub and Van Loan [1996: section 5.2].

There is also a symmetric QR iterative process that is a useful computational tool (Golub and Van loan [1996: section 8.2]).

16.43. (Tridiagonal Matrix) If \( T = QR \) is a QR decomposition of a symmetric tridiagonal matrix \( T \), all matrices being \( n \times n \), then \( Q \) has lower bandwidth 1, \( R \) has upper bandwidth 2, and

\[ T_1 = RQ = (Q'Q)RQ = Q'TQ \]

is also symmetric and tridiagonal. (The upper bandwidth is the number of nonzero diagonals above the main diagonal, and the lower bandwidth is the number of nonzero diagonals below the main diagonal; all other elements except possibly those in the main diagonal are zero.) The factorization can be computed by applying a sequence of \( n - 1 \) Givens rotations.

**Proofs.** Section 16.5.


### 16.6 FURTHER DIAGONAL OR TRIDIAGONAL REDUCTIONS

16.44. (Spectral Decomposition Theorem) Let \( A \) be any \( n \times n \) real symmetric (respectively Hermitian) matrix. Then there exists an orthogonal (respectively unitary) matrix \( Q = (q_1, q_2, \ldots, q_n) \) such that

\[ Q'AQ = \text{diag}(\lambda_1, \lambda_2, \ldots, \lambda_n) = \Lambda, \text{ say,} \]

where \( \lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n \) are the ordered eigenvalues of \( A \) (which we know are real). When \( A \) is Hermitian, \( Q' \) is replaced by \( Q^* \). With the above ordering, \( \Lambda \) is unique and \( Q \) is unique up to a postfactor of

\[ S = \begin{pmatrix} S_1 & 0 & \cdots & 0 \\ 0 & S_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & S_k \end{pmatrix}, \quad S_i \in \mathbb{Q}(m_i), \]

where \( k \) is the number of different eigenvalues of \( A \); \( m_1, m_2, \ldots, m_k \) are the algebraic multiplicities, that is \( \lambda_1 = \lambda_2 = \cdots = \lambda_{m_1} \geq \lambda_{m_1+1} = \cdots = \lambda_{m_1+m_2} \), and so on;
and $Q(m_i)$ stands for the set of all $m_i \times m_i$ orthogonal (respectively unitary) matrices.

If all the eigenvalues are distinct, each $m_i = 1$ and $S$ reduces to a diagonal matrix with diagonal elements equal to $\pm 1$. In this case the columns $q_i$ of $Q$ are unique except for their signs. If we stipulate, for example, that the element of $q_i$ with the largest magnitude is positive, then $S = I_n$ and $Q$ is unique. We note that:

(a) $A = QAQ' = \sum_{i=1}^n \lambda_i q_i q_i' = \sum_{i=1}^n \lambda_i F_i$, where the $F_i$ are symmetric, idempotent, and satisfy $F_i F_j = 0$ for all $i, j \neq i$.

(b) If $x = Qy$, then $x'Ax = y'Q'AQy = \lambda_1 y_1^2 + \cdots + \lambda_n y_n^2$. An algorithm for carrying out this reduction by completing the square rather than finding eigenvalues and eigenvectors (known as Lagrange’s reduction) is described by Rao and Bhimasankaram [2000: 333].

(c) If $A$ has rank $r$, $A_r$ contains the $r$ nonzero eigenvalues, and $Q_r$ contains the corresponding right eigenvectors of $A$, then $A = Q_r A_r Q_r'$, where $Q_r' Q_r = I_r$.

16.45. (Tridiagonal Reduction) Suppose $A$ is a real symmetric $n \times n$ matrix.

(a) There exists an orthogonal matrix $Q$ such that

$$Q'AQ = B,$$

where $B$ is tridiagonal. This is a very useful reduction used in numerical analysis because it provides an intermediate step for speeding up a diagonalization process. If $Q = (q_1, q_2, \ldots, q_n)$, then the $q_i$ are called Lanczos vectors (cf. Golub and Van Loan [1996: 473])

(b) If $q_1$ is defined in (a), then

$$Q'(q_1, Aq_1, \ldots, A^{n-1}q_1) = R,$$

where $R$ is upper-triangular. The matrix in brackets is a Krylov matrix. If $R$ is nonsingular, then $B$ of (a) has no zero subdiagonal elements.

16.46. (Normal Matrix)

(a) (Diagonal Reduction) An $n \times n$ complex matrix is normal (i.e., $AA^* = A^*A$) if and only if there exists a unitary matrix $Q$ such that $Q^*AQ = \text{diag}(\lambda_1, \lambda_2, \ldots, \lambda_n)$, where the $\lambda_i$ are the eigenvalues of $A$.

(b) (Tridiagonal Reduction)

(i) Let $A$ be a real $n \times n$ matrix. Then $A$ is normal (i.e., $AA' = A'A$) if and only if there is a real orthogonal matrix $Q$ such that

$$Q'AQ = \text{diag}(A_1, A_2, \ldots, A_k) = D_1, \quad 1 \leq k \leq n,$$

where tridiagonal $D_1$ is a real block-diagonal matrix, and $A_j$ is either a real $1 \times 1$ matrix or a real $2 \times 2$ matrix of the form

$$A_j = \begin{pmatrix} \alpha_j & \beta_j \\ -\beta_j & \alpha_j \end{pmatrix}.$$
(ii) If \( A \) is a real skew-symmetric matrix (i.e., \( A' = -A \)), then \( A \) is normal. It then follows that \( A \) is skew-symmetric if and only if there exists a real orthogonal matrix \( Q \) such that

\[
Q' AQ = \text{diag}(0, 0, \ldots, 0, A_1, A_2, \ldots, A_t) = D_2,
\]

where \( D_2 \) is a real block diagonal matrix with each \( A_j \) having the form

\[
A_j = \begin{pmatrix}
0 & \beta_j \\
-\beta_j & 0
\end{pmatrix}.
\]

(iii) If \( A \) is an orthogonal matrix, then it is normal. It follows that \( A \) is orthogonal if and only if there exists a real orthogonal matrix \( Q \) such that

\[
Q' AQ = \text{diag}(\lambda_1, \lambda_2, \ldots, \lambda_r, A_1, A_2, \ldots, A_s) = D_3,
\]

where \( D_3 \) is a real block diagonal matrix with each \( \lambda_j = \pm 1 \) and each matrix \( A_j \) having the form

\[
A_j = \begin{pmatrix}
\cos \theta_j & \sin \theta_j \\
-\sin \theta_j & \cos \theta_j
\end{pmatrix}.
\]

16.47. (Hermitian matrix) If \( A \) is an \( n \times n \) Hermitian matrix of rank \( r \), then there exists a nonsingular matrix \( S \) such that \( S^* AS = D \), where

\[
D = \text{diag}(1, 1, \ldots, 1, -1, -1, \ldots, -1, 0, 0, \ldots, 0).
\]

The number of +1’s and -1’s are the same as the number of positive and negative eigenvalues of \( A \) (say \( r_+ \) and \( r_- \), respectively), and the number of zeros is \( r_0 = n - r \). The result obviously holds for a real symmetric matrix and real \( S \) (e.g., Anderson [2003: 640]). Clearly the signature, defined below, is unique.

**Definition 16.13.** Refering to (16.47) above, if \( A \) is a Hermitian matrix, the triple \((r_+, r_-, r_0)\) is called the **inertia** of \( A \), while \( r_+ - r_- \) is called the **signature** of \( A \).

**Proofs.** Section 16.6.

16.44. Harville [1997: 534–539].
16.46b(i). Horn and Johnson [1985: 105].
16.47. Horn and Johnson [1985: 221–222].
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16.48. (Sylvester's Law of Inertia) Let $A$ and $B$ be $n \times n$ Hermitian matrices. There exists an $n \times n$ nonsingular matrix $S$ such that $A = SBS^*$ if and only if $A$ and $B$ have the same inertia (cf. 16.47).

16.49. (Ostrowski) Let $A$ be Hermitian and $S$ nonsingular, both $n \times n$ matrices. Then, for each $i = 1, 2, \ldots, n$, there exists a positive real number $\theta_i$ such that $\lambda_{\max}(SS^*) \geq \theta_i \geq \lambda_{\min}(SS^*)$ and

$$\lambda_i(SAS^*) = \theta_i \lambda_i(A).$$

16.50. Let $A$ and $B$ be $n \times n$ real or complex symmetric matrices. There exists a nonsingular $S$ such that $A = SBS^*$ if and only if $A$ and $B$ have the same rank.

Proofs. Section 16.7.


16.8 SIMULTANEOUS REDUCTIONS

16.51. Let $A$ and $B$ be $n \times n$ real symmetric matrices.

(a) (i) There exists a real orthogonal matrix $Q$ such that $Q'AQ$ and $Q'BQ$ are both diagonal if and only if $AB = BA$ (that is $AB$ is symmetric).

(ii) The previous result holds for more than two matrices. A set of real symmetric matrices are simultaneously diagonalizable by the same orthogonal matrix $Q$ if and only if they commute pairwise.

(iii) The above result also holds for Hermitian matrices and unitary $Q$.

(b) If a real linear combination of $A$ and $B$ is positive definite, then there exists a nonsingular matrix $R$ such that $R'AR$ and $R'BR$ are diagonal.

(c) If $A$ is also positive definite, there exists a nonsingular $S$ such that $S'AS = I_n$ and $S'BS = \text{diag}(\lambda_1, \lambda_2, \ldots, \lambda_n)$, where the $\lambda_i$ are the roots of $|\lambda A - B| = 0$, i.e., are the eigenvalues of $A^{-1}B$ (or $BA^{-1}$ or $A^{-1/2}BA^{-1/2}$). The $\lambda_i$ are real.

(d) If $A$ and $B$ are both non-negative definite, there exists a nonsingular matrix $R$ such that $R'AR$ and $R'BR$ are both diagonal.

16.52. Let $A$ and $B$ be $n \times n$ complex matrices.

(a) If $A$ and $B$ are both symmetric, there exists a unitary $U$ such that $UAU'$ and $UBU'$ are both diagonal if and only if $AB$ is normal; that is, $A^*B = B^*A$.

(b) If $A$ is Hermitian and $B$ is symmetric, there exists a unitary $U$ such that $UAU^*$ and $UBU'$ are both diagonal if and only if $AB$ is symmetric; that is $AB = BA$. 
(c) If $A$ is Hermitian positive definite and $B$ is symmetric, then there exists a nonsingular matrix $S$ such that $S^*AS$ and $S^*BS$ are both diagonal.

(d) Let $A$ be a Hermitian matrix, $B$ be a Hermitian non-negative definite matrix with rank $r \leq n$, and $N$ be an $n \times n - r$ matrix of rank $n - r$ such that $N^*B = 0$. Then:

(i) There exists an $n \times r$ matrix $L$ such that $L^*BL = I_r$ and $L^*AL = \Delta$, where $\Delta$ is an $r \times r$ diagonal matrix.

(ii) A necessary and sufficient condition that there exists a nonsingular matrix $R$ such that $R^*AR$ and $R^*BR$ are both diagonal is that $\text{rank}(N^*A) = \text{rank}(N^*AN)$.

(iii) A necessary and sufficient condition that there exists a nonsingular matrix $R$ such that $R^*BR$ and $R^{-1}A(R^{-1})^*$ are both diagonal is $\text{rank}(BA) = \text{rank}(BAB)$.

(iv) If, in addition, $A$ is Hermitian non-negative definite, there exists a nonsingular matrix $R$ such that $R^*AR$ and $R^*BR$ are both diagonal.

(v) If, in addition, $A$ is Hermitian non-negative definite, then there exists a nonsingular matrix $R$ such that $R^*BR$ and $R^{-1}A(R^{-1})^*$ are both diagonal.

For other results like (a)-(c) see the table of Horn and Johnson [1985: 229].

16.53. (Simultaneous Upper-Triangular Reductions) Let $A$ and $B$ be $n \times n$ complex matrices.

(a) There exist unitary matrices $P$ and $Q$ such that $P^*AQ = T$ and $P^*BQ = S$ are upper-triangular. If the diagonal elements $s_{ii}$ of $S$ are all nonzero, then $\lambda_i(AB^{-1}) = t_{ii}/s_{ii}$ for $i = 1, 2, \ldots, n$.

(b) If $A$ and $B$ are real, there exist real orthogonal matrices $P$ and $Q$ such that $P^*AQ$ is upper quasi-triangular (upper Hessenberg) and $P^*BQ$ is upper-triangular.

(c) If $AB = BA$, then there exists a unitary matrix $U$ such that $U^*AU$ and $U^*BU$ are both upper-triangular. This result holds for any family of commuting matrices (Horn and Johnson [1985: 81]).

16.54. (Simultaneous Singular Value Decompositions)

(a) (Two Matrices) Let $A$ and $B$ be $m \times n$ matrices. There exist unitary matrices $P_{m \times m}$ and $Q_{n \times n}$ such that $A = P_1R_1Q^*$ and $B = P_2R_2Q^*$, where $R_i (i = 1, 2)$ are $m \times n$ diagonal matrices, if and only if if $AB^*$ and $B^*A$ are both normal.

(b) (More Than Two Matrices) Given $m \times n$ matrices $A_i (i = 1, 2, \ldots, k)$, there exist unitary matrices $P$ and $Q$ such that $A = P\Sigma Q^*$ for all $i$, where the $\Sigma_i$ are all diagonal, if and only if each $A_i^*A_j^*(i \neq j)$ is normal and all the pairs of $A_i^*A_j^*(i \neq j)$ commute.
16.55. (Diagonalizable Matrices)

(a) (Two Matrices) Two diagonalizable \( n \times n \) matrices are simultaneously diagonalizable; that is, there is a single nonsingular matrix \( R \) such that \( R^{-1}AR \) and \( R^{-1}BR \) are diagonal, if and only if \( A \) and \( B \) commute (i.e., \( AB = BA \)). Commuting matrices play a major role in simultaneous factorizations as we have seen in (16.53c) and (16.54) above. For details see Horn and Johnson [1985: chapter 2].

(b) Let \( S \) be an arbitrary (finite or infinite) set of \( n \times n \) matrices in which every pair commutes. Then:

(i) There is a vector \( x \in \mathbb{C}^n \) that is an eigenvector of every \( A \in S \).

(ii) The members of \( S \) can be simultaneously diagonalized.

Proofs. Section 16.8.

16.48a(iii). Horn and Johnson [1985: 228; they also give other equivalent conditions for the simultaneous diagonalization of two Hermitian matrices] and Rao and Rao [1998: 185–186].
16.52c. Horn and Johnson [1985: 466].
16.52d. For proofs of (d) and further results, see Rao and Mitra [1971: chapter 6].
16.53b. Stewart [1972].
16.54a. Horn and Johnson [1985: 426, exercise 26].
16.9 POLAR DECOMPOSITION

16.56. Let \( A \) be an \( m \times n \) complex matrix of rank \( r \) \((r \leq \min\{m, n\})\).

(a) Suppose \( m \leq n \). Then, using the thin complex version of the singular value decomposition (cf. Section 16.3) we have the polar decomposition

\[
A = P \Delta_m Q_m^* = (P \Delta_m P^*)(Q_m P^*) = BW,
\]

where \( B = (AA^*)^{1/2} \) is an \( m \times m \) unique Hermitian non-negative definite matrix of rank \( r \), and \( W \) is \( m \times n \) with orthonormal rows (that is, \( WW^* = I_m \)). If rank \( A = m \), then the matrix \( W \) is unique and \( B \) is Hermitian positive definite. If \( A \) is real, then both \( B \) and \( W \) can be taken as real.

(b) If \( m = n \), then \( W \) is unitary. Furthermore, if \( A \) is nonsingular, then \( W \) is uniquely determined as \( B^{-1}A \).

(c) Let \( m \geq n \). By applying (a) to \( A^* \) we can write \( A = VC \), where the \( m \times n \) matrix \( V \) has orthonormal columns and \( C \) is an \( n \times n \) unique non-negative definite Hermitian matrix of rank \( r \). If \( A \) nonsingular, then \( V = W \).

(d) \( B = C \) if and only if \( A \) is normal.

16.57. Suppose that the \( n \times n \) matrix \( A \) has a polar decomposition \( A = BW \). Then it follows from (16.56d) above that \( A \) is normal if and only if \( BW = WB \).

Proofs. Section 16.9.


16.10 MISCELLANEOUS FACTORIZATIONS

16.58. (Takagi Factorization) Let \( A = (a_{ij}) \) be a real or complex symmetric \( n \times n \) matrix. Then \( A \) can be expressed in the form \( A = QDQ' \) (note \( Q' \) and not \( Q^* \)), where \( Q \) is an \( n \times n \) unitary matrix and \( D \) is a real non-negative diagonal matrix. The columns of \( Q \) are an orthogonal set of right eigenvectors of \( A \hat{A} \), and the corresponding diagonal elements of \( D \) are the non-negative square roots of the corresponding eigenvalues of \( A \hat{A} \).

16.59. Any square matrix \( A \) can be factorized as \( A = SQDQ'S^{-1} \), where \( S \) is nonsingular, \( Q \) is unitary, and \( D \) is diagonal with non-negative main diagonal entries; all matrices are \( n \times n \).

16.60. For any square matrix \( A \), there exists a unitary \( Q \) and upper-triangular matrix \( V \) such that \( A = QVQ' \), where all matrices are \( n \times n \), if and only if the eigenvalues of \( A \hat{A} \) are real and non-negative. When this condition is true, the main diagonal elements of \( V \) may be chosen to be non-negative.
16.61. If \( H \) is Hermitian, there exists a unitary matrix \( Q \) such that \( Q^*AQ \) is tridiagonal (and also Hermitian).

16.62. (Upper Hessenberg Reduction) For any square matrix \( A \) there exists a unitary matrix \( Q \) such that \( QAQ^* \) is upper Hessenberg.

Proofs. Section 16.10.


CHAPTER 17

DIFFERENTIATION

Methods of differentiation and differentials involving scalars, vectors, and matrices are used extensively in statistics. Applications include maximum likelihood and least squares estimation, large sample theory, statistical computing, and Jacobians, the subject of the next chapter. Turkington [2002], for example, applies first and second order differentiation to find maximum likelihood estimates and variance estimates for linear regression models, autoregressive time series, seemingly unrelated regression equations, and linear simultaneous equations models. Magnus and Neudecker [1999] do a similar thing with multivariate models, errors-in-variables models, nonlinear regression, and simultaneous equation models.

Differentiation is also used in sensitivity analysis and perturbation methods, which endeavor to determine the perturbation in a system when there are small changes in the parameters. It is also used in the derivation of elasticities (a term from economics), where one determines the proportional perturbation when there is a proportional change in a parameter. Some examples are model fitting (e.g., Seber and Wild [1989: 121–126, 668]), ecological population dynamics (Caswell [2001, 2007]), and multivariate elliptical linear regression models (Liu [2002b]). The chapter closes with a few results on difference equations.

17.1 INTRODUCTION

I have endeavored to categorize the methods of differentiation for easy reference, though some results, especially relating to a function of a function, fit into more than
one category. There is also some overlap of topics as one can consider differentiation either with respect to a vector or matrix, or with respect to an element of a vector or a matrix. A helpful survey of the subject including an historical overview is given by Nel [1980]. He also considers differentiation with respect to patterned matrices (cf. Section 18.3.5).

17.2 SCALAR DIFFERENTIATION

For some analytical background to the subject in a statistical context, the reader is referred to Abadir and Magnus [2005: chapter 13], Magnus and Neudecker [1999], and Schott [2005: chapter 9].

17.2.1 Differentiation with Respect to \( t \)

**Definition 17.1.** We first define the derivative of a matrix or vector with respect to a scalar. If \( A(t) = (a_{ij}(t)) \), then \( \frac{\partial A(t)}{\partial t} \) is defined to be \( \frac{\partial a_{ij}(t)}{\partial t} \); that is, the derivative of \( A(t) \) is obtained by differentiating each element of \( A \). The same is true for a vector \( a(t) = (a_i(t)) \).

Unless specified (e.g., \( A \) is symmetric), we assume that the elements of all the matrices differentiated are functionally independent (i.e., unconstrained). Also, the following apply when we have a vector \( \mathbf{t} = (t_1, t_2, \ldots, t_r)' \) and \( \partial t \) is replaced by \( \partial t_i \).

17.1. We have from the definition:

\[
\begin{align*}
\text{(a)} \quad & \frac{\partial \{AX(t)B\}}{\partial t} = A \frac{\partial X(t)}{\partial t} B, \\
\text{(b)} \quad & \frac{\partial \text{vec} X(t)}{\partial t} = \text{vec} \frac{\partial X(t)}{\partial t}.
\end{align*}
\]

17.2. (Products) Noting that \( \otimes \) is the Kronecker product, the following result is used extensively in the next section.

\[
\begin{align*}
\text{(a)} \quad & \frac{\partial (A(t)B(t)C(t))}{\partial t} = \frac{\partial A(t)}{\partial t} BC + A \frac{\partial B(t)}{\partial t} C + AB \frac{\partial C}{\partial t}, \\
\text{(b)} \quad & \frac{\partial (A(t) \otimes B(t))}{\partial t} = \frac{\partial A(t)}{\partial t} \otimes B + A \otimes \frac{\partial B(t)}{\partial t}.
\end{align*}
\]

17.3. (Inverse)

\[
\begin{align*}
\text{(a)} \quad & \text{Differentiating } A^{-1} A = I \text{ for nonsingular } A(t), \text{ we get} \\
& \quad \frac{\partial A^{-1}(t)}{\partial t} = -A^{-1} \frac{\partial A(t)}{\partial t} A^{-1}. \\
\text{(b)} \quad & \text{If } R \text{ does not depend on } t, \text{ then differentiating } [R'A(t)R]^{-1}R'A(t)R = I \text{ gives us} \\
& \quad \frac{\partial [R'A(t)R]^{-1}}{\partial t} = [R'A(t)R]^{-1}R' \frac{\partial A(t)}{\partial t} R[R'A(t)R]^{-1}.
\end{align*}
\]
(c) If $A$ is symmetric and $B(t) = R[R'A(t)R]^{-1}R'$, where $R$ does not depend on $t$, then, using (b), we obtain

$$\frac{\partial B}{\partial t} = -B\frac{\partial A}{\partial t}B.$$ 

(d) If $A^{-1}(t)$ is a weak inverse of $A(t)$, then differentiating $AA^{-1} = A$ gives us

$$A\frac{\partial A^{-1}(t)}{\partial t}A = -AA^{-1}\frac{\partial A}{\partial t}A^{-1}A.$$ 

Further details are given in (17.8) below.

(e) $A\frac{\partial [(A'A)^{-1}]}{\partial t}A' = -A(A'A)\frac{\partial (AA')}{\partial t}(A'A)^{-1}A'$.

17.4. (Determinants) If $A(t)$ is nonsingular, then

$$\frac{\partial \log(\det A)}{\partial t} = \text{trace} \left[A^{-1}\frac{\partial A}{\partial t}\right].$$

The result is also true if $A$ is symmetric. A further result follows by noting that

$$\frac{\partial \det A}{\partial t} = \det A \frac{\partial \log(\det A)}{\partial t}.$$ 

17.5. (Trace) $\frac{\partial \text{trace}(A(t))}{\partial t} = \text{trace} \left[\frac{\partial A(t)}{\partial t}\right].$

17.6. (Exponential) $\frac{\partial e^{At}}{\partial t} = Ae^{At}$.

Proofs. Section 17.2.1.

17.2. Graham [1981: 38].

17.3d–e. Searle [1982: 335].


17.6. Abadir and Magnus [2005: 368].

17.2.2 Differentiation with Respect to a Vector Element

We now consider the special case when $t$ is an element of an $n \times 1$ vector $x = (x_1)$. The results in this section still apply if $F$ is a matrix function of a matrix $X = (x_{ij})$, and we replace $x_i$ by $x_{ij}$.

17.7. Let $F$ be a square matrix function of a vector $x = (x_1, x_2, \ldots, x_n)'$, then from (17.4) and (17.3a) we have the following.

(a) $\frac{\partial \text{trace}(F(x))}{\partial x_i} = \text{trace} \left(\frac{\partial F}{\partial x_i}\right)$. 

(b) Suppose $F$ is nonsingular.

(i) \( \frac{\partial \det[F(x)]}{\partial x_i} = (\det F) \text{trace} \left( F^{-1} \frac{\partial F}{\partial x_i} \right) \).

(ii) \( \frac{\partial \log \det[F(x)]}{\partial x_i} = \frac{1}{\det F} \frac{\partial \det F}{\partial x_i} = \text{trace} \left( F^{-1} \frac{\partial F}{\partial x_i} \right) \).

(iii) \( \frac{\partial F^{-1}}{\partial x_i} = -F^{-1} \frac{\partial F}{\partial x_i} F^{-1} \).

(iv) \( \frac{\partial \log \det(AF^{-1}B)}{\partial x_i} = -\text{trace} \left[ F^{-1}B(AF^{-1}B)^{-1}AF \frac{\partial F}{\partial x_i} \right] \).

(v) If \( \text{adj}F \) is the adjoint matrix of \( F \), then \( \text{adj}F = (\det F)F^{-1} \) and

\[ \frac{\partial \text{adj}F}{\partial x_i} = \frac{\partial \det F}{\partial x_i} F^{-1} + \det F \frac{\partial F^{-1}}{\partial x_i}. \]

(c) (Kronecker Product) Let \( F \) and \( G \) be \( p \times q \) and \( r \times s \) matrix functions of \( x \).

(i) \( \frac{\partial (F \otimes G)}{\partial x_i} = F \otimes \frac{\partial G}{\partial x_i} + \frac{\partial F}{\partial x_i} \otimes G \).

We can replace \( F \) by \( \text{vec}F \) and \( G \) by \( \text{vec}G \) in the above equation.

(ii) \( \frac{\partial \text{vec}(F \otimes G)}{\partial x_i} = (I_q \otimes K_{sp} \otimes I_r) \frac{\partial (\text{vec}F \otimes \text{vec}G)}{\partial x_i} \),

where \( K_{sp} \) (= \( I_{(p,s)} \)) is the commutation matrix.

17.8. Let \( F \) be a \( p \times q \) matrix function of \( x \). If \( F^- \) is a weak inverse of \( F \), then, under certain analytical conditions including continuous differentiability and constant rank in some neighborhood, we have

\[ F \frac{\partial F^-}{\partial x_i} F = -FF^- \frac{\partial F}{\partial x_i} F^- F. \]

In particular, there exists a weak inverse \( G \) of \( F \) such that \( \frac{\partial G}{\partial x_i} = -G \frac{\partial F}{\partial x_i} G. \)

17.9. Let \( F \) be a \( p \times q \) matrix function of \( x \). If \( F^+ \) is the Moore–Penrose inverse of \( F \), then, under certain analytical conditions including continuous differentiability and constant rank in some neighborhood, we obtain

\[ \frac{\partial F^+}{\partial x_i} = \]

\[ -F^+ \frac{\partial F}{\partial x_i} F^+ + F^+(F^+)' \left( \frac{\partial F}{\partial x_i} \right)' \left( I_p - FF^+ \right) + \left( I_q - F^+ F \right) \left( \frac{\partial F}{\partial x_i} \right)' (F^+)' F^+. \]

17.10. (Eigenvalue and Eigenvector) Let \( F \) be a symmetric matrix function of an \( n \times 1 \) vector \( x \). Let \( \lambda \) be a simple eigenvalue of \( F \) (i.e., one with an algebraic multiplicity of 1) and corresponding right eigenvector \( u \) of unit length. Then, given \( Fu = \lambda u \) and \( H^+ \), the Moore–Penrose inverse of \( H = F - \lambda I \), we obtain

\[ \frac{\partial \lambda}{\partial x_i} = u \frac{\partial F}{\partial x_i} u \quad \text{and} \quad \frac{\partial u}{\partial x_i} = -H^+ \frac{\partial F}{\partial x_i} u. \]
17.11. Consider the idempotent matrix \( P = X(X'WX)^{-1}X'W \), where \( X \) is \( n \times p \) and \( W \) is an \( n \times n \) positive definite matrix such that the elements of \( W \) and/or \( X \) are functions of a vector \( z \). Then, under certain analytical conditions including continuous differentiability and constant rank in some neighborhood, we obtain

\[
\frac{\partial P}{\partial z_i} = (I_n - P) \frac{\partial X}{\partial z_i} (X'WX)^{-1}X'W + X(X'WX)^{-1}(\frac{\partial X}{\partial z_i})'W(I_n - P)
\]

\[
+ X(X'WX)^{-1}X' \frac{\partial W}{\partial z_i} (I_n - P).
\]

17.12. Suppose \( X = X(\phi) \), where \( X \) is \( n \times p \) of rank \( p \) and is a function of \( \phi = (\phi_1, \phi_2, \ldots, \phi_k)' \). Then,

\[
\frac{\partial \det(X'X)}{\partial \phi_i} = \det(X'X) \operatorname{trace} \left( X^+ \frac{\partial X}{\partial \phi_i} \right),
\]

where \( X^+ \) is the Moore–Penrose inverse of \( X \). This theory arises in nonlinear modeling.

**Proofs.** Section 17.2.2.


17.9. Harville [1997: 511].


17.11. Harville [1997: 315]. Derivatives are also given for \( WP \) and \( W - WP \).


### 17.2.3 Differentiation with Respect to a Matrix Element

**Definition 17.2.** We define the matrix \( E_{ij} \) to be an \( m \times n \) matrix with 1 in the \( i,j \)th position and zeros elsewhere. Thus \( E_{ij} = e_{i,m}e'_{n,j} \), where \( e_{i,m} \) is the \( i \)th column of \( I_m \) and \( e_{j,n} \) is the \( j \)th column of \( I_n \).

In what follows, we consider the special case of \( t = x_{ij} \), an element of the real \( m \times n \) matrix \( X \), and include differentiation with respect to a vector element. Results in this section can be derived using the properties given in the previous section along with (17.13) below. We assume that the elements of \( X \) are functionally independent (i.e., are “unconstrained”), unless stated otherwise. When \( m = n \), then \( E_{ij} = E'_{ji} \).

17.13. (Basic Result)

(a) It is straightforward to show that

\[
\frac{\partial X}{\partial x_{ij}} = \begin{cases}
   E_{ij}, & X \text{ unconstrained,} \\
   E_{ij} + E_{ij}' - \delta_{ij}E_{ii}, & X \text{ symmetric,}
\end{cases}
\]

where \( \delta_{ij} = 1 \) when \( i = j \) and \( \delta_{ij} = 0 \) when \( i \neq j \).
(b) \( \frac{\partial X'}{\partial x_{ij}} = \left( \frac{\partial X}{\partial x_{ij}} \right)' \).

(c) To convert a result given below about an unconstrained \( X \) into one for symmetric \( X \), we simply replace \( E_{ij} \) by \( E_{ij} + E_{ij}' - \delta_{ij}E_{ii} \).

17.14. (Products) We assume that the following matrices are conformable and \( X \) is unconstrained. The results follow directly from (17.1) and (17.2). Further results can be obtained by setting \( A \) and/or \( B \) equal to the identity matrix.

(a) \( \frac{\partial (AXB)}{\partial x_{ij}} = A \frac{\partial X}{\partial x_{ij}} B = AE_{ij}B. \)

(b) \( \frac{\partial (AXB)}{\partial x_{ij}} = AE_{ij}B. \)

(c) \( \frac{\partial (X'AXB)}{\partial x_{ij}} = \frac{\partial X'}{\partial x_{ij}} AXB + X' \frac{\partial (AXB)}{\partial x_{ij}} = E_{ij}'AXB + X'AE_{ij}B. \)

(d) \( \frac{\partial (XAXB)}{\partial x_{ij}} = E_{ij}AX'B + XAE_{ij}B. \)

(e) \( \frac{\partial (X'X'B)}{\partial x_{ij}} = XAX'B + AXX'B. \)

(f) \( \frac{\partial (AXB)}{\partial x_{ij}} = E_{ij}AXB + XAE_{ij}B. \)

(g) \( \frac{\partial (X'B)}{\partial x_{ij}} = E_{ij}'AXB + XAE_{ij}'B. \)

(h) \( \frac{\partial (X'B)}{\partial x_{ij}} = E_{ij}X'X + XX'E_{ij}. \)

17.15. (Inverses)

(a) If \( BXC \) is nonsingular, we differentiate \( (BXC)(BXC)^{-1} = I \) to get (cf. 17.3a)
\[ \frac{\partial \{A(BXC)^{-1}D\}}{\partial x_{ij}} = -A(BXC)^{-1}BE_{ij}C(BXC)^{-1}D. \]

(b) Suppose \( X \) is \( m \times m \) and nonsingular. From (a) we have
\[ \frac{\partial X^{-1}}{\partial x_{ij}} = -X^{-1}E_{ij}X^{-1} = -X^{-1}e_{i,m}e_{j,m}X^{-1} = -y_iz_j', \]
where \( y_i \) is the ith column and \( z_j' \) is the jth row of \( X^{-1} \).

If \( X \) is symmetric, then using (17.13c) we have
\[ \frac{\partial X^{-1}}{\partial x_{ij}} = \begin{cases} -y_i'y_i', & \text{if } i = j, \\ -y_i'y_j - y_j'y_i', & \text{if } i > j, \end{cases} \]
where \( y_i \) is the ith column of \( X^{-1} \).
17.16. (Determinants) Suppose $X$ is square and $\xi_{ij}$ is the cofactor of $x_{ij}$. Then

$$\frac{\partial \det X}{\partial x_{ij}} = \begin{cases} \xi_{ij}, & X \text{ unconstrained,} \\ (2 - \delta_{ij})\xi_{ij}, & X = X', \end{cases}$$

where $\delta_{ij} = 1$ when $i = j$ and 0 otherwise.

17.17. (Powers) Let $X$ be nonsingular, and let $k$ be a positive integer.

(a) We can prove by induction that

$$\frac{\partial X^k}{\partial x_{ij}} = \sum_{r=0}^{k-1} X^r E_{ij} X^{k-r-1}$$

for $k = 1, 2, \ldots$, where $X^0 = I_n$.

(b) Differentiating $X^k X^{-k} = I$ gives us

$$\frac{\partial X^{-k}}{\partial x_{ij}} = -X^{-k} \frac{\partial X^k}{\partial x_{ij}} X^{-k}.$$

17.18. (Some Matrix Functions) Let $Y$ be a nonsingular matrix function of $X$, where $X$ is unconstrained.

(a) $\frac{\partial \det Y}{\partial x_{ij}} = \text{trace}\left( (\text{adj} Y) \left( \frac{\partial Y}{\partial x_{ij}} \right) \right) = (\det Y) \text{trace}\left( Y^{-1} \frac{\partial Y}{\partial x_{ij}} \right)$.

When $X$ is symmetric we can use (17.13c) in the following applications.

(i) If $Y = AXB$, then (from 17.14a)

$$\frac{\partial \det(AXB)}{\partial x_{ij}} = \det(AXB) \text{trace}[(AXB)^{-1} A E_{ij} B] = \det(AXB)\{[B(AXB)^{-1} A']_{ij}\}.$$

(ii) If $Y = X'AX$, then (from 17.14c)

$$\frac{\partial \det(X'AX)}{\partial x_{ij}} = \det(X'AX) \text{trace}\{(X'AX)^{-1} [E_{ij} AX + X'AE_{ij}]\}.$$

(b) $\frac{\partial \text{vec} Y}{\partial x_{ij}} = \text{vec} \frac{\partial Y}{\partial x_{ij}}$.

(c) $\frac{\partial \text{trace} Y}{\partial x_{ij}} = \text{trace} \left( \frac{\partial Y}{\partial x_{ij}} \right)$.

(d) $\frac{\partial Y^{-1}}{\partial x_{ij}} = -Y^{-1} \frac{\partial Y}{\partial x_{ij}} Y^{-1}$.

We can get a corresponding result for $(Y^{-1})'$ by simply replacing $Y$ by $Y'$, as $(Y^{-1})' = (Y')^{-1}$. 
17.19. (Eigenvalue and Eigenvector) Let \( X \) be a symmetric \( n \times n \) matrix with simple eigenvalue \( \lambda \) (i.e., has an algebraic multiplicity of 1), and corresponding eigenvector \( u = (u_i) \) of unit length. Then

\[
\frac{\partial \lambda}{\partial x_{ij}} = 2uu' - \text{diag}(u_1^2, u_2^2, \ldots, u_n^2).
\]

Also, if \( g_j \) is the \( j \)th column of \( H^+ \), the Moore–Penrose inverse of \( H = X - \lambda I_n \), we have

\[
\frac{\partial u}{\partial x_{ij}} = \begin{cases} -u_i g_i, & \text{if } j = i, \\ -(u_j g_i + u_i g_j), & \text{if } j < i. \end{cases}
\]

Proofs. Section 17.2.3.

17.15b. Harville [2001: 130, exercise 21].
17.18. Harville [1997: section 15.8].

17.3 VECTOR DIFFERENTIATION: SCALAR FUNCTION

17.3.1 Basic Results

Definition 17.3. If \( f \) is a function of \( x \), we denote the vector of partial derivatives \((\partial f/\partial x_i)\) by the column vector \( \partial f/\partial x \), that is, \( \frac{\partial f}{\partial x} = \left( \frac{\partial f}{\partial x_i} \right) \). We also define the row vector \( \partial f/\partial x' = (\partial f/\partial x)'. \) Some authors (e.g., Dhrymes [2000]) reverse the notation.

17.20. (Basic Results) Let \( x \) and \( a \) be \( n \times 1 \) vectors, and let \( A \) an \( n \times n \) matrix.

(a) \( \frac{\partial x'a}{\partial x} = a = \frac{\partial a'x}{\partial x} \).

(b) \( \frac{\partial x'Ax}{\partial x} = (A + A')x \), or \( 2Ax \) if \( A \) is symmetric.

17.21. (Chain Rule) If \( z \) is a differentiable scalar function of \( y \), and \( y \) is a differentiable function of \( x \), then

\[
\frac{\partial z}{\partial x_i} = \sum_j \frac{\partial z}{\partial y_j} \frac{\partial y_j}{\partial x_i},
\]

which can be expressed in the form of the row vector

\[
\frac{\partial z}{\partial x'} = \frac{\partial z}{\partial y'} \cdot \frac{\partial y'}{\partial x'}.
\]
In terms of column vectors,
\[
\frac{\partial z}{\partial x} = \left( \frac{\partial y}{\partial x} \right)' \frac{\partial z}{\partial y}.
\]
The function \(z\) might include functions such as the trace, the determinant, and quadratic expressions.

**Proofs.** Section 17.3.1.

17.20. Abadir and Magnus [2005: 356, transposed].

17.3.2 \(x = \text{vec } X\)

In applying the following results using the chain rule above, it can be more convenient to work with \(\partial (\text{vec } X)'\) instead of \(\partial \text{vec } X\). The right-hand side is then transposed, as indicated in (17.22) below. Some authors use the reverse notation (e.g., Dhrymes [2000]). Note that the following derivatives are all column vectors.

17.22. If \(f(X)\) is a scalar function of the matrix \(X\), then
\[
\frac{\partial f(X)}{\partial \text{vec } X} = \text{vec } \left( \frac{\partial f(X)}{\partial X} \right) = \left( \frac{\partial f(X)}{\partial (\text{vec } X)'} \right)'.
\]

17.23. (Trace)

(a) \(\frac{\partial \text{trace}(AXB)}{\partial \text{vec } X} = \text{vec } (A'B')\).

We can obtain this result directly by noting that

\[
\text{trace}(AXB) = \text{trace}(BAX) = \text{vec } (A'B')' \text{vec } X,
\]
and using (17.20a). We can set \(A\) or \(B\) equal to \(I\).

(b) \(\frac{\partial \text{trace}(X'AXB)}{\partial \text{vec } X} = [(B' \otimes A) + (B \otimes A')] \text{vec } X\).

Provided that the appropriate matrices are square, other results follow from \(\text{trace}(CD) = \text{trace}(DC)\) and \(\text{trace } C = \text{trace } C'\). For example,

\[
\text{trace}(X'AXB) = \text{trace}(AXBX') = \text{trace}(XBX'A) = \text{trace}(BX'AX).
\]

17.24. (Determinants and Log Determinants) The following matrices \(X\) and \(Y\) are nonsingular, and we use the result \(\text{vec } (AXB) = (B' \otimes A) \text{vec } X\).

(a) \(\frac{\partial \det X}{\partial \text{vec } X} = \text{vec } [(\text{adj } X)'] = (\det X) \text{vec } (X^{-1'})\).

(b) If \(Y = X'AX\), then
\[
\frac{\partial \det Y}{\partial \text{vec } X} = \det Y[(Y^{-1'} \otimes A) + (Y^{-1} \otimes A')] \text{vec } X.
\]
When $A$ is symmetric, then $Y$ is also symmetric and
\[ \frac{\partial \det Y}{\partial \text{vec } X} = 2 \det Y [(Y^{-1} \otimes A) \text{vec } X]. \]

(c) If $Y = XBX'$, then
\[ \frac{\partial \det Y}{\partial \text{vec } X} = \det Y [B \otimes (Y^{-1})'] + (B' \otimes Y^{-1}) \text{vec } X. \]

When $B$ is symmetric, then $Y$ is symmetric and
\[ \frac{\partial \det Y}{\partial \text{vec } X} = 2 \det Y [B \otimes (Y^{-1})] \text{vec } X. \]

(d) If $Y$ is one of the above functions, then
\[ \frac{\partial (\log \det Y)}{\partial \text{vec } X} = \frac{1}{\det Y} \frac{\partial \det Y}{\partial \text{vec } X}. \]

**Proofs.** Section 17.3.2.


17.24a–d. Turkington [2002: chapter 4].

### 17.3.3 Function of a Function

17.25. Suppose $y = w'Az$, where $A$ is $m \times n$ and $w$, $z$, and $A$ are all functions of $x$. We wish to find the row vector $\partial y/\partial x'$. We first note from (11.16b) and (11.15c) that
\[ y = \text{vec } y = (z' \otimes w') \text{vec } A = (z \otimes w)' \text{vec } A = [\text{vec } (wz')]' \text{vec } A. \]

Then using $w'Az = z'A'w$, we get
\[ \frac{\partial y}{\partial x'} = z'A'\frac{\partial w}{\partial x'} + [\text{vec } (wz')]' \frac{\partial \text{vec } A}{\partial x'} + w'A \frac{\partial z}{\partial x'}. \]

17.26. Let $y = \text{trace}[F(Z)]$, where $F$ is a square matrix function of $Z$ and $Z$ is a function of $x$. Then, by the chain rule (17.21), we obtain
\[ \frac{\partial y}{\partial x'} = \frac{\partial y}{\partial (\text{vec } Z)'} \cdot \frac{\partial \text{vec } Z}{\partial x'}, \]

where $\partial y/\partial (\text{vec } Z)'$ can be obtained from (17.23) and transposing. We give three examples from Dhrymes [2000: section 5.4].

(a) \[ \frac{\partial \text{trace}(AZB)}{\partial x'} = \text{vec } (A'B')' \frac{\partial \text{vec } Z}{\partial x'}. \]
VECTOR DIFFERENTIATION: VECTOR FUNCTION

\[ \frac{\partial \text{trace}(AZ'BZ)}{\partial x'} = (\text{vec } Z)'(A' \otimes B + A \otimes B') \frac{\partial \text{vec } Z}{\partial x'} \]

\[ \frac{\partial \text{det } Z}{\partial x'} = \text{vec } [(\text{adj } Z)']' \frac{\partial \text{vec } Z}{\partial x'} \]

Proofs. Section 17.3.3.


17.26a. The result follows from (17.23a).

17.26b. We use (17.23b) transposed with A and B interchanged.

17.26c. We use (17.24a).

17.4 VECTOR DIFFERENTIATION: VECTOR FUNCTION

Definition 17.4. Let \( x \) and \( y \) be \( n \times 1 \) vectors. We define

\[ \frac{\partial y}{\partial x'} = \left( \frac{\partial y_i}{\partial x_j} \right) \]

I find this notation easy to remember because \( y \), being a column vector, means that \( i \) refers to the row number, and \( x' \), being a row vector, means that \( j \) refers to the column number. This notation is used, for example, by Magnus and Nuedeker [19] and Harville [1997]. However, other notations are used in the literature. For example, Dhrymes [200] calls the above expression \( \partial y/\partial x \), while Graham [1981], Searle [1982], and Turkington [2002] define \( \partial y/\partial x = (\partial y_j/\partial x_i) \), the transpose of our definition. However, such a definition does not adapt so well to the chain rule below in (17.29) and in the derivation of Jacobians, which are discussed in the next chapter.

If \( Y = F(X) \) is a matrix function of \( X \), we shall also be interested in the derivative \( \partial \text{vec } Y/(\partial \text{vec } X)' \). Rao and Rao [1998: Section 6.5] denoted the latter expression by "\( \partial Y/\partial X \)" and list a number of results. The Kronecker product "\( \otimes \)" is very useful in this regard, along with (17.60). Many of the results are proved using the method of differentials (Section 17.8).

17.27. Since the Kronecker product \( x \otimes a \) is a vector, we have the following.

\[ \frac{\partial (x \otimes a)}{\partial x'} = I_n \otimes a. \]

\[ \frac{\partial (a \otimes x)}{\partial x'} = a \otimes I_n. \]

17.28. If \( y = Ax \), then

\[ \frac{\partial y}{\partial x'} = A. \]

Similarly, if \( \text{vec } Y = B \text{ vec } X \), then

\[ \frac{\partial \text{vec } Y}{\partial (\text{vec } X)'} = B. \]
17.29. (Chain Rule) If \( z \) is a differentiable vector function of \( y \) and \( y \) is a differentiable function of \( x \), then, arguing as in (17.21),

\[
\frac{\partial z}{\partial x'} = \frac{\partial z}{\partial y'} \cdot \frac{\partial y}{\partial x'}
\]

This result also holds if \( z \) is a scalar (cf. 17.21), and then \( \partial z/\partial x' \) is a row vector.

17.30. (Matrices with Functionally Independent Elements) In what follows we can obtain special cases by putting some of the matrices equal to the identity matrix. Also \( I_{(m,n)}(= K_{mn}) \) is the vec-permutation (commutation) matrix.

(a) \( \frac{\partial \text{vec} X}{\partial (\text{vec} X)'} = I \).

(b) If \( Y = AXB \), then from (11.16b), \( \text{vec} Y = (B' \otimes A) \text{vec} X \) and

\[
\frac{\partial \text{vec} Y}{\partial (\text{vec} X)'} = B' \otimes A.
\]

(c) If \( Y = AX'B \) and \( X \) is \( m \times n \), then \( \text{vec} Y = (B' \otimes A) \text{vec} X' \), \( \text{vec} X' = I_{(n,m)} \text{vec} X \) and, from (a) and (11.16b),

\[
\frac{\partial \text{vec} Y}{\partial (\text{vec} X)'} = (B' \otimes A) I_{(n,m)}.
\]

(d) If \( X \) is nonsingular and \( Y = AX^{-1}B \), then

\[
\frac{\partial \text{vec} Y}{\partial (\text{vec} X)'} = -(X^{-1}B)' \otimes (AX^{-1}).
\]

We can set \( A = B = I \).

(e) If \( X \) is nonsingular and \( Y = X^k \), where \( k \) is a positive integer, then

\[
\frac{\partial \text{vec} Y}{\partial (\text{vec} X)'} = \sum_{i=1}^{k} ((X')^{k-i} \otimes X^{i-1}).
\]

(f) If \( X \) is \( m \times n \) and \( Y = X'AX \), then

\[
\frac{\partial \text{vec} Y}{\partial (\text{vec} X)'} = (X'A' \otimes I_n) I_{(n,m)} + (I_n \otimes X'A).
\]

If \( A \) is symmetric, we get \((I_{n^2} + I_{(n,n)})(I_n \otimes X'A)\).

(g) If \( X \) is \( m \times n \) and \( Y = XBX' \), then

\[
\frac{\partial \text{vec} Y}{\partial (\text{vec} X)'} = (XB' \otimes I_m) + (I_m \otimes XB) I_{(n,m)}.
\]

If \( B \) is symmetric, we get \((I_{m^2} + I_{(m,m)})(XB \otimes I_m)\).
(h) If \( X \) is \( m \times n \), \( U \) is a \( p \times q \) matrix function of \( X \), and \( V \) is a \( q \times r \) matrix function of \( X \), then
\[
\frac{\partial \text{vec} (UV)}{\partial \text{vec} X'} = (V \otimes I_p)' \frac{\partial \text{vec} U}{\partial \text{vec} X'} + (I_r \otimes U) \frac{\partial \text{vec} V}{\partial \text{vec} X'}.
\]

17.31. Let \( F(X) = Z(Y(X)) \), then by the chain rule (17.29),
\[
\frac{\partial \text{vec} F}{\partial \text{vec} X'} = \left. \frac{\partial \text{vec} Z(V)}{\partial \text{vec} Y} \right|_{V = Y(X)} \frac{\partial \text{vec} Y(X)}{\partial \text{vec} X'}.
\]

17.32. (Symmetric Matrices) Let \( X \) be an \( n \times n \) symmetric matrix.

(a) If \( Y = AXA' \), then \( \text{vech} Y = H_n (A \otimes A) G_n \text{vech} X \) (cf. 11.30), where \( H_n \) can be replaced by \( G_n^+ (= D_n^+) \), and
\[
\frac{\partial \text{vech} Y}{\partial \text{vech} X'} = H_n (A \otimes A) G_n.
\]

Here \( G_n \) is the duplication matrix.

(b) If \( Y = X^{-1} \), then \( Y = X^{-1}XX^{-1} \), and from (a),
\[
\frac{\partial \text{vech} Y}{\partial \text{vech} X'} = -H_n (X^{-1} \otimes X^{-1}) G_n.
\]

(c) If \( Y = X^k \), where \( k = 2, 3, \ldots \), then
\[
\frac{\partial \text{vech} Y}{\partial \text{vech} X'} = H_n \sum_{i=1}^{k} (X^{k-i} \otimes X^{i-1}) G_n.
\]

(d) If \( Y = X^+ \), then
\[
\frac{\partial \text{vech} Y}{\partial \text{vech} X'} = G_n^+ \{[X^+X^+ \otimes (I_n - X^+X)]

+ (I_n - XX^+) \otimes X^+X^+]I_{n,n} - (X^+ \otimes X^+) \} G_n,
\]

where \( I_{(n,n)} \) is the vec-permutation (commutation) matrix.

17.33. Let \( F \) be a \( p \times q \) matrix whose elements are a function of \( x = (x_1, x_2, \ldots, x_n)' \). (Here \( x \) can be vec \( X \).) The following results mirror (17.30) and (17.32):

(a) \[
\frac{\partial \text{vec} (AFB)}{\partial x'} = (B' \otimes A) \frac{\partial \text{vec} F}{\partial x'}.
\]

(b) If \( F \) is nonsingular, \[
\frac{\partial \text{vec} F^{-1}}{\partial x'} = -(F^{-1} \otimes F^{-1}) \frac{\partial \text{vec} F}{\partial x'}.
\]

(c) If \( F = X \) and \( x = \text{vec} X \), then \[
\frac{\partial \text{vec} F}{\partial x'} = I_{pq}.
\]

(d) If \( F \) is \( n \times n \), then
\[
\frac{\partial \text{vec} (F^k)}{\partial x'} = \sum_{i=1}^{k} [(F^{i-1})' \otimes F^{k-i}] \frac{\partial \text{vec} F}{\partial x'} \quad (F^0 = I_n).
\]
(e) If $F$ is symmetric and $n \times n$, then:

1. $\frac{\partial \text{vech} (AFA')}{\partial x'} = H(\text{vec } A \otimes A) G_n \frac{\partial \text{vech } F}{\partial x'}$.

2. $\frac{\partial \text{vech } F^{-1}}{\partial x'} = -H_n(\text{vec } F^{-1} \otimes F^{-1}) G_n \frac{\partial \text{vech } F}{\partial x'}$.

17.34. Let $F$ and $G$ be $m \times n$ and $p \times q$ matrices, respectively, which are functions of $x$.

(a) (Kronecker Product) From (17.7c) we have:

1. $\frac{\partial (\text{vec } F \otimes \text{vec } G)}{\partial x'} = \left( \text{vec } F \otimes \frac{\partial \text{vec } G}{\partial x'} \right) + \left( \frac{\partial \text{vec } F}{\partial x'} \otimes \text{vec } G \right)$.

(b) (Hadamard Product) If $F$ and $G$ are both $m \times n$ matrix functions of $x$, then

$$\frac{\partial \text{vec } (F \circ G)}{\partial x'} = D(F) \frac{\partial \text{vec } G}{\partial x'} + D(G) \frac{\partial \text{vec } F}{\partial x'},$$

where "o" represents the Hadamard product, and for any $m \times n$ matrix $A$,

$$D(A) = \text{diag}(a_{11}, a_{12}, \ldots, a_{1n}, a_{21}, a_{22}, \ldots, a_{2n}, \ldots, a_{m1}, a_{m2}, \ldots, a_{mn}).$$

17.35. Suppose $y = Az$, where $A$ is $m \times n$ and $A$ and $z$ are functions of $x$. We want to find $\frac{\partial y}{\partial x'}$. Since $y = \text{vec } y = \text{vec } (Az) = (z' \otimes I_m) \text{vec } A$, we have

$$\frac{\partial y}{\partial x'} = \left[ \frac{\partial \text{vec } (Az)}{\partial x'} \right]_A \text{ constant } + \left[ \frac{\partial (Az)}{\partial x'} \right]_A \text{ constant } = (z' \otimes I_m) \frac{\partial \text{vec } A}{\partial x'} + A \frac{\partial z}{\partial x'}.$$

Proofs. Section 17.4.


17.32c. Henderson and Searle [1979: 74].

17.33. Harville [1997: section 16.6]; for (d) see Harville [2001: 157, exercise 31].

17.34a(ii). Harville [2001: 158, exercise 31].


17.5 MATRIX DIFFERENTIATION: SCALAR FUNCTION

17.5.1 General Results

**Definition 17.5.** Let $y = f(X)$ be a scalar function of the elements $x_{ij}$ of the $m \times n$ matrix $X$. Then the derivative of $y$ with respect to $X$, written $\partial y/\partial X$, is the matrix with $(i,j)$th element $\partial y/\partial x_{ij}$, that is,

$$
\begin{align*}
\frac{\partial f(X)}{\partial X} &= \left( \frac{\partial f(X)}{\partial x_{ij}} \right).
\end{align*}
$$

If $X$ is a vector $x$, then we write $\partial y/\partial x$, a column vector with $i$th element $\partial y/\partial x_i$. Thus

$$
\begin{align*}
\frac{\partial f(x)}{\partial x} &= \left( \frac{\partial f(x)}{\partial x_i} \right).
\end{align*}
$$

It is assumed that $X$ and $x$ have functionally dependent elements, unless stated to the contrary (e.g., $X$ is symmetric). Note that

$$
\begin{align*}
\frac{\partial f(X)}{\partial X} &= \left( \frac{\partial f(X)}{\partial X} \right)'.
\end{align*}
$$

A special case is when $y_{rs} = F_{rs}(X)$, where $y_{rs}$ is the $(r,s)$th element of $Y = F(X)$.

We remind the reader that $\text{diag}(A)$ is the diagonal matrix whose diagonal elements are the same as the diagonal elements of $A$. Such matrices feature frequently below. Many of the results in this section can be derived using the method of differentials, as demonstrated in (17.57).

17.36. (Chain Rules)

(a) If $y = f(X)$ and $z = g(y)$, then $\frac{\partial z}{\partial x_{ij}} = \frac{\partial z}{\partial y} \cdot \frac{\partial y}{\partial x_{ij}}$, which leads to

$$
\begin{align*}
\frac{\partial z}{\partial X} &= \frac{\partial z}{\partial y} \cdot \frac{\partial y}{\partial X}. 
\end{align*}
$$

(b) If $Y = F(X)$ and $z = g(Y)$, then

$$
\begin{align*}
\frac{\partial z}{\partial x_{ij}} &= \sum_r \sum_s \frac{\partial z}{\partial y_{rs}} \cdot \frac{\partial y_{rs}}{\partial x_{ij}} = \text{trace} \left( \frac{\partial z}{\partial Y} \cdot \frac{\partial Y'}{\partial x_{ij}} \right).
\end{align*}
$$
We can also write the above equation in the form
\[ \frac{\partial g(Y)}{\partial X} = \sum_r \sum_s \frac{\partial g}{\partial y_{rs}} \frac{\partial y_{rs}}{\partial X}. \]

Nel [1980: 150–151] used this equation to derive some of the results below.

**17.37.** (Symmetric X) If \( y = f(X) \), where \( X \) is symmetric, then
\[ \frac{\partial f}{\partial X} \left\{ \frac{\partial f(Y)}{\partial Y} + \frac{\partial f(Y)}{\partial Y'} - \text{diag} \left( \frac{\partial f(Y)}{\partial Y} \right) \right\}_{Y=X}. \]

In working out the derivative \( \frac{\partial f(Y)}{\partial Y} \), we pretend that the function \( f(\cdot) \) is defined on the class of matrices \( Y \) with all independent components, and then the derivative is formed. Rao and Rao [1998: 231] give some helpful examples of the method.

**Proofs.** Section 17.5.1.


**17.5.2 f = trace**

We now give various matrix derivatives for the trace of matrix products. Variations of the following can be obtained by using the results \( \text{trace} C = \text{trace} C' \), \( \text{trace}(DE) = \text{trace}(ED) \), \( \text{trace}(AXB) = \text{trace}(BAX) \), and \( a'Xb = \text{trace}(a'Xb) \) for square \( C, DE, \) and \( AXB \). In what follows, we assume \( X \) to be \( m \times n \) and unconstrained, unless otherwise stated. If \( X \) is symmetric, we assume it to be \( n \times n \).

We can also set \( A = I \) and/or \( B = I \), to get special cases. The following can be readily derived from the basic simple result
\[ \frac{\partial \text{trace} Y}{\partial x_{ij}} = \text{trace} \left( \frac{\partial Y}{\partial x_{ij}} \right) \]
and then using the results of (17.13c) and (17.14). We also use the fact that if \( W = (w_{ij}) \), then \( \text{trace}(E_{ij}W) = \text{trace}(WE_{ij}) = w_{ij} \) and \( \text{trace}(E_{ij}W) = \text{trace}(WE_{ij}) = w_{ii} \), where \( E_{ij} \) has 1 in the \( i,j \)th position and zeros elsewhere.

**17.38.** If \( y = \text{trace}[(U(X)V(X))] \), where \( U \) and \( V \) are matrix functions of \( X \), then
\[ \frac{\partial y}{\partial X} = \frac{\partial \text{trace}[(U(X)V(Y))]}{\partial X}|_{Y=X} + \frac{\partial \text{trace}[(U(Y)V(X))]}{\partial X}|_{Y=X}. \]

**17.39.** Using (17.14a) and (17.13), we obtain
\[ \frac{\partial \text{trace}(AXB)}{\partial X} = \begin{cases} C', & X \text{ unconstrained}, \\ C + C' - \text{diag} C, & X \text{ symmetric; } A, B \text{ square,} \end{cases} \]
where \( C = BA \).

To obtain further results we use \( \text{trace}(AX'B) = \text{trace}(B'XA') \), and also set \( A \) or \( B \) equal to \( I \).
17.40. If \( A \) is \( m \times m \), \( B \) is \( n \times n \), and \( X \) is unconstrained, we have from (17.14c) that
\[
\frac{\partial \text{trace}(X'AXB)}{\partial X} = \frac{\partial \text{trace}(XBX'A)}{\partial X} = AXB + A'XB'.
\]
An important special case is when \( B = I \) and \( A \) is symmetric. Then
\[
\frac{\partial \text{trace}(X'AX)}{\partial X} = 2AX.
\]

17.41. Using (17.14f) and (17.13), we obtain
\[
\frac{\partial \text{trace}(XAXB)}{\partial X} = \begin{cases} 
H' & \text{if } X \text{ unconstrained,} \\
H + H' - \text{diag}(H) & \text{if } X \text{ symmetric,}
\end{cases}
\]
where \( H = BXA + AXB \). We can get the special case of \( \text{trace}[(AX)^2] \) by noting that \( \text{trace}[(AX)^2] = \text{trace}(XAXA) = \text{trace}(XAXA) \). Also, we can set \( B = I \).

17.42. If \( X \) is nonsingular and unconstrained, we have from (17.15a):

(a) \[
\frac{\partial \text{trace}[A(BXC)^{-1}D]}{\partial X} = -[C(BXC)^{-1}DA(BXC)^{-1}B]'.
\]

(b) From (a) we have \[
\frac{\partial \text{trace}(AX^{-1}B)}{\partial X} = -(X^{-1}BAX^{-1})'.
\]

(c) A useful special case is \[
\frac{\partial \text{trace } X^{-1}}{\partial X} = -(X^{-2})'.
\]

(d) When \( X \) is symmetric, we have from (17.13) that
\[
\frac{\partial \text{trace } X^{-1}}{\partial X} = -2(X^{-2}) + \text{diag}(X^{-2}).
\]

17.43. Using (17.17a) and (17.13), we have for \( k = 2, 3, \ldots \)
\[
\frac{\partial \text{trace } X^k}{\partial X} = \begin{cases} 
2kX^{k-1} - k \text{diag}(X^{k-1}) & \text{if } X \text{ symmetric.}
\end{cases}
\]

17.44. Suppose \( X \) is unconstrained.

(a) \[
\frac{\partial \text{trace } e^X}{\partial X} = (e^X)'.
\]

(b) \[
\frac{\partial e^{\text{trace}(X^2)}}{\partial X} = 2e^{\text{trace}(X^2)}X'.
\]

Proofs. Section 17.5.2.

17.44a. Abadir and Magnus [2005: 368, exercise 13.29].
17.44b. The derivative is \( e^{\text{trace}(X^2)} \frac{\partial \text{trace}(X^2)}{\partial X} \), and then use (17.14f) with \( A = B = I \).
17.5.3 $f = \text{determinant}$

In this section we assume that all the determinants are nonzero and that $X$ is unconstrained, unless otherwise stated. Most of the following results for $X$ unconstrained are derived in Dwyer [1967]. The constrained case follows from the unconstrained case using (17.13) above.

17.45. From (17.18a(i)),

$$\frac{\partial \det X}{\partial X} = \begin{cases} (\text{adj}X)' = (\det X)(X^{-1})', & X \text{ unconstrained,} \\ \det(X)[2X^{-1} - \text{diag}(X^{-1})], & X \text{ symmetric.} \end{cases}$$

17.46. From (17.45),

$$\frac{\partial \log(\det X)}{\partial X} = (\det X)^{-1}\frac{\partial \det X}{\partial X} = \begin{cases} (X^{-1})', & X \text{ unconstrained,} \\ 2X^{-1} - \text{diag}(X^{-1}), & X \text{ symmetric.} \end{cases}$$

17.47.

$$\frac{\partial \det(AXB)}{\partial X} = \begin{cases} \det(AXB)C', & X \text{ unconstrained,} \\ \det(AXB)[C + C' - \text{diag}C], & X \text{ symmetric,} \end{cases}$$

where $C = B(AXB)^{-1}A$.

17.48. If $k$ is a positive integer and $X$ is unconstrained,

$$\frac{\partial (\det X)^k}{\partial X} = k(\det X)^{k-1}\frac{\partial \det X}{\partial X}.$$ 

In particular,

$$\frac{\partial (\det X)^2}{\partial X} = 2(\det X)^2(X^{-1})'.$$

17.49. Assuming $X'AX$ is nonsingular,

(a) \[
\frac{\partial \det(X'AX)}{\partial X} = \det(X'AX)(AX(X'AX)^{-1} + A'(X'AX)^{-1}').
\]

This result is linked to (17.24b).

(b) Setting $A = I$ we get

\[
\frac{\partial \det(X'X)}{\partial X} = 2[\det(X'X)]X(X'X)^{-1} = 2\det(X'X)X^+,
\]


(c) Replacing $X$ by $X'$, we get

\[
\frac{\partial \det(XX')}{\partial X} = 2[\det(XX')](XX')^{-1}X.
\]
17.50. Let $F(X)$ be a square nonsingular matrix function of $X$, and let $G(X) = C[F(X)]^{-1}A$. Then

$$
\frac{\partial \det[F(X)]}{\partial X} = \begin{cases}
\det[F(X)](GXB + G'XB'), & \text{if } F(X) = AXBX'C, \\
\det[F(X)](BXG + B'XG'), & \text{if } F(X) = AX'BXC, \\
\det[F(X)](GX + BXG'), & \text{if } F(X) = AXBXC.
\end{cases}
$$

17.51. If $X$ is nonsingular,

$$
\frac{\partial \det(AX^{-1}B)}{\partial X} = \begin{cases}
-\det(AX^{-1}B)C', & X \text{ unconstrained}, \\
-\det(AX^{-1}B)(C + C' - \text{diag } C), & X \text{ symmetric},
\end{cases}
$$

where $C = [X^{-1}B(AX^{-1}B)^{-1}AX^{-1}]$.

17.52. If $F$ is a nonsingular matrix function of $X$ with $\det F > 0$, then

$$
\frac{\partial \log \det F}{\partial X} = (\det F)^{-1} \frac{\partial \det F}{\partial X}.
$$

This can be applied to all the previous results.

Proofs. Section 17.5.3.

17.45. Mathai [1997: 9] and Searle [1982: 337]; see also (17.57b).

17.46. Henderson and Searle [1979: 76] and Searle [1982: 33]; see also (17.57d).

17.47. Rogers [1980: 52]; see also (17.57d).


17.49a. This result also follows from (17.50).


17.49c. Magnus and Neudecker [1999: 179].

17.50. Quoted by Magnus and Neudecker [1999: 180].

17.51. Rogers [1980: 52].

17.5.4 $f = y_{rs}$

17.53. In what follows we assume that $X$ and $E_{ij}$ (with 1 in the $(i,j)$th position and zeros elsewhere) are both $m \times n$ matrices.

(a) $\frac{\partial (AXB)_{rs}}{\partial X} = A'E_{rs}B'$.

(b) $\frac{\partial (AX'B)_{rs}}{\partial X} = BE'_{rs}A$.

(c) $\frac{\partial (AX^{-1}B)_{rs}}{\partial X} = -(X^{-1})'A'E_{rs}B'(X^{-1})'$.
(d) \[ \frac{\partial (X'AX)}{\partial X} = AXE_{rs} + A'XE_{rs}. \]

(e) \[ \frac{\partial (XAX)}{\partial X} = E_{rs}X'A' + A'XE_{rs}. \]

(f) \[ \frac{\partial (X'AX')}{\partial X} = AX'E_{rs} + E_{rs}X'A'. \]

(g) If \( k \) is a positive integer, \[ \frac{\partial (X^k)}{\partial X} = \sum_{j=0}^{k-1} (X')^j E_{rs} (X')^{n-j-1}, \]
where \( X^0 = I. \)

Proofs. Section 17.5.4.


17.5.5 \( f = \text{eigenvalue} \)

17.54. If \( \lambda \) is a nonrepeated (simple) eigenvalue of the square matrix \( X \) with left eigenvector \( v \) and right eigenvector \( u \), then

(a) \[ \frac{\partial \lambda}{\partial X} = v(v'u)^{-1}u'. \]

(b) If \( \lambda_i \) is a simple eigenvalue, \( X \) is symmetric, and \( u_0 \) is the normalized right eigenvector (i.e., \( u_0'u_0 = 1 \)), which is also the left eigenvalue, then

\[ \frac{\partial \lambda}{\partial X} = u_0'u_0. \]

Proofs. Section 17.5.5.

17.54a. Lancaster [1964] and Nel [1980: 141].

17.54b. Lancaster [1964] and Magnus and Neudecker [1999: 180].

17.6 \textbf{TRANSFORMATION RULES}

We now give some transformation rules that enable us to use the results from one type of differentiation to obtain results for other types.

17.55. Let \( X \) be an \( m \times n \) matrix, and let \( Y \) be a function of \( X \). The following equivalent expressions (adapted from Graham’s [1981: 65, 74] two “transformation principles”) apply for all conformable \( A_t, B_t, C_v, \) and \( D_v \), including functions of \( X \), and are simply different ways of writing \( \partial y_{rs}/\partial x_{ij} \). If we obtain an expression like (1) or (2) below, for example, in the process of differentiation, then we can immediately obtain (3), which may be more difficult to get directly.
It should be noted that $E_{rs}$ and $E_{ij}$ may be of different sizes. We also recall (cf. 11.19a) that if $C$ and $D$ are both $m \times n$, then

$$I_{(m,n)}(D \otimes C') = (C' \otimes D)I_{(n,m)}.$$

### 17.7 MATRIX DIFFERENTIATION: MATRIX FUNCTION

**Definition 17.6.** Let $Y = F(X)$, where $Y$ is $p \times q$ and $X$ is $m \times n$. Then the derivative of $Y$ with respect to $X$ can be defined in different ways. One method is to use the $mp \times nq$ matrix (MacRae [1974] and Rogers [1980])

$$dY = \begin{pmatrix}
\frac{\partial y_{11}}{\partial X} & \frac{\partial y_{12}}{\partial X} & \cdots & \frac{\partial y_{1q}}{\partial X} \\
\frac{\partial y_{21}}{\partial X} & \frac{\partial y_{22}}{\partial X} & \cdots & \frac{\partial y_{2q}}{\partial X} \\
\vdots & \vdots & \ddots & \vdots \\
\frac{\partial y_{p1}}{\partial X} & \frac{\partial y_{p2}}{\partial X} & \cdots & \frac{\partial y_{pq}}{\partial X}
\end{pmatrix} = Y \otimes \frac{\partial}{\partial X},$$

where the multiplication of a matrix element by a derivative operator corresponds to the operation of differentiation. Some authors—for example, Vetter [1970]—have used the reverse order $(d/dX) \otimes Y$ in the above definition. Rogers defines the latter to be

$$\begin{pmatrix}
\frac{\partial Y}{\partial x_{11}} & \frac{\partial Y}{\partial x_{12}} & \cdots & \frac{\partial Y}{\partial x_{1n}} \\
\frac{\partial Y}{\partial x_{21}} & \frac{\partial Y}{\partial x_{22}} & \cdots & \frac{\partial Y}{\partial x_{2n}} \\
\vdots & \vdots & \ddots & \vdots \\
\frac{\partial Y}{\partial x_{m1}} & \frac{\partial Y}{\partial x_{m2}} & \cdots & \frac{\partial Y}{\partial x_{mn}}
\end{pmatrix}.$$

This is the definition for $dY/dX$ used by Graham [1981: chapter 6].

The above definitions can also be used when $X$ or $Y$ are vectors. Magnus and Neudecker [1999: chapter 9] and Rao and Rao [1988: 233] discuss the relative merits of the above definitions and recommend a third alternative definition of a matrix derivative, namely $\partial \text{vec } Y / \partial (\text{vec } X)'$ as the only appropriate definition. This ties in nicely with the use of Jacobians; such derivatives and Jacobians are discussed in the next chapter. Kollo and von Rosen [2005: 127] define $dY/dX = \partial (\text{vec } Y)' / \partial \text{vec } X$, the transpose of the former definition. Their notation has the advantage in that it is consistent with the case $\partial \phi(X) / \partial \text{vec } X$, where $\phi$ is a scalar function. For those interested in results relating to the two previous displayed definitions, the reader is referred to Graham [1981], MacRae [1974], Neudecker [2003], Rogers [1980], and the references therein.
17.8 MATRIX DIFFERENTIALS

We mentioned some transformation rules for finding matrix derivatives in (17.55) above. There is, however, another powerful method for finding derivatives based on matrix differentials using another transformation rule given in (17.60) below. They can be used to derive some of the expressions given above, as indicated in the next chapter, Section 18.2. A good reference for this method is Abadir and Magnus [2005: chapter 13].

**Definition 17.7.** If \( y = f(x) \) is a scalar function of \( x = (x_1, x_2, \ldots, x_n)' \), then the differential \( dy \) is defined to be

\[
dy = \sum_{i=1}^{n} \frac{\partial f}{\partial x_i} dx_i = \sum_{i=1}^{n} \frac{\partial y}{\partial x_i} dx_i.
\]

If \( X = (x_{ij}) \) is an \( m \times n \) matrix, then we define the differential \( dX \) to be the matrix of differentials \( dx_{ij} \), that is, \( dX = (dx_{ij}) \). In the case of a vector \( x = (x_i) \), we have \( dx = (dx_i) \), so that we can therefore express \( dX \) as a vector using \( \text{vec} dX = d\text{vec} X \). For some analytical details see Abadir and Magnus [2005: chapter 13], Magnus and Neudecker [1999], and Schott [2005: sections 9.2, 9.3]. In what follows, \( X \) can be replaced by \( F(X) \), a matrix function of \( X \), when obtaining differentials so that \( dX \) is replaced by \( dF \).

**17.56. (Basic Properties)** Let \( X \) be an \( m \times n \) matrix.

(a) If \( A \) is a matrix of constants, then \( d(AX) = A dX \).

(b) \( d(X \pm Y) = dX \pm dY \).

(c) \( d(XY) = (dX)Y + X dY \).

(d) \( d(X') = (dX)' \).

(e) \( \text{dvec} X = \text{vec} dX \).

(f) \( \text{dvec} X' = \text{vec} (dX') = I_{(n,m)} \text{vec} (dX) \) (cf. Definition 11.6 above (11.18)).

(g) If \( X \) is an \( n \times n \) matrix, we obtain

\[
d(\text{trace } X) = \text{trace}(dX) = \text{trace}(I_n dX) = \text{vec} (I_n)' d(\text{vec } X),
\]

from (11.17a).

(h) (Kronecker product) \( d(X \otimes Y) = (dX) \otimes Y + X \otimes dY \).

(i) (Hadamard product) \( d(X \circ Y) = (dX) \circ Y + X \circ dY \).

(j) \( d(\det X) = (\det X) \text{trace}(X^{-1} dX) \).

(k) \( dX^{-1} = -X^{-1} (dX) X^{-1} \).

**17.57. (A Scalar Transformation Rule)** If \( y = f(X) \) is a scalar function of \( X \), then \( dy = \text{trace}(A' dX) \) if and only if \( \frac{\partial f}{\partial X} = A \). Furthermore, from (11.17a), we have

\[
dy = \text{trace}(A' dX) = (\text{vec } A)' \text{dvec } X \quad \text{if and only if} \quad \frac{\partial f}{\partial (\text{vec } X)} = \text{vec } A.
\]
Here \( A \) may be a function of \( X \). Examples follow with \( X \) unconstrained (Abadir and Magnus [2005: 357]).

(a) If \( y = \text{trace}(X'X) \), then \( dy = 2 \text{trace}(X'dX) \) (by (17.56c) and (17.56g)), from which we get \( \frac{\partial y}{\partial X} = 2X \).

(b) If \( y = \det X \), where \( X \) is nonsingular, then \( dy = (\det X)\text{trace}(X^{-1}dX) \) (by 17.56j) and \( \frac{\partial y}{\partial x} = (\det X)X^{-1}' \). We also have
\[
d \log(\det X) = (\det X)^{-1}d(\det X).
\]

(c) If \( y = \text{trace}(XAX'B) \), then
\[
d y = \text{trace}[d(XAX'B)] = \text{trace}[(dX)AX'B] + \text{trace}[XA(dX)'B]
\]
and
\[
\frac{\partial y}{\partial X} = (AX'B + A'X'B')'.
\]

(d) If \( y = \det(AXB) \), where \( Y = AXB \) is nonsingular, then from (b)
\[
d(\det Y) = \det Y \text{trace}(Y^{-1}dY) = \det Y \text{trace}[Y^{-1}A(dX)B] = \det Y \text{trace}[B(AXB)^{-1}AdX] = \det Y \text{trace}(CdX), \text{ say,}
\]
and \( \frac{\partial y}{\partial X} = (\det Y)C', \) where \( C = B(AXB)^{-1}A \).

(e) If \( y = \det(X'X) \), where \( Y = X'X \) is nonsingular, then from (a) we obtain
\[
d(\det Y) = \det Y \text{trace}(Y^{-1}dY) = \det Y \text{trace}[Y^{-1}d(X'X)] = 2 \det Y \text{trace}[Y^{-1}X'dX]
\]
and \( \frac{\partial y}{\partial X} = 2(\det Y)(XY^{-1}). \)

17.58. (A Vector Transformation Rule) If the vector \( y \) is a differentiable function of the vector \( x \), then we have \( dy = Adx \) if and only if
\[
\frac{\partial y}{\partial x'} = \left( \frac{\partial y_i}{\partial x_j} \right) = A.
\]

Here \( A \) can be a function of \( x \), and we can substitute \( x = \text{vec} X \), and so on, as in the next result. For example, if \( y = Ax \), where \( A \) is a function of \( x \), then since \( (dA)x = \text{vec} [(dA)x] \), we have from (11.16a, third equation)
\[
dy = (dA)x + Adx = (x' \otimes I)d\text{vec} A + Adx
\]
\[
\frac{\partial y}{\partial x'} = (x' \otimes I) \frac{\partial \text{vec } A}{\partial x'} + A.
\]

17.59. (A Matrix Transformation Rule) Let \( Y \) be a differentiable function of \( X_{m \times n} \). Then we have the following:

(a) \( \text{d vec } Y = \text{vec } (\text{d } Y) = B \text{ vec } (\text{d } X) = B \text{ vec } dX \) if and only if

\[
\frac{\partial \text{vec } Y}{\partial (\text{vec } X)'} = B.
\]

(b) \( \text{vec } (\text{d } Y) = B \text{ vec } (\text{d } X') = BI_{(n,m)} \text{ vec } (\text{d } X) \) (by 17.56f) if and only if

\[
\frac{\partial \text{vec } Y}{\partial (\text{vec } X)'} = BI_{(n,m)}).
\]

In the above, \( B \) may be a function of \( X \), but not of \( dX \).

17.60. (Equivalent Representations) Let \( X \) be \( m \times n \). If \( \otimes \) is the Kronecker product, then the following three statements are equivalent.

(1) \( dY = A(dX)B + C(dX')D \).

(2) \( \text{vec } (dY) = (B' \otimes A)\text{vec } (dX) + (D' \otimes C)\text{vec } (dX') \).

(3) \( \frac{\partial \text{vec } Y}{\partial (\text{vec } X)'} = B' \otimes A + (D' \otimes C)I_{(n,m)}. \)

Here \( I_{(n,m)} \) is the vec-permutation (commutation) matrix, and the matrices \( A, B, C, \) and \( D \) may all be functions of \( X \). Examples follow for \( X \) unconstrained.

(a) Let \( R, S, \) and \( T \) be matrices of constants. If \( Y = RX'SXT \), where \( X \) is \( m \times n \), then from (17.56a) and (17.56c) above we obtain

\[
\text{d } Y = RX'S(dX)T + Rd(X')SXT,
\]

and by (17.60(3)) we obtain

\[
\frac{\partial \text{vec } Y}{\partial (\text{vec } X)'} = T' \otimes (RX'S) + [(SXT)']' \otimes R]I_{(n,m)}.
\]

(b) If \( X \) and \( C \) are \( m \times n \), \( B \) is an \( m \times m \) symmetric matrix, and \( Y = (X - C)'B(X - C) \), then from (a) with \( D = B(X - C) \) we have

\[
\text{d } Y = (dX)'D + D'dX,
\]

so that

\[
\frac{\partial \text{vec } Y}{\partial (\text{vec } X') = I_n \otimes D' + (D' \otimes I_n)I_{(n,m)} = I_{(n,n)}(I_n \otimes D') + I_{n^2}(I_n \otimes D') = 2I_n(I_n \otimes D').
\]
Here $P_n = N_n$ is the symmetrizer matrix in Definition 11.9 (see also (11.29h(ii)). The case $Y = X'X$ was given by Abadir and Magnus [2005: 363].

(c) If $Y = X^{-1}$, where $X$ is nonsingular, then from (17.56k) we have

$$dY = -X^{-1}(dX)X^{-1}.$$  

(i) \[ \frac{\partial \text{vec} X^{-1}}{\partial (\text{vec} X)'} = -(X^{-1} \otimes X^{-1}). \]

(ii) \[ \text{trace}[X \, d(X^{-1})] = -\text{trace}[XX^{-1}(dX)X^{-1}] = -\text{trace}(X^{-1}dX). \]

(d) If $T$ is orthogonal and $\det(T + I) \neq 0$, then there exists a one-to-one relation between $T$ and the skew symmetric matrix $S$, namely, $S = 2(T + I)^{-1} - I$, where $T = 2(S + I)^{-1} - I$ (cf. 5.19). Then from (b),

$$dT = -\frac{1}{2}(T + I)(dS)(T + I).$$

17.61. (Moore–Penrose Inverse) If $X$ is $m \times n$ with Moore–Penrose $X^+$, then, provided that rank $X$ is constant (over a suitable set), we obtain

$$dX^+ = (I_n - X^+X)(dX')X^+X^+ + X^+X^+X(dX')(I_m - XX^+) - X^+(dX)X^+.$$  

Hence, using rule (3) in (17.60), we have

$$\frac{\partial \text{vec} X^+}{\partial (\text{vec} X)'} = (X'^+X^+ \otimes (I_n - X^+X) + (I_m - XX^+) \otimes X^+X^+)I_{(n,m)} - (X'^+ \otimes X^+).$$

17.62. (Idempotent Matrix) Let $X = (x_1, x_2, \ldots, x_p)$ be $n \times p$ of rank $p$, and define $M = I_n - X(X'X)^{-1}X'$. Then:

(a) $dM = -M(dX)(X'X)^{-1}X' - X(X'X)^{-1}(dX'M).$

(b) \[ \frac{\partial \text{vec} M}{\partial (\text{vec} X)'} = -(I_{n^2} + I_{(n,n)})[X(X'X)^{-1} \otimes M]. \]

(c) From $dX = (dx_j)e_j'$, we obtain

$$dM = -M(dx_j)e_j'(X'X)^{-1}X' - X(X'X)^{-1}e_j(dx_j)'M,$$

where $e_j$ is the $j$th column of $I_p$.

(d) \[ \frac{\partial \text{vec} M}{\partial x_j'} = -(I_{n^2} + I_{(n,n)})[X(X'X)^{-1}e_j \otimes M]. \]

17.63. (Eigenvalue and Eigenvector) Let $X$ be a symmetric $n \times n$ matrix with distinct eigenvalue $\lambda_i$ and corresponding normalized eigenvector $\gamma_i$ (with unit length). Then:

(a) $d\lambda_i = \gamma_i'(dX)\gamma_i$ and $d\lambda_i = d\text{vec} \lambda_i = (\gamma_i' \otimes \gamma_i')d\text{vec} X$. Since $\text{vec} X = G_n \text{vech} X$ we have

$$\frac{\partial \lambda_i}{\partial \text{vech} X} = (\gamma_i' \otimes \gamma_i')G_n.$$
\[ \frac{\partial \gamma_i}{\partial \text{vech } X} = -(X - \lambda_i I_n)^+ \gamma_i \quad \text{and} \quad \frac{\partial \lambda_i}{\partial \text{vech } X} = -\{\gamma_i \otimes (X - \lambda_i I_n)^+\} G_n, \]

where \((X - \lambda_i I_n)^+\) is the Moore–Penrose inverse of \((X - \lambda_i I_n)\).

17.64. (Sensitivity Analysis in Regression) From Section 20.7.1, the ordinary least squares (OLS) estimate of a full-rank regression model is \(\hat{\beta} = (X'X)^{-1}X'y\), where \(X = (x_1, x_2, \ldots, x_p)\) is \(n \times p\) of rank \(p\), and the residual is \(r = (I_n - X(X'X)^{-1}X')y\). Then:

(a) \[ \frac{\partial \hat{\beta}}{\partial (\text{vec } X)'} = (X'X)^{-1} \otimes r' - [\hat{\beta}'(\otimes (X'X)^{-1}X')]. \]

(b) \[ \frac{\partial \hat{\beta}}{\partial x_j} = -(X'X)^{-1}(\hat{\beta}_j X' - e_j r'). \]

(c) \[ \frac{\partial r}{\partial (\text{vec } X)'} = -\hat{\beta}' \otimes M - X(X'X)^{-1} \otimes r'. \]

(d) \[ \frac{\partial r}{\partial x_j} = -(\hat{\beta}_j M + X(X'X)^{-1}e_j r'). \]

Proofs. Section 17.8.


17.57b. Mathai [1997: 71]

17.57c. Abadir and Magnus [2005: 359].

17.60d. Deemer and Olkin [1951: 364–365].


17.63. Magnus and Neudecker [1999: 159–160, differentials only; they also give the complex case, and some second differentials] and Schott [2005: 369].

17.64. Abadir and Magnus [2006: 375–376].

17.9 PERTURBATION USING DIFFERENTIALS

An important problem is that of finding a Taylor expansion for a function of \(X + dX\), when the elements of \(dX\) are small. We begin by writing \(dX = \epsilon Y\), where \(\epsilon\) is small, so that \(X + \epsilon Y\) represents a small perturbation of \(X\). If \(f\) is a vector function of \(X\), then a Taylor expansion would take the form

\[ f(X + \epsilon Y) = f(X) + \sum_{i=1}^{\infty} \epsilon^i g_i(X, Y), \]
where $g_i(X, Y)$ represents some vector function of $X$ and $Y$. Similarly, if we have a matrix function $F$, then the expansion would take the form

$$F(X + \epsilon Y) = F(X) + \sum_{i=1}^{\infty} \epsilon^i G_i(X, Y),$$

where $G_i$ is now a matrix function. Schott [2005: section 9.6] demonstrated the method with several examples, and some of the results of these are given below. He also demonstrated how the method can be used for finding differentials and, ultimately, Jacobians.

17.65. Suppose that $X$ is nonsingular and $F(X) = X^{-1}$. Then

$$(X + dX)^{-1} = X^{-1} - X^{-1}(dX)X^{-1} + X^{-1}(dX)X^{-1}(dX)X^{-1} - X^{-1}(dX)X^{-1}(dX)X^{-1}(dX)X^{-1} + \cdots.$$

17.66. Let $X$ be a real symmetric $n \times n$ matrix with spectral decomposition $X = Q\Lambda Q'$, where $\Lambda = \text{diag}(\lambda_1, \lambda_2, \ldots, \lambda_n)$ and $\lambda_i = \lambda_i(X)$ is a distinct eigenvalue of $X$ corresponding to the eigenvector $q_i$, the $i$th column of $Q$. Let $\lambda_i(X + dX)$ and $\gamma_i$ be the eigenvalue and corresponding eigenvector of $X + dX$. If $dX = Q'WQ$, where $W$ is “small” and symmetric, then we have the following:

(a) $\lambda_i(X + dX) = \lambda_i + q_i'Wq_i + \cdots.$

(b) $\gamma_i(X + dX) = q_i - (Z - \lambda_iI_n)Wq_i + \cdots.$

Proofs. Section 17.9.


17.10 MATRIX LINEAR DIFFERENTIAL EQUATIONS

17.67. If $x = x(t)$ is an $n \times 1$ vector with elements that are functions of $t$ and $A$ is an $n \times n$ constant matrix, then

$$\frac{\partial x(t)}{\partial t} = Ax(t), \quad x(0) = x_0$$

has a formal solution $x = e^{At}x_0$. If $A$ is not a diagonal matrix, then the system of equations is said to be coupled. This coupling, which links $\partial x_i(t)/\partial t$ to the other components of $x(t)$, makes the solution harder to actually find. If $A$ can be transformed to a diagonal or near diagonal form, then the problem may be easier to solve. For example, if $A = SJ_0S^{-1}$, where $J_0$ is the Jordan canonical form of $A$, then the differential equation becomes

$$\frac{\partial y(t)}{\partial t} = J_0y(t), \quad y(0) = y_0,$$

where $x(t) = Sy(t)$ and $y_0 = S^{-1}x_0$. However, if $A$ is diagonalizable, then $J_0 = \text{diag}(\lambda_1, \ldots, \lambda_n)$, where the $\lambda_i$ are the eigenvalues of $A$. The transformed equations are now uncoupled and have solutions

$$y_i(t) = y_i(0)e^{\lambda_it}, \quad i = 1, 2, \ldots, n.$$
For further details see Horn and Johnson [1985: 133-134].

17.68. If \( x = x(t) \), then \( \frac{\partial x(t)}{\partial t} = Ax(t) + b(t) \) and \( x(t_0) = x_0 \) has solution

\[
x(t) = e^{A(t-t_0)}x_0 + e^{At} \int_{t_0}^{t} e^{-As}b(s)ds.
\]

Further details are given by Seber and Wild [1989: section 8.3]. For solutions of the more general case

\[
A \frac{\partial x(t)}{\partial t} + Bx(t) = b(t),
\]

where \( A \) may be nonsingular, see Campbell and Meyer [1979: section 9.2].

17.69. If \( X = X(t) \) is an \( m \times n \) matrix with elements that are functions of \( t \), then

\[
\frac{\partial X(t)}{\partial t} = AX + XB, \quad X(0) = X_0
\]

has solution \( X = e^{At}X_0 e^{Bt} \).

Proofs. Section 17.10.


17.11 SECOND-ORDER DERIVATIVES

Second-order derivatives are often required for determining the stationary values of a function. Below we give some techniques for finding Hessians.

**Definition 17.8.** Let \( f(X) \) be a scalar function of the \( m \times n \) matrix \( X \) that is twice differentiable inside the domain of \( f \). Then the **Hessian** of \( f \) is defined to be

\[
\nabla^2 f(X) = \frac{\partial^2 f(X)}{\partial \text{vec } X \partial (\text{vec } X)'} = \frac{\partial}{\partial \text{vec } X} \left( \frac{\partial f(X)}{\partial (\text{vec } X)'} \right).
\]

If \( X \) is a vector, say \( x \), then

\[
\nabla^2 f(x) = \frac{\partial^2 f}{\partial x \partial x'} = \left( \frac{\partial^2 f}{\partial x_i \partial x_j} \right).
\]

If \( Y \) is a matrix function of \( X \), we also define the **second differential** \( d^2Y = d(dY) \); and in deriving this in applications, we note that \( d^2X = 0 \). For some analytical details see Abadir and Magnus [2005: chapter 13], Harville [1997: section 15.1], Magnus and Neudecker [1999: chapter 6], and Nel [1980]. A number of examples are given by Nel [1980: section 7.2].
17.70. The Hessian as defined above is symmetric.

17.71. (Identification Rules)

(a) \( d^2 f(X) = (\text{vec } dX)'B(\text{vec } dX) \) if and only if \( \nabla^2 f(X) = \frac{1}{2}(B + B') \), where \( B \) may depend on \( X \) but not on \( dX \).

For example, if \( f(X) = \text{trace}(AXBX'C) \), where \( A, B, \) and \( C \) are square matrices (not necessarily of the same size) of constants, then taking differentials twice and setting \( d^2 X = 0 \) and \( d(dX)' = 0 \) we have, interchanging “\( d \)” and “\( \text{trace} \)”, and noting that \( \text{trace } F = \text{trace } F' \),

\[
d f(X) = \text{trace}[A(dX)BX'C + AXB(dX)'C],
\]

and

\[
d^2 f(X) = 2 \text{trace}[A(dX)B(dX)'C]
\]

\[
= 2 \text{trace}[(dX)'CA(dX)B]
\]

\[
= 2(\text{vec } dX)'(B' \otimes CA)(\text{vec } dX),
\]

since \( \text{trace}(D'E) = (\text{vec } D)'\text{vec } E \) and \( \text{vec } (DEF) = (F' \otimes D)\text{vec } E \). Here “\( \otimes \)” is the Kronecker product. We thus have from (a) the following rule:

(b) \( d^2 f(X) = \text{trace}[A(dX)B(dX)'C] \) if and only if

\[
\nabla^2 f(X) = \frac{1}{2}(B' \otimes CA + B \otimes A'C').
\]

Similarly, by using \( \text{trace}(FG) = \text{trace}(GF) \), we see that

\[
d^2 f(X) = \text{trace}[B(dX')C(dX)] \) if and only if
\]

\[
\nabla^2 f(X) = \frac{1}{2}(B' \otimes C + B \otimes C').
\]

For example, if \( f(X) = \text{trace}(X'AX) \), then \( d^2 f(X) = 2 \text{trace}[(dX')AdX] \) and

\[
\nabla^2 f(X) = I \otimes (A + A').
\]

(c) \( d^2 f(X) = \text{trace}[B(dX)C(dX)] \) if and only if

\[
\nabla^2 f(X) = \frac{1}{2}I_{(m,n)}(B' \otimes C + C' \otimes B),
\]

where \( X \) is \( m \times n \) and \( I_{(m,n)} \) is the commutation (vec-permutation) matrix. We have the following examples for \( n \times n \) \( X \).

(i) If \( f(X) = \text{trace}(X^{-1}) \), then \( d^2 f(X) = 2 \text{trace}[X^{-2}(dX)X^{-1}dX] \) and

\[
\nabla^2 f(X) = I_{(n,n)}(X^{-2} \otimes X^{-1} + X^{-1} \otimes X^{-2}).
\]

(ii) If \( f(X) = \det X \), then

\[
\nabla^2 f(X) = -\det X[I_{(n,n)}(X^{-1} \otimes X^{-1}) - (\text{vec } X^{-1})(\text{vec } X^{-1})'].
\]
(d) We also have the following special case for vectors.
\[ d^2 f(x) = (dx)'A(dx) \text{ if and only if } \nabla^2 f(x) = \frac{1}{2}(A + A'). \]

For example, if \( f(x) = x'Bx \), where \( B \) is a symmetric constant matrix, then \( df = 2x'Bdx \) and \( d^2 f = 2(dx)'Bdx \). Here \( A \) can be a function of \( x \).

17.72. Suppose \( X \) has \( L \)-structure (e.g., is symmetric or triangular) so that \( \text{vec } X = \Delta \phi(X) \) (cf. Section 18.3.5 for notation), then
\[
\frac{\partial^2 f(X)}{\partial \phi(X) \partial (\phi(X))'} = \Delta' \nabla^2 f(X) \Delta.
\]

If \( X \) is symmetric and \( n \times n \), then \( \phi(X) = \text{vech } X \) and \( \Delta = G_n \), the duplication matrix.

We demonstrate the above theory with the example \( f(X) = \text{trace}(X^{-1}) \). From (17.71c(i)) we obtain
\[
\nabla^2 f(X) = I_{(n,n)}(X^{-1} \otimes X^{-2} + X^{-2} \otimes X^{-1}).
\]

If \( X \) is symmetric, then
\[
\frac{\partial^2 f(X)}{\partial \phi(X) \partial (\phi(X))'} = \Delta' \nabla^2 f(X) \Delta = 2\Delta'(X^{-1} \otimes X^{-2})\Delta,
\]
since \( I_{(n,n)} \Delta = I_{(n,n)} G_n = G_n = \Delta \), by (11.29d).

17.73. Let \( F(t) \), with \( r, s \)th elements \( f_{rs}(t) \), be a nonsingular matrix function of \( t \).

(a)
\[
\frac{\partial^2 \det F}{\partial t_i \partial t_j} = (\det F) \left[ \text{trace} \left( F^{-1} \frac{\partial^2 F}{\partial t_i \partial t_j} \right) + \text{trace} \left( F^{-1} \frac{\partial F}{\partial t_i} \right) \text{trace} \left( F^{-1} \frac{\partial F}{\partial t_j} \right) \right. \\
- \text{trace} \left( F^{-1} \frac{\partial F}{\partial t_i} F^{-1} \frac{\partial F}{\partial t_j} \right) \left].
\]

(b)
\[
\frac{\partial^2 \log(\det F)}{\partial t_i \partial t_j} = \text{trace} \left( F^{-1} \left( \frac{\partial^2 F}{\partial t_i \partial t_j} \right) \right) - \text{trace} \left( F^{-1} \frac{\partial F}{\partial t_i} F^{-1} \frac{\partial F}{\partial t_j} \right).
\]

(c)
\[
\frac{\partial^2 F^{-1}}{\partial t_i \partial t_j} = -F^{-1} \frac{\partial^2 F}{\partial t_i \partial t_j} F^{-1} + F^{-1} \frac{\partial F}{\partial t_i} F^{-1} \frac{\partial F}{\partial t_j} F^{-1} + F^{-1} \frac{\partial F}{\partial t_j} F^{-1} \frac{\partial F}{\partial t_i} F^{-1}.
\]
17.74. Let $d(\theta) = \det[X(\theta)'X(\theta)]$, where $X$ is $n \times p$ of rank $p$ for $\theta \in \Omega$, and let $k(\theta) = \frac{1}{2} \log d(\theta)$. Then from (17.12),

$$k_r = \frac{\partial k(\theta)}{\partial \theta_r} = \text{trace}(X^+X_r),$$

where $X_r = \partial X/\partial \theta_r$. Also

$$k_{rs} = \frac{\partial^2 k(\theta)}{\partial \theta_r \partial \theta_s} = - \text{trace}(X^+X_rX^+X_s) + \text{trace}[X^+(X^+)'X_r'(I_n - XX^+)X_s]$$

$$+ \text{trace}(X^+X_{rs}),$$

where $X^+$ is the Moore–Penrose of $X$. The Hessian $H(\theta) = (h_{rs})$ of $d(\theta)$ is given by

$$h_{rs} = \frac{\partial^2 d(\theta)}{\partial \theta_r \partial \theta_s} = 2d(\theta)(k_{rs} + 2k_rik_s).$$

**Proofs.** Section 17.11.

17.70. Magnus and Neudecker [1999: 105–106].


17.71d. Abadir and Magnus [2005: 353]

17.72. Magnus [1988: 155].

17.73. Harville [1997: section 15.9].


17.12 VECTOR DIFFERENCE EQUATIONS

**Definition 17.9.** The vector difference equation

$$A_0y_t + A_1y_{t-1} + \ldots + A_r y_{t-r} = g(t),$$

with $A_0$ nonsingular and all vectors $n$-dimensional functions of $t$, is called an $r$th-order vector difference equation with constant coefficients. Since $A_0$ is nonsingular, we can set $A_0 = I_d$ without loss of generality. Difference equations arise in discrete time stochastic processes and in iterative procedures that converge. The case when $A_0$ is singular can be handled using the Drazin inverse of $A_0$ (Campbell and Meyer [1979: 181–184]).
**17.75.** The above difference equation can be reduced to a first-order equation as follows. Let \( z_t = (y_t', y_{t-1}', \ldots, y_{t-r+1}')' \) and

\[
B = \begin{pmatrix}
-A_1 & -A_2 & \cdots & -A_{r-1} & -A_r \\
I_d & 0 & \cdots & 0 & 0 \\
0 & 0 & \cdots & I_d & 0
\end{pmatrix}.
\]

Then \( z_t = Bz_{t-1} + e_1 \otimes g(t) \), where \( e_1 \) is an \( r \)-dimensional vector \( (1, 0, \ldots, 0)' \) and “\( \otimes \)” is the Kronecker product. The solution of this was studied by Dhrymes [2000: 175-178]. He applies it to the general linear structural econometric model.

**17.76.** If \( x_t = Ax_{t-1} + d \), where \( A \) and \( x_0 \) are known, then provided that \( A^t \to 0 \) as \( t \to \infty \) and \( (I - A)^{-1} \) exists, we have \( x_t = A^t x_0 + (I - A^t)(I - A)^{-1}d \) and \( x_t \to (I - A)^{-1}d \) as \( t \to \infty \).

**Definition 17.10.** (Linear Stationary Iterations) Let \( Ax = b \), with \( A \) an \( n \times n \) and expressible in the form \( A = M - N \), where \( M^{-1} \) exists. Let \( H = M^{-1}N \), the iteration matrix, and let \( d = M^{-1}b \). Given an initial \( n \times 1 \) vector \( x(0) \), then a linear stationary iteration is

\[
x(k) = Hx(k-1) + d, \quad k = 1, 2, 3, \ldots.
\]

**17.77.** Given the notation above, if \( \rho(H) < 1 \), where \( \rho \) is the spectral radius, then \( A \) is nonsingular and

\[
\lim_{k \to \infty} x(k) = x = A^{-1}b
\]

for every initial vector \( x(0) \). For details and methods see Meyer [2000a: 620-626].

**Proofs.** Section 17.12.

17.76. Searle [1982: 289].

17.77. Meyer [2000a: 621].
JACOBIANS

Jacobians play a fundamental role in statistical distribution theory. Formulae for Jacobians and their proofs are given in many places, especially in the appendices of statistics books. In the case of complicated transformations, it is not always clear what the sign of the Jacobian is as it will depend on how the variables are ordered. Fortunately, the ordering only affects the sign of the Jacobian, which usually does not matter as in applications we are mainly interested in the absolute value of the Jacobian.

18.1 INTRODUCTION

Before listing a number of results, we look at the meaning of a Jacobian and give a number of different techniques for finding Jacobians.

Definition 18.1. Suppose \( f : x \rightarrow y = f(x) \), where \( x \) and \( y \) belong to \( \mathbb{R}^n \), is a one-to-one (bijective) differentiable function, i.e., it has an inverse function \( g = f^{-1} \). Then \( \frac{\partial x}{\partial y'} = (\frac{\partial x_i}{\partial y_j}) \) is called the Jacobian matrix of the transformation \( x \rightarrow y \), and its determinant

\[
J_{x \rightarrow y} = \det \left( \frac{\partial x}{\partial y'} \right)
\]

is called the Jacobian of the transformation. (Some authors call the absolute value \(|J_{x \rightarrow y}|\) the Jacobian.) For further comments on this definition see Section 17.7.
In the above definition we want to differentiate \( x \) with respect to \( y \), so it is more natural to use \( x = g(y) \), as does Muirhead [1982: chapter 2], for example. However, as most of the references use \( y = f(x) \), I have decided to stay with the latter in this chapter. As it can be a source of possible confusion, Daniel L. Solomon gives the following mnemonic rule (Searle [1982: 339]) to help get the order of the variables right: If “o” represents the old coordinates \( (x) \) and “n” represents the new coordinates \( (y) \), then \( J_{o \rightarrow n} \) is correct, but \( J_{n \rightarrow o} \) is not (spells no).

If we interchange two elements of \( y \), we change the sign of \( J_{y \rightarrow x} \). However, it does not matter in what order we list the elements of \( x \) and \( y \). Several authors—for example, Mathai [1997], whom I will refer to frequently in this chapter—get around this problem by stating that the sign of a particular Jacobian should be ignored. I shall tend to use absolute values throughout.

As already mentioned, if we want to differentiate \( x \) with respect to \( y \), we can endeavor to express the transformation in the form \( x = g(y) \). However, it may be easier to find \( J_y \rightarrow x \) first as \( J_x \rightarrow y = J^{-1}_y \rightarrow x \). To see this, we have \( x = g(f(x)) \) and

\[
I_n = \left( \frac{\partial x_i}{\partial x_j} \right) = \left( \sum_r \frac{\partial g_r}{\partial y_r} \cdot \frac{\partial y_r}{\partial x_j} \right) = \frac{\partial x}{\partial y'} \cdot \frac{\partial y}{\partial x'}.
\]

Then

\[
1 = \det \left\{ \frac{\partial x}{\partial y'} \cdot \frac{\partial y}{\partial x'} \right\} = \det \left\{ \frac{\partial x}{\partial y'} \right\} \cdot \det \left\{ \frac{\partial y}{\partial x'} \right\} = J_{x \rightarrow y} J_{y \rightarrow x}.
\]

We note that \( J_y \rightarrow x \) will be expressed in terms of \( x \), which in applications usually has to be replaced by its function of \( y \). For example, two important statistical applications of Jacobians are (i) change of variables in integration, that is,

\[
\int \cdots \int h(x_1, x_2, \ldots, x_n) dx_1 dx_2 \cdots dx_n = \int \cdots \int h(g(y)) |J_x \rightarrow y| dy_1 dy_2 \cdots dy_n,
\]

and (ii) probability density functions for functions of random variables, namely

\[
f_Y(y) = f_X(g(y)) |J_{x \rightarrow y}|.
\]

If \( x \) and \( y \) are replaced by matrices with \( Y = F(X) \), we define

\[
J_{X \rightarrow Y} = J_{\text{vec } x \rightarrow \text{vec } y} = \det \left( \frac{\partial \text{vec } X}{\partial (\text{vec } Y)'} \right),
\]

and, if \( X \) and \( Y \) are symmetric or lower-triangular, we define

\[
J_{x \rightarrow y} = J_{\text{vech } x \rightarrow \text{vech } y} = \det \left( \frac{\partial \text{vech } X}{\partial (\text{vech } Y)'} \right).
\]

For upper-triangular matrices we can use \( \text{vech } (X') \).

In order to evaluate the above Jacobians, various properties of the Kronecker product and of the vec and vech operators are required from Chapter 11. In this chapter we shall concentrate on finding \( J_{y \rightarrow x} \) or \( |J_{y \rightarrow x}| \), which can then be inverted. Unless otherwise stated, all matrices and scalars are real. We now give some techniques for finding Jacobians; some of these techniques are demonstrated by Olkin [2002].
18.2 METHOD OF DIFFERENTIALS

Differentials were introduced in Section 17.8 along with some rules that provide a powerful method for finding Jacobians.

18.1. A key result from (17.28) for vectors is as follows. If dy = A dx, where A may be a function of x, then

\[ \frac{\partial y}{\partial x'} = A \quad \text{and} \quad J_{y \rightarrow x} = \det A. \]

In the case of matrices, if d vec Y = B d vec X, then

\[ \frac{\partial \text{vec } Y}{\partial (\text{vec } X)'} = B \quad \text{and} \quad J_{Y \rightarrow X} = \det B, \]

where B may be a function of X. Also d vec X = vec (dX).

18.2. We recall the following equivalent statements from (17.60), where X is \( m \times n \).

1. \( dY = A(dX)B + C(dX')D \).

2. vec \((dY) = (B' \otimes A) \text{vec } (dX) + (D' \otimes C) \text{vec } (dX')\), or, equivalently,

\[ d \text{ vec } Y = \{(B' \otimes A) + (D' \otimes C)I_{(n,m)}\} d \text{ vec } X. \]

When the above hold, we see from (2) and (3) that

\[ J_{Y \rightarrow X} = J_{\text{vec } Y \rightarrow \text{vec } X} = J_{d \text{ vec } Y \rightarrow d \text{ vec } X}. \]

We demonstrate how these results can be used by working through two examples.

Example 1 Let \( Y_{m \times n} = A_{m \times m}X_{m \times n}B_{n \times n} \), where A and B are nonsingular. Then \( dY = A(dX)B \) and \( \text{vec } (dY) = (B' \otimes A) \text{vec } (dX) \). Using (17.1l(ii)), we get

\[ J_{Y \rightarrow X} = \det(B' \otimes A) = (\det B)^m(\det A)^n. \]

Thus, \( J_{X \rightarrow Y} = (\det B)^{-m}(\det A)^{-n} \).

Example 2 Let \( Y = X^{-1} \), where X is a nonsingular \( n \times n \) matrix. Since \( YX = I_n \), we have \( 0 = d(YX) = YdX + (dY)X \), or \( dY = -X^{-1}(dX)X^{-1} \). Thus, from Example 1 with \( A = -X^{-1} \) and \( B = X^{-1} \), we have

\[ J_{Y \rightarrow X} = (-1)^n(\det X)^{-2n}, \]

and \( J_{X \rightarrow Y} = (-1)^n(\det Y)^{-2n} \).

18.3 FURTHER TECHNIQUES

In addition to the method of differentials, there are a number of other useful related techniques that we now describe.
18.3.1 Chain Rule

One useful technique makes use of the chain rule (17.21). This rule leads to the result that if we have the transformations \( x \to y \) and \( y \to z \), then \( J_{x \to z} = J_{x \to y} J_{y \to z} \), i.e., Jacobians multiply. If the Jacobian of \( x \to z \) is hard to derive, it may be possible to find an intermediary variable \( y \) such that \( J_{x \to y} \) and \( J_{y \to z} \) are easy to find. This method was used frequently by Deemer and Olkin [1951] and Olkin [1953], and several examples of it appear later.

18.3.2 Exterior (Wedge) Product of Differentials

This elegant technique is described in detail by Muirhead [1982: chapter 2] and used extensively by Mathai [1997]. We assume that \( y \) and \( x \) are \( n \times 1 \) vectors, and we introduce a skew-symmetric product “\( \wedge \)” of differentials called the exterior or wedge product, satisfying (i) \( dy_i \wedge dy_j = -dy_j \wedge dy_i \) and (ii) \( dy_i \wedge dy_i = 0 \) (a consequence of (i)). To evaluate \( \det(\partial y/\partial x') \), we begin with

\[
\begin{align*}
\sum_{j=1}^{n} \frac{\partial y_i}{\partial x_j} \, dx_j,
\end{align*}
\]

and multiply these together using the above two properties of the exterior product to get

\[
\begin{align*}
dy_1 \wedge dy_2 \wedge \cdots \wedge dy_n = \det \left( \frac{\partial y}{\partial x'} \right) \, dx_1 \wedge dx_2 \wedge \cdots \wedge dx_n.
\end{align*}
\]

This result is readily demonstrated for \( n = 2 \). We have

\[
\begin{align*}
dy_1 \wedge dy_2 & = \left( \frac{\partial y_1}{\partial x_1} \, dx_1 + \frac{\partial y_1}{\partial x_2} \, dx_2 \right) \wedge \left( \frac{\partial y_2}{\partial x_1} \, dx_1 + \frac{\partial y_2}{\partial x_2} \, dx_2 \right) \\
& = \frac{\partial y_1}{\partial x_1} \cdot \frac{\partial y_2}{\partial x_1} \, dx_1 \wedge dx_1 + \frac{\partial y_1}{\partial x_2} \cdot \frac{\partial y_2}{\partial x_1} \, dx_1 \wedge dx_2 \\
& \quad + \frac{\partial y_1}{\partial x_2} \cdot \frac{\partial y_2}{\partial x_2} \, dx_2 \wedge dx_1 + \frac{\partial y_1}{\partial x_2} \cdot \frac{\partial y_2}{\partial x_2} \, dx_2 \wedge dx_2 \\
& = 0 + \left( \frac{\partial y_1}{\partial x_1} \cdot \frac{\partial y_2}{\partial x_2} - \frac{\partial y_1}{\partial x_2} \cdot \frac{\partial y_2}{\partial x_1} \right) \, dx_1 \wedge dx_2 + 0 \\
& = \det \left( \begin{array}{cc} \frac{\partial y_1}{\partial x_1} & \frac{\partial y_1}{\partial x_2} \\ \frac{\partial y_2}{\partial x_1} & \frac{\partial y_2}{\partial x_2} \end{array} \right) \, dx_1 \wedge dx_2 \\
& = \det \left( \frac{\partial y}{\partial x'} \right) \, dx_1 \wedge dx_2.
\end{align*}
\]

We shall define the wedge product for a vector \( x \) as

\[
d_w x = \wedge_{i=1}^{n} dx_i.
\]

This approach extends to matrices by setting \( y = \vec{y} \) and defining \( d_w Y = \wedge_{i,j \in \mathcal{D}} dy_{ij} \), where \( \mathcal{D} \) denotes the ordered set of distinct elements of \( Y \), ordered according to \( y \). I have deliberately made this notation different from that of Muirhead.
[1982] and Mathai [1997] to avoid confusion, because they use brackets like (dX) with opposite meanings.

If Y is symmetric or lower-triangular, we can use y = vech Y for the distinct elements of Y and define d_w Y = d_w y = d_w vech Y. In the case of a skew-symmetric matrix, the diagonal elements are ignored, as they are zero. However, as already noted, the order in which the distinct elements of these matrices are listed is not important in applications.

18.3. It follows from the above that if vec Y = y and vec X = x, then
\[ d_w Y = \frac{\partial y}{\partial x} d_w X. \]

Since, as already mentioned, the order of the variables can be arbitrary, we have
\[ d_w Y = (\det C)d_w X \implies |J_Y - X| = |\det C|. \]

Example 3 Let \((y_1, y_2, \ldots, y_n) = Y = AX = (Ax_1, Ax_2, \ldots, Ax_n).\) Then, from (18.1), \(d_w y_i = (\det A)d_w x_i,\) so that \(d_w Y = \bigwedge_{i=1}^n d_w y_i = (\det A)^n d_w X,\) and \(|J_Y - X| = |\det A|^n.\) Alternatively, vec Y = diag(A, A, A) vec X and, from (18.1), \(|\det C| = |\det \{\text{diag}(A, A, \ldots, A)\}| = |\det A|^n,\) as before.

Example 4 Let \(Y = BX,\) where the matrices are all \(n \times n\) lower-triangular matrices so that \((y_1, y_2, \ldots, y_n) = (Bx_1, Bx_2, \ldots, Bx_n).\) For \(r = 1, 2, \ldots, n,\) let \(y(r) = (y_{r, r}, y_{r+1, r}, \ldots, y_{n, r})^T\) be \(y_r\) without its leading zeros; \(x(r)\) is similarly defined. Note that \(y(n) = y_{n, n} = b_{n, n} x_{n, n} = b_{n, n} x(n).\) Then
\[ a_n = \det \left( \frac{\partial y_{n, n}}{\partial x_{n, n}} \right) = b_{n, n}, \]
\[ a_{n-1} = \det \left( \begin{array}{cc} y_{n-1, n-1} & y_{n-1, n} \\ x_{n-1, n-1} & x_{n-1, n} \end{array} \right) = \det \left( \begin{array}{cc} b_{n-1, n-1} & b_{n-1, n} \\ 0 & b_{n, n} \end{array} \right) = b_{n, n} b_{n-1, n-1}, \]
and so on. Hence
\[ d_w Y = \bigwedge_{r=1}^n d_w y(r) = \prod_{r=1}^n a_r d_w y(r) = \prod_{r=1}^n b_{r, r}^r d_w X \]
and \(|J_Y - X| = |\prod_{r=1}^n b_{r, r}^r|.| \]

18.3.3 Induced Functional Equations

Olkin and Sampson [1972] described a method whereby one sets up an equation satisfied by the Jacobian and then solves the equation.

Example 5 Suppose \(Y = AXA',\) where A is nonsingular and Y is symmetric. To find the Jacobian of this transformation, let \(Z = BYB',\) where B is nonsingular and Z is symmetric, so that \(Z = ABX(AB)'\). Then
\[ |J_{Z - X}| = |J_{Z - Y}| \cdot |J_{Y - X}|. \]
As the transformation is linear in $X$, $|J_{Y\to X}|$ is a positive function of $A$ above, say $h(A)$. Then, by the above equation,

$$h(AB) = h(A)h(B),$$

which, for this example, has solution $h(A) = |\det A|^c$, for some $c$. Setting $A = \text{diag}(a_1, 1, 1, \ldots, 1)$ and finding $J_{Y\to X}$ for this simple case, leads to $c = n+1$ (Olkin and Sampson [1972: 263]).

Olkin and Sampson [1972] derive solutions of the equation $h(AB) = h(A)h(B)$ for diagonal, triangular, orthogonal, and symmetric matrices. Their paper can be referred to for details (see also Mathai [1997: 40-44] for a summary of the main results).

### 18.3.4 Jacobians Involving Transposes

Consider the transformation $Y = X'$, where $X$ is an $m \times n$ unconstrained matrix. Then, by (11.18b(i)) and (11.18f(i)),

$$\text{vec } Y = \text{vec } X' = I_{(n,m)} \text{vec } X,$$

$$J_{Y\to X} = \det I_{(n,m)} = (-1)^{\frac{1}{2}m(m-1)n(n-1)}, \text{ and } |J_{Y\to X}| = 1.$$

**Example 6** Consider the transformation $Y_{m\times n} = A_{m\times n}X'_{m\times n}B_{n\times n}$, where $A$ and $B$ are nonsingular. Setting $W = X'$ and $Y = AWB$, we have, from Example 1 above and the chain rule (17.21),

$$J_{Y\to X} = J_{Y\to W}J_{W\to X} = (\det B)^m(\det A)^n(-1)^{\frac{1}{2}m(m-1)n(n-1)}.$$

In practice, we are more interested in absolute values so that we do not need to distinguish between $X$ and $X'$ in linear transformations like the above, as $|J_{W\to X}| = |J_{X'\to X}| = 1$ and $|J_{Y\to X}| = |J_{Y\to W}|$.

**Example 7** Suppose we know the Jacobian for the transformation $Y = AX$, and we want to find the Jacobian for $Y = XA$. Taking transposes, we obtain $Y' = A'X'$ or $W = A'Z$. Then

$$J_{Y\to X} = J_{Y\to Y'}J_{Y'\to X'}J_{X'\to X} = J_{Y\to Y'}J_{W\to Z}J_{X'\to X}$$

and, by Example 6, $|J_{Y\to X}| = |J_{W\to Z}|$. Hence the absolute value of the Jacobian for $Y = XA$ can be obtained from the one for $Y = AX$ by simply replacing $A$ by $A'$. Example 7 is, of course, a special case of Example 6, but the method is instructive.

### 18.3.5 Patterned Matrices and L-Structures

Sometimes the matrices involved are "patterned" or structured in some way such as symmetric or triangular. We are therefore interested in this case where $\text{vec } X$ (where $X$ is $m \times n$) will be in a linear subspace $D_s$ of $\mathbb{R}^{mn}$. For example, if $X$ is $n \times n$ and lower-triangular, then $\text{vec } X$ will contain zeros in a certain pattern.
Magnus [1988] proposed a method based on linear structures, a linear structure being the set of all real matrices of a specified order, say $m \times n$, that satisfy a set of linear restrictions. He gives the following definition.

**Definition 18.2.** Let $D_s$ be an $s$-dimensional subspace of $\mathbb{R}^{mn}$ and let $\delta_1, \delta_2, \ldots, \delta_s$ be a set of basis vectors for $D_s$. Then the $mn \times s$ matrix

$$\Delta_{mn \times s} = (\delta_1, \delta_2, \ldots, \delta_s)$$

is called a basis matrix for $D_s$, and the collection of real $m \times n$ matrices

$$L(\Delta_{mn \times s}) = \{X : X \in \mathbb{R}^{mn}, \text{vec} \ X \in D_s\}$$

is called a linear structure (L-structure), $s$ is called the dimension of the L-structure, and $m \times n$ is called the order of the L-structure. Here $\Delta$ is not unique, but once defined, there exists a unique $s \times 1$ vector $\phi(X)$ such that $\text{vec} \ X = \Delta \phi(X)$ or $\phi(X) = \Delta^+ \text{vec} \ X$, where $\Delta^+$ is the Moore–Penrose inverse. Typically, $\phi(X)$ is the vector containing the "free" elements of $X$ in an appropriate order so that $\Delta$ is then unique.

For example, if $X$ is a real symmetric $n \times n$ matrix, then among its $n^2$ elements $x_{ij}$ there exist $\frac{1}{2}n(n-1)$ linear relationships of the form $x_{ij} = x_{ji}$ ($i < j$). Here $s = n^2 - \frac{1}{2}n(n-1) = \frac{1}{2}n(n+1)$. In particular, for $n = 2$, $D_3 \subset \mathbb{R}^4$ and a basis matrix for $D_3$ is the $4 \times 3$ matrix

$$\Delta_{4 \times 3} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$ 

Thus if $(a, b, c)' \in \mathbb{R}^3$, then

$$\Delta_{4 \times 3} \begin{pmatrix} a \\ b \\ c \end{pmatrix} = \begin{pmatrix} a \\ b \\ c \end{pmatrix} = \text{vec} \begin{pmatrix} a & b \\ b & c \end{pmatrix} = \text{vec} \ X.$$ 

We note that

$$\phi(X) = (a, b, c)' = \text{vech} \ X, \quad \text{and} \quad \Delta_{4 \times 3} = G_2,$$

the so-called duplication matrix. A general theory for finding such basis matrices is given by Kollo and von Rosen [2005: section 1.3.6]. We now give a key result.

**18.4.** Suppose $Y = F(X)$ is a one-to-one function representing a relationship between $s$ variables $x_{ij}$ and $s$ variables $y_{ij}$, where $Y \in L(\Delta_2)$ for every $X \in L(\Delta_1)$ with the dimensions of $L(\Delta_1)$ and $L(\Delta_2)$ both equal to $s$. Then, from Magnus [1988: 34],

$$J_{Y \rightarrow X} = \det \left[ \Delta_2^+ \left( \frac{\partial \text{vec} \ Y}{\partial \text{vec} \ X}' \right) \Delta_1 \right],$$

where $\frac{\partial \text{vec} \ Y}{\partial \text{vec} \ X}'$ is calculated ignoring the a priori knowledge about the L-structures.
Henderson and Searle [1979: 74-76] discussed the same idea, but from a slightly different perspective. They define $\text{vecp}_z(Z)$ as the vector of the distinct elements with pattern $p_z$, where $Z = X$ or $Y$ (they use $X_1$ and $X_2$). Then

$$\text{vecp}_z(Z) = P_z \text{vec} Z \quad \text{and} \quad \text{vec} Z = Q_z \text{vecp}_z(Z) = Q_z P_z \text{vec} Z,$$

where $P_z$ and $Q_z$ correspond to $H$ and $G$ of Section 11.5.1. In particular, $P_z Q_z = I$, $Q_z$ has full column rank, and $P_z = (Q_z' Q_z)^{-1} Q_z'$ is one possible choice for $P_z$.

Finally,

$$J_{X \rightarrow Y} = \det \left[ P_X \frac{\partial \text{vec} X}{\partial (\text{vec} Y)' Q_Y} \right].$$

Derivatives for patterned matrices are also discussed by Nel [1980: section 61]. Kollo and von Rosen [2005: 135-149] develop derivatives for structured matrices, but use a derivative notation $Y \otimes \partial / \partial X$.

We are now going to systematically list Jacobians. If the order of the variables is not well defined, $|J|$ will be quoted instead of $J$.

18.4 VECTOR TRANSFORMATIONS

The following transformations between $n \times 1$ vectors are one-to-one.

18.5. If $y = Ax$, where $A$ is nonsingular, then from (17.28) we have

$$|J_{Y \rightarrow X}| = |\det A|.$$

When $A = aI_n$, $|J_{Y \rightarrow X}| = |a|^n$.

18.6. (Symmetric Functions) Let $y_i = x_{(i)}$, $i = 1, 2, \ldots, n$, where $x_{(i)}$ is the so-called (elementary) symmetric function representing the sum of all the products of $x_j$ taken $i$ at a time. Thus $y_1 = x_1 + \cdots + x_n$, $y_2 = x_1 x_2 + x_1 x_3 + \cdots + x_{n-1} x_n$, and $y_n = x_1 x_2 \cdots x_n$. Then for each $x_j > 0$,

$$|J_{Y \rightarrow X}| = \prod_{i=1}^{n-1} \prod_{j=i+1}^{n} |x_i - x_j|.$$

18.7. If

$$y_1 = x_1 + x_2 + \cdots + x_n,$$
$$y_2 = x_1^2 + x_2^2 + \cdots + x_n^2,$$
$$\vdots$$
$$y_{n-1} = x_1^{n-1} + x_2^{n-1} + \cdots + x_n^{n-1},$$
$$y_n = x_1 x_2 \cdots x_n,$$

then, for each $x_j > 0$,

$$|J_{Y \rightarrow X}| = (n - 1) \prod_{i=1}^{n-1} \prod_{j=i+1}^{n} |x_i - x_j|. $$
18.8. (Polar Coordinates)

(a) Consider the transformation

\[\begin{align*}
x_1 &= r \sin \theta_1 \sin \theta_2 \cdots \sin \theta_{n-2} \sin \theta_{n-1}, \\
x_2 &= r \sin \theta_1 \sin \theta_2 \cdots \sin \theta_{n-2} \cos \theta_{n-1}, \\
x_3 &= r \sin \theta_1 \sin \theta_2 \cdots \cos \theta_{n-2}, \\
\vdots &= \vdots \\
x_{n-1} &= r \sin \theta_1 \cos \theta_2, \\
x_n &= r \cos \theta_1,
\end{align*}\]

where \(r > 0, 0 < \theta_i \leq \pi (i = 1, 2, \ldots, n - 2),\) and \(0 < \theta_{n-1} \leq 2\pi.\) Then, if \(\theta = (\theta_1, \theta_2, \ldots, \theta_n)',\) we have

\[|J_{x \to r, \theta}| = r^{n-1} |(\sin \theta_1)^{n-2}(\sin \theta_2)^{n-3} \cdots \sin \theta_{n-2}|\]

(b) If we reverse the order of the \(x_i\) and replace \(\theta_i\) by \(\frac{\pi}{2} - \theta_i\) in (a), we get

\[\begin{align*}
x_1 &= r \sin \theta_1, \\
x_j &= r \cos \theta_1 \cos \theta_2 \cdots \cos \theta_{j-1} \sin \theta_j, \quad j = 2, 3, \ldots, n - 1, \\
x_n &= r \cos \theta_1 \cos \theta_2 \cdots \cos \theta_{n-1},
\end{align*}\]

where \(r > 0, -\frac{\pi}{2} < \theta_i \leq \frac{\pi}{2} (i = 1, \ldots, n - 2),\) and \(-\pi < \theta_{n-1} \leq \pi.\) Then

\[|J_{x \to r, \theta}| = r^{n-1} |(\cos \theta_1)^{n-2}(\cos \theta_2)^{n-3} \cdots \cos \theta_{n-2}|.\]

Proofs. Section 18.4.

18.7. Mathai [1997: 45].
18.8b. Mathai [1997: 45].

18.5 JACOBIANS FOR COMPLEX VECTORS AND MATRICES

We demonstrate the meaning of a Jacobian for complex variables using a simple example taken from Mathai [1997: 175–176]. Let \(y = y_1 + iy_2\) and \(x = x_1 + ix_2,\) where the \(x_i\) and \(y_i\) are all real \(n \times n\) vectors. Consider the transformation \(y = Ax\) where \(A\) is real. Then \(y_i = Ax_i\) for \(i = 1, 2,\) and

\[\begin{pmatrix} y_1 \\ y_2 \end{pmatrix} = \begin{pmatrix} A & 0 \\ 0 & A \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = Bx.\]

We define the Jacobian of the transformation to be \(J_{y_1, y_2 \to x_1, x_2}.\) From (18.5) this is \(\det B = (\det A)^2\) (\(= |\det A|^2,\) say).
If $A$ is complex and $A = A_1 + iA_2$, then
\[
y = y_1 + iy_2 = (A_1 + iA_2)(x_1 + ix_2) = (A_1x_1 - A_2x_2) + i(A_1x_2 + A_2x_1),\]
and we have $y_1 = A_1x_1 - A_2x_2$ and $y_2 = A_1x_2 + A_2x_1$. Then $\partial y_1/\partial x'_1 = A_1$, $\partial y_1/\partial x'_2 = -A_2$, $\partial y_2/\partial x'_1 = A_2$, and $\partial y_2/\partial x'_2 = A_1$. Hence, from Section 5.1.2,
\[
|J_{y_1, y_2 \rightarrow x_1, x_2}| = \left| \begin{array}{cc}
A_1 & -A_2 \\
A_2 & A_1
\end{array} \right| = (|\det A|^2 = |\det (AA^*)|).
\]

Thus the above equation is true for both the real and complex cases.

When vectors are replaced by matrices, the expression $J_{Y_1, Y_2 \rightarrow X_1, X_2}$ denotes the Jacobian of the transformation, where $Y_1$ and $Y_2$ are written as functions of $X_1$ and $X_2$, or where $Y = Y_1 + iY_2$ is a function of $X = X_1 + iX_2$, the elements of $X$ being functionally independent. As we have seen from the above example, we can typically go from the real to the complex case by squaring absolute values of determinants or by replacing $|\det A|$ by $|\det AA^*| = |\det A|^2$. We shall also see below that a term like $|x_{ii}|$ for a real diagonal element $x_{ii}$ remains the same for a complex element except that $|\cdot|$ now refers to the modulus of a complex number.

### 18.6 MATRICES WITH FUNCTIONALLY INDEPENDENT ELEMENTS

#### 18.9
If $Y_{m \times n} = aX_{m \times n}$, then $J_{Y \rightarrow X} = a^{mn}$ and $|J_{Y \rightarrow X}| = |a|^{mn}$. For complex matrices the latter Jacobian becomes $|a|^{2mn}$.

#### 18.10
If $Y_{m \times n} = A_{m \times m}X_{m \times n}B_{n \times n}$, where $A$ and $B$ are nonsingular then, from Example 1 above in Section 18.2,
\[
|J_{Y \rightarrow X}| = |\det B|^m \cdot |\det A|^n.
\]
The transformation is clearly one-to-one. In particular, if $y = Ax$, then
\[
|J_{y \rightarrow x}| = \left| \frac{\partial y}{\partial x'} \right| = |\det A|.
\]
Other cases follow by setting $A$ or $B$ equal to the identity matrix.

If the matrices are complex, we find that we simply replace $A$ by $AA^*$ and $B$ by $BB^*$ in the above expressions.

#### 18.11
Let $Y = AXA' \pm BXB'$, where all the matrices are $n \times n$ and $A \otimes A \pm B \otimes B$ are nonsingular. Then $\text{vec } Y = (A \otimes A \pm B \otimes B)\text{vec } X$, so that the transformation is one-to-one, and
\[
|J_{Y \rightarrow X}| = \prod_{i=1}^{n} \prod_{j=1}^{n} |\alpha_i \alpha_j \pm \beta_i \beta_j|,
\]
where the $\alpha_i$ and $\beta_j$ are the respective eigenvalues of $A$ and $B$.

#### 18.12
Let $Y = X^{-1}$, where $X$ is $n \times n$ and nonsingular.

(a) From Example 2 in Section 18.2 above, $|J_{Y \rightarrow X}| = (|\det X|)^{-2n}$. 

(b) When $X$ is complex, we replace $X$ by $XX^*$. 

18.13. Let $Y = (\det X)X^{-1}$, where $X$ is $n \times n$, and $\det X > 0$ to ensure the transformation is one-to-one.

(a) (i) If $X$ is real, $|J_{Y \rightarrow X}| = (n - 1)(|\det X|)^{n(n-2)}$.

(ii) If $X$ is complex, then

$$|J_{Y_1, Y_2 \rightarrow X_1, X_2}| = (n - 1)^2 |\det X|^{2n(n-2)}.$$ 

(b) (i) If $X$ is real and $Z = Y^{-1} = X/\det X$, then

$$|J_{Z \rightarrow X}| = (n - 1)|\det X|^{n^2}.$$ 

This follows from $J_{Z \rightarrow X} = J_{Z \rightarrow Y} J_{Y \rightarrow X}$ and (18.12).

(ii) When $X$ is complex,

$$|J_{Z_1, Z_2 \rightarrow X_1, X_2}| = (n - 1)^2 |\det X|^{−2n^2}.$$ 

18.14. If $Y = AX^{-1}B$ and all matrices are $n \times n$ and nonsingular, then the transformation is one-to-one and

$$|J_{Y \rightarrow X}| = |(\det B)^n (\det X)^{−2n} (\det A)^n|.$$ 

This can be proved from (18.12) using $Y = AZB$, $Z = X^{-1}$, and the chain rule.

18.15. Let $Y = X^k$, where $X$ is $n \times n$ and nonsingular, and $k$ is a positive integer.

(a) If $X$ has nonzero, not necessarily distinct, real eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_n$, then

(i) $|J_{Y \rightarrow X}| = |\prod_{i=1}^{n} \prod_{j=1}^{n} \sum_{r=1}^{k} \lambda_i^{k-r} \lambda_j^{r-1}|.$

We note that the transformation is generally not one-to-one.

(ii) If the eigenvalues are distinct, an alternative expression is given by

$$|J_{Y \rightarrow X}| = |k^n (\det X)^{k-1} \prod_{i=1}^{n} \prod_{j=i+1}^{n} \left( \frac{\lambda_i^k - \lambda_j^k}{\lambda_i - \lambda_j} \right)^2 |$$

$$= |k^n (\det X)^{k-1} \prod_{i=1}^{n} \prod_{j \neq i}^{n} \left( \frac{\lambda_i^k - \lambda_j^k}{\lambda_i - \lambda_j} \right) |,$$

which, by noting that $\det X = \prod_i \lambda_i$, is readily shown to be the same as the expression in (i).

(b) Suppose $k = 2$, that is, $Y = X^2$.

(i) From (a),

$$|J_{Y \rightarrow X}| = \prod_{i=1}^{n} \prod_{j=1}^{n} |\lambda_i + \lambda_j|.$$ 

(ii) When $X$ is complex and the eigenvalues are distinct, then

$$|J_{Y_1, Y_2 \rightarrow X_1, X_2}| = \prod_{i=1}^{n} \prod_{j=1}^{n} |\lambda_i + \lambda_j|^2.$$
Proofs. Section 18.6.


18.15a(i). Henderson and Searle [1979: 73].


18.15b(i). Henderson and Searle [1979: 73].


18.7 SYMMETRIC AND HERMITIAN MATRICES

Let $X$ and $Y$ be $n \times n$ real symmetric matrices, unless otherwise stated. We note that if $X = X_1 + iX_2$ is Hermitian, then $X_1$ is real symmetric and $X_2$ is real skew-symmetric.

18.16. The following transformations are one-to-one.

(a) If $Y = aX$, then $|J_{Y - X}| = |a^{n(n+1)/2}|$.

(b) If $Y = AXA'$, where $A$ is nonsingular, then $|J_{Y - X}| = (|\det A|)^{n+1}$.

(c) If $Y = AX^{-1}A'$, where $A$ and $X$ are nonsingular, then

$$|J_{Y - X}| = (|\det A|^{n+1}(\det X)^{-(n+1)})|.$$

(d) If $X = X_1 + iX_2$ is Hermitian, then $Y = Y_1 + iY_2 = AXA'$ is Hermitian and $|J_{Y_1,Y_2 - X_1,X_2}| = |\det A|^{2n}$.

18.17. Let $A$ and $B$ be real nonsingular matrices, and assume that $A \otimes A \pm B \otimes B$ are nonsingular.

(a) The transformation $Y = AXA' \pm BXB'$ is one-to-one since, from (11.30),

$$\text{vech } Y = [H(A \otimes A \pm B \otimes B) \mathbf{G}] \text{vech } X.$$
The matrix in square brackets is nonsingular because, from (11.29c) and (11.29g), $H$ has full row rank and $G$ full column rank.

(i) If $\lambda_i$ (i = 1, 2, ..., n) are the eigenvalues of $AB^{-1}$, then

$$|J_{X \rightarrow Y}| = |(\det B)^{n+1} \prod_{i=1}^{n} \prod_{j=i}^{n} (1 \pm \lambda_i \lambda_j)|.$$

(ii) Alternatively, if $\alpha_i$ and $\beta_i$ (i = 1, 2, ..., n) are the eigenvalues of $A$ and $B$, respectively, then

$$|J_{X \rightarrow Y}| = \prod_{i=1}^{n} \prod_{j=i}^{n} (\alpha_i \alpha_j \pm \beta_i \beta_j)|.$$

When $B = 0$, it can be shown that the above result reduces to (18.16b).

(iii) If $A$ and $B$ are lower-triangular with respective diagonal elements $a_{ii}$ and $b_{ii}$, then

$$|J_{Y \rightarrow X}| = \prod_{i=1}^{n} \prod_{j=i}^{n} (a_{ii} a_{jj} \pm b_{ii} b_{jj})|.$$

This is the same as (ii) as the diagonal elements of a triangular matrix are its eigenvalues.

(b) If $Y = AXB' + BXA'$, then

$$|J_{X \rightarrow Y}| = |(\det B)^{n+1} \prod_{i=1}^{n} \prod_{j=i}^{n} (\lambda_i + \lambda_j)|,$$

where $\lambda_i$ (i = 1, 2, ..., n) are the eigenvalues of $AB^{-1}$. We need $B \otimes A + A \otimes B$ to be nonsingular for the transformation to be one-to-one.

18.18. Suppose $Y = X^{-1}$, where $X$ is nonsingular and symmetric.

(a) From (18.16c) with $A = I$, $|J_{Y \rightarrow X}| = |\det X|^{-(n+1)}$.

(b) If $X = X_1 + iX_2$ is Hermitian, then $Y = Y_1 + iY_2$ is also Hermitian and

$$|J_{Y_1, Y_2 \rightarrow X_1, X_2}| = |\det (XX^*)|^{-n} = |\det X|^{-2n}.$$

18.19. Let $Y = (\det X)X^{-1}$, where $X$ is positive definite. (The latter condition is sufficient for the transformation to be one-to-one.)

(a) We have:

(i) $\det Y = (\det X)^{n-1}$ and

$$|J_{Y \rightarrow X}| = (n-1)(\det X)^{(n+1)(n-2)/2}.$$

(ii) If $X = X_1 + iX_2$ is Hermitian and positive definite, and $Y = Y_1 + iY_2$, then

$$|J_{Y_1, Y_2 \rightarrow X_1, X_2}| = (n-1)|\det X|^{n(n-2)}.$$
(b) Suppose $Z = Y^{-1} = X / \det X$. Then

(i) $|J_{Z \rightarrow X}| = (n - 1)|\det X|^{-n(n+1)/2}$.

(ii) If $X = X_1 + iX_2$ is Hermitian and positive definite, and $Z = Z_1 + iZ_2$, then

$$|J_{Z_1, Z_2 \rightarrow X_1, X_2}| = (n - 1)|\det X|^{-n^2}.$$

18.20. Let $Y = X^k$, $k = 2, 3, \ldots$, and let $\lambda_i$ ($i = 1, 2, \ldots, n$) be the eigenvalues of $X$.

(a) (i) $|J_{Y \rightarrow X}| = k^n |(\det X)^{k-1}| \prod_{i=1}^{n} \prod_{j=i+1}^{n} |\mu_{ij}|$, where

$$\mu_{ij} = \begin{cases} \frac{\lambda_i^k - \lambda_j^k}{\lambda_i - \lambda_j}, & \text{if } \lambda_i \neq \lambda_j, \\ k\lambda_i^{k-1}, & \text{if } \lambda_i = \lambda_j. \end{cases}$$

(ii) If the eigenvalues are distinct, then $k^n(\det X)^{k-1} = \prod_{i=1}^{n} k\lambda_i^{k-1}$ and

$$|J_{Y \rightarrow X}| = \prod_{i=1}^{n} \prod_{j=i+1}^{n} \left|\frac{\lambda_i^k - \lambda_j^k}{\lambda_i - \lambda_j}\right| \prod_{i=1}^{n} k\lambda_i^{k-1}$$

$$= \prod_{i=1}^{n} \prod_{j=i+1}^{n} \left|\lambda_i^{k-1} + \lambda_i^{k-2}\lambda_j + \ldots + \lambda_j^{k-1}\right|$$

$$= \prod_{i=1}^{n} \prod_{j=i+1}^{n} \sum_{r=1}^{k} \lambda_i^{k-r}\lambda_j^{r-1}.$$

(b) When $k = 2$ we have:

(i)

$$|J_{Y \rightarrow X}| = \prod_{i=1}^{n} \prod_{j=i}^{n} |\lambda_i + \lambda_j|.$$

The transformation $Y = X^2$ is generally not one-to-one.

(ii) When $X = X_1 + iX_2$ is Hermitian, and $Y = Y_1 + iY_2$, then

$$|J_{Y_1, Y_2 \rightarrow X_1, X_2}| = 2^n |\det X| \prod_{i=1}^{n} \prod_{j=i+1}^{n} |\lambda_i + \lambda_j|^2.$$

18.21. If $Y = XAX$, where $A$ is symmetric, and $\lambda_i$ ($i = 1, 2, \ldots, n$) are the eigenvalues of $XA$, then, since $\det(XA) = \prod_i \lambda_i$, we have

$$|J_{Y \rightarrow X}| = 2^n |\det(A)\det(X)| \prod_{i=1}^{n} \prod_{j=i+1}^{n} (\lambda_i + \lambda_j) = \prod_{i=1}^{n} \prod_{j=i}^{n} (\lambda_i + \lambda_j)|.$$

If $A$ and $X$ are positive definite and the $\lambda_i$ are such that $\lambda_1 > \cdots > \lambda_n > 0$, then the transformation is one-to-one.
Proofs. Section 18.7.

18.16c. Mathai [1997: 60].
18.18b. Mathai [1997: 190].
18.19a(i). Deemer and Olkin [1951: 357, theorem 4.4; they also give the Jacobian of $Y^{-1}$ in corollary 4.4], Magnus [1988: 128], and Mathai [1997: 74].
18.19b(i). Mathai [1997: 75].

18.8 SKEW-SYMMETRIC AND SKEW-HERMITIAN MATRICES

Let $X$ and $Y$ be $n \times n$ matrices with $X$ real skew-symmetric, that is, $X' = -X$. Then, for the following transformations, $Y$ is also skew-symmetric. Note that if $X = X_1 + iX_2$ is skew-Hermitian, then $X_1$ is real skew-symmetric and $X_2$ is real symmetric.

18.22. If $Y = aX$, then $|J_{Y-X}| = |a|^{n(n-1)/2}$.

18.23. Let $Y = AXA'$. Then the following hold.

(a) $|J_{Y-X}| = (|\det A|)^{n-1}$.

(b) If $X = X_1 + iX_2$ is skew-Hermitian and $Y = Y_1 + iY_2 = AXA^*$, then $Y$ is skew-Hermitian and

$$|J_{Y-X}| = |\det(AXA^*)|^n = |\det A|^{2n},$$
18.24. Let $A$ and $B$ be nonsingular, and let $\lambda_i (i = 1, 2, \ldots, n)$ be the eigenvalues of $AB^{-1}$.

(a) If $Y = AXA' \pm BXB'$, then $|J_{X \rightarrow Y}| = |(\det B)^{-1} \prod_{i=1}^{n} \prod_{j=i+1}^{n} (1 \pm \lambda_i \lambda_j)|$. If $A$ and $B$ are lower-triangular, then

$$|J_{Y \rightarrow X}| = \prod_{i=1}^{n} \prod_{j=i+1}^{n} (a_{ii}a_{jj} \pm b_{ii}b_{jj}).$$

The above transformations are one-to-one if $(A \otimes A \pm B \otimes B)$ are nonsingular.

(b) If $Y = AXB' + BXA'$, then

$$|J_{X \rightarrow Y}| = |(\det B)^{-1} \prod_{i=1}^{n} \prod_{j=i+1}^{n} (\lambda_i + \lambda_j)|.$$

The above transformation is nonsingular if $(B \otimes A + A \otimes B)$ is nonsingular.

18.25. Let $Y = AX^{-1}A'$, where $A$ is nonsingular.

(a) $|J_{Y \rightarrow X}| = |\det A|^{n-1} |\det X|^{-(n-1)}$.

(b) If $Y = X^{-1}$, we can set $A = I$ in (a).

(i) $|J_{Y \rightarrow X}| = |\det X|^{-(n-1)}$.

(ii) If $X = X - 1 + iX_2$ is skew-Hermitian and $Y = Y_1 + iY_2$, then $|J_{Y_1 \rightarrow X_1, Y_2 \rightarrow X_2}| = |\det(XX^*)|^{-n} = |\det X|^{-2n}$, the same as for the Hermitian case of (18.18b).

18.26. If $Y = (\det X)X^{-1}$, where $\det X \neq 0$, then

$$|J_{Y \rightarrow X}| = (n - 1)|\det X|^{(n-1)(n-2)/2}.$$  

18.27. Let $Y = X^k$, $k = 3, 5, \ldots$, and let $\lambda_i (i = 1, 2, \ldots, n)$ be the eigenvalues of $X$. Then we have

$$|J_{Y \rightarrow X}| = \prod_{i=1}^{n} \prod_{j=i+1}^{n} \mu_{ij},$$

where

$$\mu_{ij} = \begin{cases}  \frac{(\lambda_i^k + \lambda_j^k)}{(\lambda_i + \lambda_j)}, & \text{if } \lambda_i \neq -\lambda_j, \\ k\lambda_i^{k-1}, & \text{if } \lambda_i = -\lambda_j. \end{cases}$$

If $Y = X^2$, then $Y$ is symmetric and the transformation is not one-to-one.

18.28. If $Y = XAX$, where $A$ is skew symmetric, then

$$|J_{Y \rightarrow X}| = \prod_{i=1}^{n} \prod_{j=i+1}^{n} (\lambda_i + \lambda_j),$$

where $\lambda_i (i = 1, 2, \ldots, n)$ are the eigenvalues of $XA$. 

Proofs. Section 18.8.


18.27. Magnus [1988: 136].


18.9 TRIANGULAR MATRICES

Any matrix with a “tilde”—for example, $\bar{X}$—will denote a $n \times n$ nonsingular lower-triangular matrix. Results for upper-triangular matrices can be obtained by taking transposes. In what follows we assume that the elements in the lower triangle of $\bar{X}$ are unconstrained (functionally independent). Also, the product of lower-triangular matrices is lower-triangular, and the inverse of a lower-triangular matrix is also lower-triangular.

18.9.1 Linear Transformations

18.29. Let $\bar{Y} = \bar{P} \bar{X} \bar{Q}$, where $\bar{P}$ and $\bar{Q}$ are lower-triangular and nonsingular.

(a) If the matrices are all real,

$$|J_{\bar{Y} \rightarrow \bar{X}}| = \prod_{i=1}^{n} p_{ii}^{i} q_{ii}^{n-i+1}|.$$

We get special cases by setting $\bar{P} = I_n$ or $\bar{Q} = I_n$.

(b) If the matrices are all complex (i.e., $\bar{Y} = \bar{Y}_1 + i\bar{Y}_2$, etc.), then we have the following results.

(i) If $\bar{Y} = \bar{P} \bar{X}$, then $|J_{\bar{Y}_1, \bar{Y}_2 \rightarrow \bar{X}_1, \bar{X}_2}| = \prod_{i=1}^{n} |p_{ii}|^{2i}$

(or $\prod_{i=1}^{n} |p_{ii}|^{2i-1}$ if the $p_{ii}$'s and $x_{ii}$'s are real).

(ii) If $\bar{Y} = \bar{X} \bar{Q}$, then $|J_{\bar{Y}_1, \bar{Y}_2 \rightarrow \bar{X}_1, \bar{X}_2}| = \prod_{i=1}^{n} |q_{ii}|^{2(n-i+1)}$

(or $\prod_{i=1}^{n} |q_{ii}|^{2(n-i)+1}$ if the $q_{ii}$'s and $x_{ii}$'s are real).
(c) Given real matrices, if $\tilde{X}$, and therefore $\tilde{Y}$, has fixed diagonal elements, then

$$|J_{\tilde{Y} \to \tilde{X}}| = \prod_{i=1}^{n} p_{ii}^{-1} q_{ii}^{n-i+1}.$$ 

(d) Given real matrices, if $\tilde{Y} = a\tilde{X}$, then

$$|J_{\tilde{Y} \to \tilde{X}}| = |a|^{n(n+1)/2}.$$ 

When the matrices and $a$ are complex, we get $|a|^{n(n+1)}$.

18.30. (Upper-Triangular) If $\tilde{Z} = \tilde{P}'\tilde{X}'\tilde{Q}'$, where $\tilde{P}$ and $\tilde{Q}$ are nonsingular, then $\tilde{Z}$ is upper-triangular.

(a) For real matrices,

$$|J_{\tilde{Z} \to \tilde{X}}| = \prod_{i=1}^{n} q_{ii}^{i-1} p_{ii}^{n-i+1}.$$ 

By interchanging $\tilde{P}$ and $\tilde{Q}$, taking the transpose, and noting that $|J_{\tilde{Z} \to \tilde{X}}| = |J_{\tilde{Z} \to \tilde{X}'}|$, we see that the above result is equivalent to (18.29a), but for upper-triangular matrices.

(b) The results for complex matrices are similar to those given in (18.29a) by transposing, and interchanging (i) and (ii).

18.31. Let $\tilde{Y} = \tilde{P}\tilde{X}\tilde{Q} + \tilde{R}\tilde{X}\tilde{S}$, where the matrices are all real.

(a) $|J_{\tilde{Y} \to \tilde{X}}| = \prod_{i=1}^{n} \prod_{j=1}^{i} (p_{ij}q_{jj} + r_{ij}s_{jj}).$

The transformation is one-to-one if $\tilde{Q}' \otimes \tilde{P} + \tilde{S}' \otimes \tilde{R}$ is nonsingular. Also, if $\tilde{R} = 0$,

$$\prod_{i=1}^{n} \prod_{j=1}^{i} (p_{ij}q_{jj}) = p_{11}(p_{22}q_{11}p_{22}q_{22})(p_{33}q_{11}p_{33}q_{22}p_{33}q_{33}) \cdots = \prod_{i=1}^{n} p_{ii} q_{ii}^{n-i+1},$$

as in (18.29a).

(b) If $\tilde{X}$ has fixed diagonal elements, then

$$|J_{\tilde{Y} \to \tilde{X}}| = \prod_{i=1}^{n} \prod_{j=1}^{i-1} (p_{ij}q_{jj} + r_{ij}s_{jj}).$$

Proofs. Section 18.9.1.


18.31b. Magnus [1988: 137].

18.9.2 Nonlinear Transformations of $X$

All matrices are real, unless otherwise stated.

18.32. Let $\tilde{Y} = \tilde{X}\hat{P}\tilde{X}$.

(a) $|J_{Y \to \tilde{X}}| = 2^n |(\det \hat{P})(\det \tilde{X}) \prod_{i=1}^{n} \prod_{j=i+1}^{n} (p_{ii}x_{ii} + p_{jj}x_{jj})|.$

(b) If $\tilde{X}$ has fixed diagonal elements, then

$$|J_{Y \to \tilde{X}}| = \prod_{i=1}^{n} \prod_{j=i+1}^{n} (p_{ii}x_{ii} + p_{jj}x_{jj})|.$$

18.33. Let $\tilde{Y} = \tilde{X}^{-1}$.

(a) We have

$$|J_{Y \to \tilde{X}}| = |\det \tilde{X}|^{-(n+1)} = |\prod_{i=1}^{n} x_{ii}^{-(n+1)}|.$$

(b) If $\tilde{X}$ has fixed diagonal elements, then

$$|J_{Y \to \tilde{X}}| = |\det \tilde{X}|^{-(n-1)} = |\prod_{i=1}^{n} x_{ii}^{-(n-1)}|.$$

18.34. Let $\tilde{Y} = (\det \tilde{X})\tilde{X}^{-1}$, where $\tilde{Y}$ and $\tilde{X}$ are both lower- or both upper-triangular matrices.

(a) Then $\det \tilde{Y} = (\det \tilde{X})^{n-1}$.

(i) $|J_{Y \to \tilde{X}}| = (n-1)|\det \tilde{X}|^{(n+1)(n-2)/2}$.

Note that $(\det \tilde{X})^{(n+1)(n-2)} > 0$ as $(n+1)(n-2)$ is divisible by 2, so we take the positive square root. For the transformation to be one-to-one, we assume $\det \tilde{X} > 0$ (for example, $x_{ii} > 0$ for all $i$) so that $\det \tilde{Y} > 0$, and define $\tilde{X} = (\det \tilde{Y})^{1/(n-1)}$, the $(n-1)$th positive root of $\det \tilde{Y}$. We can then write

$$|J_{Y \to \tilde{X}}| = (n-1) \prod_{i=1}^{n} x_{ii}^{(n+1)(n-2)/2}.$$
Similar comments apply to (b) and (c) below.

(ii) When $\tilde{X} = \tilde{X}_1 + i\tilde{X}_2$ is complex and $\tilde{Y} = \tilde{Y}_1 + i\tilde{Y}_2$, then

$$|J_{\tilde{Y}_1, \tilde{Y}_2 - \tilde{X}_1, \tilde{X}_2}| = (n - 1)|\det \tilde{X}|^{(n+1)(n-2)}.$$ 

(b) If $\tilde{X}$ has fixed diagonal elements, then

$$|J_{\tilde{Y} - \tilde{X}}| = (n - 1)(\det \tilde{X})^{(n-1)(n-2)/2}.$$ 

(c) If $\tilde{Z} = \tilde{Y}^{-1} = \tilde{X}/\det \tilde{X}$, then

(i) $|J_{\tilde{Z} - \tilde{X}}| = (n - 1)(\det \tilde{X})^{-n(n+1)/2}$.

(ii) When $\tilde{X} = \tilde{X}_1 + i\tilde{X}_2$ is complex and $\tilde{Z} = \tilde{Z}_1 + i\tilde{Z}_2$,

$$|J_{\tilde{Z}_1, \tilde{Z}_2 - \tilde{X}_1, \tilde{X}_2}| = (n - 1)|\det \tilde{X}|^{-n(n+1)}.$$

18.35. Let $\tilde{Y} = \tilde{X}^k$, $k = 2, 3, \ldots$

(a) $|J_{\tilde{Y} - \tilde{X}}| = k^n|(\det \tilde{X})^{k-1} \prod_{i=1}^{n} \prod_{j=i+1}^{n} \mu_{ij}|$, where

$$\mu_{ij} = \begin{cases} (x_{ii}^k - x_{jj}^k)/(x_{ii} - x_{jj}), & \text{if } x_{ii} \neq x_{jj}, \\ kx_{ii}^{k-1}, & \text{if } x_{ii} = x_{jj}. \end{cases}$$

(b) If $\tilde{X}$ has fixed diagonal elements, then

$$|J_{\tilde{Y} - \tilde{X}}| = \prod_{i=1}^{n} \prod_{j=i+1}^{n} \mu_{ij}|.$$

Proofs. Section 18.9.2.

18.34a(ii). Mathai [1997: 201].
18.34b. Magnus [1988: 137].
18.34c(i). Mathai [1997: 65].
18.9.3 Decompositions with One Skew-Symmetric Matrix

If $S$ is an $n \times n$ skew-symmetric matrix, then $I_n + S$ is nonsingular (cf. 5.19). Also, $T = 2(S + I_n)^{-1} - I_n$ is orthogonal and represents a one-to-one transformation as $S = 2(T + I_n)^{-1} - I_n$. (This is a special case of the Caley transformation mentioned in Section 18.12.) Any nonsingular matrix $Y$ can expressed in the form $Y = \bar{X}T$, where $\bar{X}$ is a nonsingular lower-triangular matrix. This representation is unique under two situations (Mathai [1997: 100]): (1) $x_{ii} > 0$ for $i = 1, 2, \ldots, n - 1$, and (2) the elements of $\bar{X}$ are unrestricted, but the elements of $S$ are restricted in some way. For example, the elements of the first row of $(S + I_n)^{-1}$, except the first, being of a specific sign such as all negative (Mathai [1997: 99]) or all positive (Deemer and Olkin [1951: 361]).

18.36. Assuming that the appropriate conditions above hold so that the representation $Y = \bar{X}[2(S + I_n)^{-1} - I_n] = \bar{X}(I_n - S)(I_n + S)^{-1}$ is unique (i.e., one-to-one), then

$$|J_{Y \rightarrow \bar{X},n}| = 2^n(n-1)/2 \left\{ \prod_{i=1}^{n} x_{ii}^{n-i} \right\} \det(S + I_n)^{-(n-1)}.$$

(Note that $YY' = \bar{X}\bar{X}'$.)

18.37. If $Y = T\bar{X}T'$ is a symmetric matrix, then transposing we have $Z = Y'$ and $\bar{X} = V'$. This implies that the absolute value of the Jacobian is the same as above.

18.38. Let $Y = T\Delta x(T')' = [2(S + I_n)^{-1} - I_n]D_x[2(S + I_n)^{-1} - I_n]'$ be a symmetric matrix, where $\Delta x = (x_1, x_2, \ldots, x_n)'$ with $x_1 > x_2 > \ldots > x_n$, and $D_x = \text{diag}(x)$. If the elements of the first row of $(S + I_n)^{-1}$ except the first are of a specific sign, then

$$|J_{x \rightarrow \Delta x, n}| = 2^n(n-1)/2 \left\{ \prod_{i=1}^{n} \prod_{j=i+1}^{n} (x_i - x_j) \right\} \det(S + I_n)^{-(n-1)} \prod_{i=1}^{n} \prod_{j=i+1}^{n} (x_i - x_j).$$

The decomposition of $Y$ is unique if we add the condition that $Y$ should not belong to a set of symmetric matrices that constitutes a set of measure zero in the $n(n+1)/2$-dimensional space. Olkin and Sampson [1972: 273] also quote the result, but their constant term is incorrectly inverted.

Proofs. Section 18.9.3.


18.9.4 Symmetric $Y$

18.39. Let $Y$ be symmetric, and let $\tilde{P} = (p_{ij})$ and $\tilde{X}$ be $n \times n$ nonsingular lower-triangular matrices. Conditions for the following transformations to be one-to-one can be found using vec and vech as in (18.11) and (18.17). For example, in (a) below, $\text{vec} Y = (I_{n^2} + I_{(n,n)})\text{vec} X$, where $I_{(n,n)}$ is the vec-permutation (commutation) matrix. We also have $\text{vech} Y = H_n \text{vec} Y$ and $\text{vec} X = G_n \text{vech} X$. The following matrices are all real, unless otherwise stated.

(a) If $Y = \tilde{X} + \tilde{X}'$, then $|J_{Y\rightarrow \tilde{X}}| = 2^n$.

(b) Suppose $\tilde{X} = \tilde{X}_1 + i\tilde{X}_2$ is complex.

(i) The Jacobian is either $2^{2n}$ or $2^n$ if the $x_{ii}$'s are real.

(ii) If $Y = \tilde{X} + \tilde{X}^*$, then $Y$ is now Hermitian and the transformation is no longer one-to-one unless the $x_{ii}$ are real. In the latter case the Jacobian is $2^n$.

(c) If $Y = \tilde{X}\tilde{P} + \tilde{P}'\tilde{X}'$ and $\tilde{P}$ is nonsingular, then

$$|J_{Y\rightarrow \tilde{X}}| = 2^n \prod_{i=1}^{n} |p_{ii}|^{n-i+1}.$$  

(d) If $Y = \tilde{P}\tilde{X} + \tilde{X}'\tilde{P}'$, then

$$|J_{Y\rightarrow \tilde{X}}| = 2^n |\prod_{i=1}^{n} |p_{ii}|^{i}|.$$  

(e) If $Y = \tilde{X}'\tilde{P} + \tilde{P}'\tilde{X}$, then

$$|J_{Y\rightarrow \tilde{X}}| = 2^n \prod_{i=1}^{n} |p_{ii}|^{i}.$$  

(f) If $Y = \tilde{P}\tilde{X}' + \tilde{X}\tilde{P}'$, then

$$|J_{Y\rightarrow \tilde{X}}| = 2^n \prod_{i=1}^{n} |p_{ii}|^{n-i+1}|.$$  

18.40. Let $Y$ be symmetric, and let $\tilde{P}$, $\tilde{Q}$, $\tilde{R}$, and $\tilde{X}$ be nonsingular lower-triangular matrices. Conditions for the following transformations to be one-to-one can be found using vec and vech.

(a) If $Y = \tilde{Q}'\tilde{X}\tilde{P} + \tilde{P}'\tilde{X}'\tilde{Q}$, then

$$|J_{Y\rightarrow \tilde{X}}| = 2^n |\det \tilde{P}(\det \tilde{Q})^{n} \prod_{i=1}^{n-1} \det C(i)|,$$

where $C(i)$ is the $i$th $(i \times i)$ leading principal minor of $C = \tilde{P}\tilde{Q}^{-1}$.
(b) If $Y = \tilde{R}'\tilde{Q}\tilde{X}\tilde{P} + \tilde{P}'\tilde{X}'\tilde{Q}'\tilde{R}$, then
\[
|J_{Y \rightarrow \tilde{x}}| = 2^n \prod_{i=1}^{n} (q_{ii} r_{ii})^{i \cdot n-i+1}.
\]

(c) If $Y = \tilde{R}\tilde{X}\tilde{P}Q' + Q\tilde{P}'\tilde{X}'\tilde{R}'$, then
\[
|J_{Y \rightarrow \tilde{x}}| = 2^n \prod_{i=1}^{n} (p_{ii} q_{ii})^{n-i+1} r_{ii}.
\]

**Proofs.** Section 18.9.4.


**18.9.5 Positive Definite $Y$**

**18.41.** Let $Y$ be positive definite, and let $\tilde{X}$ be lower-triangular and nonsingular, with positive diagonal elements (which implies the existence of a unique Cholesky decomposition).

(a) If $Y = \tilde{X}'\tilde{X}$, then
\[
|J_{Y \rightarrow \tilde{x}}| = 2^n \prod_{i=1}^{n} x_{ii}^i.
\]

(b) If $Y = \tilde{X}\tilde{X}'$, then
\[
|J_{Y \rightarrow \tilde{x}}| = 2^n \prod_{i=1}^{n} x_{ii}^{n-i+1}.
\]

(c) Let $Y = \tilde{X}\tilde{X}'$, where $y_{ii} = 1$, and $\sum_{j=1}^{i} x_{ij}^2 = 1$ ($i = 1, 2, \ldots, n$). Then
\[
|J_{Y \rightarrow \tilde{x}}| = \prod_{i=1}^{n} x_{ii}^{n-i}.
\]

**Proofs.** Section 18.9.5.

18.41c. Olkin [1953: 44, theorem 5].
18.9.6 Hermitian Positive Definite Y

18.42. Suppose $Y$ is an Hermitian positive definite matrix. Let $\tilde{X} = \tilde{X}_1 + i\tilde{X}_2$ be a complex lower-triangular matrix, with $\tilde{X}_i$ a real lower-triangular matrix ($i = 1, 2$), and let $V$ be a complex upper-triangular matrix. Both $X$ and $V$ are assumed to have real positive diagonal elements, which implies the existence of the unique Cholesky decompositions given below.

(a) If $Y = \tilde{X}\tilde{X}^*$, then $|J_{Y_{1,2}}| = 2^n \prod_{i=1}^{n} x_{ii}^{2(n-i)+1}$.

If, in addition, $y_{ii} = 1$ and $\sum_{k=1}^{i} x_{ik} \overline{x}_{ik} = \sum_{k=1}^{i} |x_{ik}|^2 = 1$ for $i = 1, 2, \ldots, n$, then

$$|J_{Y_{1,2}}| = \prod_{i=1}^{n} x_{ii}^{2(n-i)}, \quad x_{11} = 1.$$ 

(b) If $Y = VV^*$, then $|J_{Y_{1,2}}| = 2^n \prod_{i=1}^{n} v_{ii}^{2(i-1)+1}$.

If, in addition, $y_{ii} = 1$ and $\sum_{k=1}^{n} |v_{ik}|^2 = 1$ for $i = 1, 2, \ldots, n$, then

$$|J_{Y_{1,2}}| = \prod_{i=1}^{n} x_{ii}^{2(i-1)}, \quad x_{nn} = 1.$$ 

Proofs. Section 18.9.6.


18.9.7 Skew-Symmetric Y

18.43. Let $\tilde{X}$ be lower-triangular with fixed diagonal elements, let $\hat{P}$, $\hat{Q}$, and $\hat{R}$ be lower-triangular, and let $Y$ be skew-symmetric.

(a) If $Y = B'\tilde{X}A - A'\tilde{X}'B$, then

$$|J_{Y_{1,2}}| = |\det B^{n-1} \prod_{i=1}^{n-1} \det C(i)|,$$

where $C(i)$ is the $i$th $(i \times i)$ leading principal minor of $C = AB^{-1}$.

(b) If $Y = \hat{R}'\hat{Q}\tilde{X}\hat{P} - \hat{P}'\tilde{X}'\hat{Q}'\hat{R}$, then

$$|J_{Y_{1,2}}| = |\prod_{i=1}^{n} (q_{ii} r_{ii})^{i-1} p_{ii}^{n-i}|.$$ 

(c) If $Y = \tilde{R}\tilde{X}\tilde{P} \hat{Q}' - \hat{Q}'\tilde{X}'\tilde{P}'\hat{R}'$, then

$$|J_{Y_{1,2}}| = |\prod_{i=1}^{n} (p_{ii} q_{ii})^{n-i} r_{ii}^{i-1}|.$$ 

Proofs. Section 18.9.7.

18.43. Magnus [1988: 138].
18.9.8 LU Decomposition

18.44. Let $Y$ be any $n \times n$ nonsingular matrix. Then, from Section 16.4, $Y$ can be expressed uniquely as a lower-triangular $L$ with unit diagonal elements and an upper-triangular $U$, that is, $Y = LU$ (or $Y = UL$, with different $U$ and $L$). In general, if $L$ is lower-triangular with fixed diagonal elements (not necessarily equal to unity), then we have the following.

(a) If $Y = \tilde{L}U$, then $|J_{Y - \tilde{L}U}| = \prod_{i=1}^{n} l^{n-i}_i u^{n-i}_i$.

(b) If $Y = U\tilde{L}$, then $|J_{Y - \tilde{L}U}| = \prod_{i=1}^{n} l^{i}_i u^{i-1}_i$.

Proofs. Section 18.9.8.

18.44. Magnus [1988: 139]. The case when $\tilde{L}$ has unit diagonal elements is proved by Mathai [1997: 92].

18.10 DECOMPOSITIONS INVOLVING DIAGONAL MATRICES

18.10.1 Square Matrices

In what follows, we define $D_w = \text{diag}(w_1, w_2, \ldots, w_n)$, where the $w_i$ are functionally independent, distinct, and nonzero. We can also use $|J_{Y - Y'}| = 1$ for any matrix $Y$. Unless stated otherwise, all matrices are real. When all the matrices are complex, we assume that $X = X_1 + iX_2$, $w = w_1 + iw_2$, and $Y = Y_1 + iY_2$, where the $X_i$, $w_i$, and $Y_i$ are all real.

18.45. Let $X$ and $Y$ be $n \times n$ matrices with $X$ having unit diagonal elements.

(a) Let $Y = D_w X$.

(i) $|J_{Y - w,X}| = \prod_{i=1}^{n} |w_i|^{n-1}$. Since $x_{ij} = y_{ij}/y_{ii}$ for $i \neq j$, and $w_i = y_{ii}$ for all $i$, the transformation is one-to-one.

(ii) For complex matrices, $|J_{Y_1, Y_2 - w_1, w_2, X_1, X_2}| = \prod_{i=1}^{n} |w_i|^{2(n-1)}$. The result is still true if the $y_{ii}$ and $w_i$ are all real and positive.

(b) If $Y = XD_w$, we get the same answers as for (a).

(c) Let $Y = D_w XD_w$, with $y_{ii} > 0$ and $w_i > 0$ for $i = 1, 2, \ldots, n$.

(i) $|J_{Y - w,X}| = 2^n \prod_{i=1}^{n} w_i^{2n-1}$. The transformation is one-to-one as $w_i = \sqrt{y_{ii}}$ for all $i$ and $x_{ij} = y_{ij}/(\sqrt{y_{ii}} \sqrt{y_{jj}})$ for $i \neq j$.

(ii) For complex $X$ and $D_w$,

$$|J_{Y_1, Y_2 - w_1, w_2, X_1, X_2}| = 2^{2n} \prod_{i=1}^{n} |w_i|^{2(2n-1)}.$$

If $y_{ii}$ and $w_i$ are real and positive, the corresponding value is $2^n \prod_{i=1}^{n} w_i^{4n-3}$ when $Y = D_w XD_w$, and $2^n \prod_{i=1}^{n} w_i^{2n-1}$ when $Y = D_w XD_w^*$ with Hermitian $X$. The transformation is no longer one-to-one.
Proofs. Section 18.10.1.

18.45a(i). Mathai [1997: 86].
18.45c(i). Mathai [1997: 86].

18.10.2 One Triangular Matrix

18.46. Suppose $\tilde{Y}$ is a lower-triangular matrix and $\tilde{X}$ is lower-triangular with fixed diagonal elements (for example, unit elements). All matrices are real, unless otherwise stated. Note that $\det \tilde{X} = \prod_{i=1}^{n} x_{ii}$.

(a) Let $\tilde{Y} = D_w \tilde{X}$.

(i) We have
\[
|J_{\tilde{Y} \rightarrow w, \tilde{X}}| = |\det \tilde{X}| \prod_{i=1}^{n} |w_i|^{i-1}.
\]

(ii) If the matrices are complex and $\tilde{X} = \tilde{X}_1 + i\tilde{X}_2$ has unit diagonal elements, then
\[
|J_{\tilde{Y}_1, \tilde{Y}_2 \rightarrow w_1, w_2, \tilde{X}_1, \tilde{X}_2}| = \prod_{i=1}^{n} |w_i|^{2(1-i)}.
\]

(b) Let $\tilde{Y} = \tilde{X}D_w$.

(i) We have
\[
|J_{\tilde{Y} \rightarrow w, \tilde{X}}| = |\det \tilde{X}| \prod_{i=1}^{n} |w_i|^{n-i}.
\]

(ii) If the matrices are complex and $\tilde{X}$ has unit diagonal elements, then
\[
|J_{\tilde{Y}_1, \tilde{Y}_2 \rightarrow w_1, w_2, \tilde{X}_1, \tilde{X}_2}| = \prod_{i=1}^{n} |w_i|^{2(n-i)}.
\]

The above transformations are one-to-one. The results for upper-triangular matrices are obtained by taking the transposes of the above. For example, if $Z = UD_w = \tilde{X}'D_w$, where $Z$ and $U$ are upper-triangular, then $Z' = D_w \tilde{X}$ and the Jacobian is given by (a). If $Z = D_w U$, then the Jacobian is given by (b).

(c) Let $Y = XD_w \tilde{X}'$, then

(i) $|J_{Y \rightarrow w, \tilde{X}}| = (\det \tilde{X})^2 \prod_{i=1}^{n} |(w_i x_{ii})|^{n-i}$.

(ii) When $X$ has unit diagonal elements, the Jacobian becomes $\prod_{i=1}^{n} |w_i|^{n-i}$. This case is also given below.
18.47. Let \( \mathbf{X} \) be lower-triangular with unit diagonal elements, and suppose \( y_{ii} > 0 \) and \( w_i > 0 \) for \( i = 1, 2, \ldots, n \).

(a) If \( \mathbf{X} \) is real, we have the following Jacobians.

(i) If \( \mathbf{Y} = \mathbf{X} \mathbf{D}_w \mathbf{X}' \), then \( |J_{\mathbf{Y} \to \mathbf{w}, \mathbf{X}|} = \prod_{i=1}^{n} w_i^{n-i} \).

(ii) If \( \mathbf{Y} = \mathbf{X}' \mathbf{D}_w \mathbf{X} \), then \( |J_{\mathbf{Y} \to \mathbf{w}, \mathbf{X}|} = \prod_{i=1}^{n} w_i^{i-1} \).

(iii) If \( \mathbf{Y} = \mathbf{D}_w^{1/2} \mathbf{X} \mathbf{X}' \mathbf{D}_w^{1/2} \), then \( |J_{\mathbf{Y} \to \mathbf{w}, \mathbf{X}|} = \prod_{i=1}^{n} w_i^{(n-1)/2} \).

(iv) If \( \mathbf{Y} = \mathbf{D}_w^{1/2} \mathbf{X}' \mathbf{X} \mathbf{D}_w^{1/2} \), then \( |J_{\mathbf{Y} \to \mathbf{w}, \mathbf{X}|} = \prod_{i=1}^{n} w_i^{(n-1)/2} \), that is, the same as (iii).

The above transformations are one-to-one as we can express \( \mathbf{Y} \) (which is positive definite) in either the form \( \mathbf{Z} \mathbf{Z}' \) or \( \mathbf{Z}' \mathbf{Z} \), where \( \mathbf{Z} \) is lower-triangular with positive diagonal elements, that is, a unique Cholesky decomposition (Section 16.5).

To get the results for upper-triangular matrices, we simply write \( \mathbf{U} = \mathbf{X}' \). For example, if \( \mathbf{Y} = \mathbf{U} \mathbf{D}_w \mathbf{U}' \), the Jacobian is given by (ii) as \( |J_{\mathbf{X} \to \mathbf{U}}| = 1 \). Similarly, if \( \mathbf{Y} = \mathbf{U}' \mathbf{D}_w \mathbf{U} \), the Jacobian is given by (i).

(b) Suppose \( \mathbf{X} = \mathbf{X}_1 + i \mathbf{X}_2 \) is complex, but \( w_i > 0 \) for all \( i \). Then:

(i) If \( \mathbf{Y} = \mathbf{X} \mathbf{D}_w \mathbf{X}' \), then \( |J_{\mathbf{Y} \to \mathbf{w}, \mathbf{X}|} = \prod_{i=1}^{n} w_i^{2(n-i)} \).

(ii) If \( \mathbf{Y} = \mathbf{D}_w^{1/2} \mathbf{X} \mathbf{X}' \mathbf{D}_w^{1/2} \), then \( |J_{\mathbf{Y} \to \mathbf{w}, \mathbf{X}|} = \prod_{i=1}^{n} w_i^{n-1} \).

(c) Suppose \( \mathbf{U} = \mathbf{U}_1 + i \mathbf{U}_2 \) is upper-triangular and complex with unit diagonal elements, and the \( w_i \) are real, positive, and distinct for all \( i \).

(i) If \( \mathbf{Y} = \mathbf{U} \mathbf{D}_w \mathbf{U}' \), then \( |J_{\mathbf{Y} \to \mathbf{w}, \mathbf{U}|} = \prod_{i=1}^{n} w_i^{2(1-i)} \).

(ii) If \( \mathbf{Y} = \mathbf{D}_w^{1/2} \mathbf{U} \mathbf{U}' \mathbf{D}_w^{1/2} \), then \( |J_{\mathbf{Y} \to \mathbf{w}, \mathbf{U}|} = \prod_{i=1}^{n} w_i^{n-1} \).

18.48. Let \( \mathbf{Y} \) and \( \mathbf{X} \) be real nonsingular lower-triangular matrices with distinct, positive diagonal elements, and let \( \mathbf{Y} \) be a positive definite matrix. Also, suppose that \( \sum_{j=1}^{i} x_{ij}^2 = 1 \) \((i = 1, 2, \ldots, n)\), and the \( w_i \) \((i = 1, 2, \ldots, n)\) are distinct and positive.

(a) If \( \mathbf{Y} = \mathbf{D}_w \mathbf{X} \), then
\[
|J_{\mathbf{Y} \to \mathbf{w}, \mathbf{X}|} = \prod_{i=1}^{n} w_i^{i-1} x_{ii}^{-1}.
\]
(For the transformation to be one-to-one we require the condition \( w_i > 0 \) for all \( i \). To see this we set \( x_{ii} = (1 - \sum_{j=1}^{i-1} x_{ij}^2)^{1/2} \), which leads to \( w_i = (\sum_{j=1}^{i} y_{ij}^2)^{1/2} \) and \( x_{ij} = y_{ij}/w_i \) for \( i > j \), so that the inverse function exists.)

(b) If \( \mathbf{Y} = \mathbf{X} \mathbf{D}_w \), then \( |J_{\mathbf{Y} \to \mathbf{w}, \mathbf{X}|} = \prod_{i=1}^{n} w_i^{n-i} x_{ii}^{-1} \).

(c) If \( \mathbf{Y} = \mathbf{D}_w^{1/2} \mathbf{X} \), then \( |J_{\mathbf{Y} \to \mathbf{w}, \mathbf{X}|} = 2^{-n} \prod_{i=1}^{n} (w_i^{1/2})^{i-2} x_{ii}^{-1} \). (This follows from (a) by replacing \( w_i \) by \( w_i^{1/2} \) and noting that \( dw_i^{1/2} = \frac{1}{2} w_i^{-1/2} dw_i \).)

(d) If \( \mathbf{Y} = \mathbf{X} \mathbf{D}_w^{1/2} \), then \( |J_{\mathbf{Y} \to \mathbf{w}, \mathbf{X}|} = 2^{-n} \prod_{i=1}^{n} (w_i^{1/2})^{n-i-1} x_{ii}^{-1} \).
(e) If \( Y = D_w^{1/2} \tilde{X}' D_w^{1/2} \), then \( |J_{Y \rightarrow w, \tilde{X}}| = \prod_{i=1}^{n} w_i^{(n-1)/2} x_{ii}^{n-i} \).

(f) If \( Y = D_w^{1/2} \tilde{X}' D_w^{1/2} \), then \( J_{Y \rightarrow w, \tilde{X}} = \prod_{i=1}^{n} w_i^{(n-1)/2} x_{ii}^{n-i} \).

(g) If \( Y = \tilde{X}' D_w \tilde{X} \), then \( |J_{Y \rightarrow w, \tilde{X}}| = \prod_{i=1}^{n} (w_i x_{ii})^{i-1} \).

(h) If \( Y = \tilde{X} D_w \tilde{X}' \), then \( |J_{Y \rightarrow w, \tilde{X}}| = \prod_{i=1}^{n} (w_i x_{ii})^{n-i} \).

(i) If \( \tilde{X} \) is complex and \( \sum_{j=1}^{i} |x_{ij}|^2 = 1 \), we replace \( w_i \) by \( w_i^2 \) in the Jacobians for (a) and (b).

**Proofs.** Section 18.10.2.

18.46a(i). Magnus [1988: 141].
18.46a(ii). Mathai [1997: 211].
18.46b(i). Magnus [1988: 141].
18.46b(ii). Mathai [1997: 211].
18.46c(i). Magnus [1988: 141].
18.46c(ii). Olkin [1953: 45].

### 18.10.3 Symmetric and Skew-Symmetric Matrices

18.49. Let \( Y = D_w X D_w \), where \( X \) is symmetric with \( x_{ii} = 1 \) (\( i = 1, 2, \ldots, n \)) and \( D_w = \text{diag}(w) \), with the \( w_i \) being distinct. Then

\[
|J_{Y \rightarrow w, X}| = 2^n \prod_{i=1}^{n} |w_i|^n.
\]

If we also add \( w_i > 0 \) for each \( i \), then \( w_i = \sqrt{y_{ii}} \) and \( x_{ij} = y_{ij}/(\sqrt{y_{ii}} \sqrt{y_{jj}}) \) so that the transformation is one-to-one as the inverse function exists.

18.50. Let \( Y = D_x + D_p X - X D_p \), where \( X \) is skew symmetric and \( D_p = \text{diag}(p_1, p_2, \ldots, p_n) \) is fixed. Then

\[
|J_{Y \rightarrow X, X}| = \prod_{i=1}^{n} \prod_{j=i+1}^{n} |p_i - p_j|.
\]

**Proofs.** Section 18.10.3.

18.50. Magnus [1988: 140].
18.11 POSITIVE DEFINITE MATRICES

18.51. If \( Y = (\det X)X^{-1} \), where \( X \) (and therefore \( Y \)), is positive definite, then

\[
|J_{Y \rightarrow X}| = (n - 1)(\det X)^{(n+1)(n-2)/2}.
\]

18.52. Let \( Y = XAX \), where all three matrices are positive definite. Then

\[
|J_{Y \rightarrow X}| = \prod_{i=1}^{n} \prod_{j=i}^{n} (\lambda_i + \lambda_j),
\]

where the \( \lambda_i \) are the eigenvalues of \( XA \), and are positive. An important special case is when \( A = I_n \) and \( X \) is the positive definite square root of \( Y \).

18.53. If \( Y = X^k \), where \( k = 2, 3, \ldots \), and \( X \) is positive definite with distinct eigenvalues \( \lambda_i \), then \( Y \) is positive definite and \( |J_{Y \rightarrow X}| \) is given by (18.20). Let \((Y)^{1/k}\) denote the \( k \)th positive definite root of \( Y \), and \( \mu_j \) \((j = 1, 2, \ldots, n)\) the eigenvalues of \( Y \). Then the transformation \( Y = X^k \) is one-to-one, and \( |J_{Y \rightarrow X}| \) can be expressed in terms of \( Y \) by noting that \( \det X = (\det Y)^{1/k} \) and \( \lambda_j = \mu_j^{1/k} \).

Proofs. Section 18.11.


18.52. Olkin and Sampson [1972: 269].

18.53. Mathai [1997: 98, example 2.5].

18.12 CALEY TRANSFORMATION

18.54. In this section we consider a particular transformation, called the Caley transformation, for nonsymmetric, symmetric, and triangular matrices, and their complex versions.

(a) Let \( Y = (A + X)^{-1}(A - X) \), where the matrices are \( n \times n \) and inverses exist so that the transformation is one-to-one.

(i) For real matrices we have

\[
|J_{Y \rightarrow X}| = 2^n^2 (|\det A|)^n (|\det (A + X)|)^{-2n}.
\]

The same result holds for \( Y = (A - X)(A + X)^{-1} \).

(ii) If the matrices are complex, we replace \( A \) by \( AA^* \), \( A + X \) by \( (A + X)(A^* + X^*) \), and \( 2^n^2 \) by \( 2^{2n^2} \) to get \( |J_{Y_1, Y_2 \rightarrow X_1, X_2}| \).

(b) Let \( Y = (I_n + X)^{-1}(I_n - X) = 2(I_n + X)^{-1} - I_n \), where \( X \) and \( Y \) are symmetric.

(i) \( |J_{X \rightarrow Y}| = 2^{n(n+1)/2} |\det (I_n + X)|^{-(n+1)} \).
(ii) If $X = X_1 + iX_2$ is Hermitian and $Y = Y_1 + iY_2$, then
\[
|J_{Y_1,Y_2 \to X_1,X_2}| = 2^{n^2} \left| \det \left\{ (I_n + X)(I_n + X^*) \right\} \right|^{-n}.
\]

(c) Let $\tilde{Y} = (\tilde{A} + \tilde{X})^{-1}(\tilde{A} - \tilde{X})$, where $\tilde{X}$, $\tilde{A}$, and $\tilde{Y}$ are all lower-triangular, $\tilde{A}$ and $\tilde{A} + \tilde{X}$ are nonsingular, and all matrices are real. Then
\[
|J_{\tilde{X} \to \tilde{Y}}| = 2^{n(n+1)/2} \left| \det (\tilde{A} + \tilde{X}) \right|^{-(n+1)} \prod_{i=1}^{n} |a_{ii}|^{n-i+1},
\]
where $\det(\tilde{A} + \tilde{X}) = \prod_{i=1}^{n} (a_{ii} + x_{ii})$. When the matrices are upper-triangular, we see, by taking transposes, that the Jacobian is given by (d).

(d) Let $\tilde{Y} = (\tilde{A} - \tilde{X})(\tilde{A} + \tilde{X})^{-1}$, where $\tilde{X}$, $\tilde{A}$, and $\tilde{Y}$ are all lower-triangular, $\tilde{A}$ and $\tilde{A} + \tilde{X}$ are nonsingular, and all matrices are real. Then
\[
|J_{\tilde{X} \to \tilde{Y}}| = 2^{n(n+1)/2} \left| \det (\tilde{A} + \tilde{Y}) \right|^{-(n+1)} \prod_{i=1}^{n} |a_{ii}|^{i}.
\]

When the matrices are all upper-triangular, the equation then becomes $\tilde{Y}' = (\tilde{A}' - \tilde{X}') (\tilde{A}' + \tilde{X})^{-1}$ so that, taking transposes, we get $\tilde{Y} = (\tilde{A} + \tilde{X})^{-1}(\tilde{A} - \tilde{X})$, and the Jacobian is given by (c) above. We now look at the complex versions of (c) and (d).

18.55. Let $\tilde{X}$, $\tilde{A}$, and $\tilde{Y}$ be complex lower-triangular matrices with $\tilde{A}$ and $\tilde{A} + \tilde{X}$ nonsingular, and $\tilde{Y} = \tilde{Y}_1 + i\tilde{Y}_2$ etc.

(a) Let $\tilde{Y} = (\tilde{A} + \tilde{X})^{-1}(\tilde{A} - \tilde{X})$.

(i) If all the elements are complex
\[
|J_{\tilde{Y}_1,\tilde{Y}_2 \to \tilde{X}_1,\tilde{X}_2}| = 2^{n(n+1)} \left| \det \left\{ (\tilde{A} + \tilde{X})(\tilde{A} + \tilde{X})^* \right\} \right|^{-(n+1)} \prod_{i=1}^{n} |a_{ii}|^{2(n-i+1)}.
\]

(ii) If all the diagonal elements of $\tilde{X}$ and $\tilde{A}$ are real and the others complex, then
\[
|J_{\tilde{Y}_1,\tilde{Y}_2 \to \tilde{X}_1,\tilde{X}_2}| = 2^{n^2} \prod_{i=1}^{n} |a_{ii} + x_{ii}|^{-2n} \prod_{i=1}^{n} |a_{ii}|^{2(n-i)+1}.
\]

When the matrices are upper-triangular, we find, by taking transposes, that the Jacobians are given by (b) below.

(b) Let $\tilde{Y} = (\tilde{A} - \tilde{X})(\tilde{A} + \tilde{X})^{-1}$. Then:

(i) If all the elements are complex,
\[
|J_{\tilde{Y}_1,\tilde{Y}_2 \to \tilde{X}_1,\tilde{X}_2}| = 2^{n(n+1)} \left| \det \left\{ (\tilde{A} + \tilde{X})(\tilde{A} + \tilde{X})^* \right\} \right|^{-(n+1)} \prod_{i=1}^{n} |a_{ii}|^{2i}.
\]
(ii) If the diagonal elements of $\tilde{X}$ and $\tilde{A}$ are real and the other elements complex, then

$$|J_{\tilde{Y}_1, \tilde{Y}_2 \rightarrow \tilde{X}_1, \tilde{X}_2}| = 2^{2n^2} \prod_{i=1}^{n} |a_{ii} + x_{ii}|^{-2n} \prod_{i=1}^{n} |a_{ii}|^{2i-1}.$$  

When the matrices are upper-triangular, we find, by taking transposes, that the Jacobians are given by (a) above.

**Proofs.** Section 18.12.

18.54a(i). Mathai [1997: 61] and Olkin [1953: 45].

18.54a(ii). Mathai [1997: 193].

18.54b(i). Mathai [1997: 61] and Olkin [1953: 45].

18.54b(ii). Mathai [1997: 193].


### 18.13 DIAGONALIZABLE MATRICES

18.56. Let $X$ be a nonsingular diagonalizable matrix with real distinct eigenvalues $\lambda_1 > \lambda_2 > \ldots > \lambda_n > 0$, that is, there exists a nonsingular $R$ such that $X = RD_{\lambda}R^{-1}$, where $D_{\lambda} = \text{diag}(\lambda_1, \lambda_2, \ldots, \lambda_n)$. Let $Y = F(X)$, where $F$ is such that $F(X) = RD_{f(\lambda)}R^{-1}$, $f$ is differentiable, and $D_{f(\lambda)} = \text{diag}(f(\lambda_1), f(\lambda_2), \ldots, f(\lambda_n))$. Then, assuming $f(\lambda_i) - f(\lambda_j) \neq 0$ and $f'(\lambda_i) \neq 0$ for all $i \neq j$ ($i, j = 1, 2, \ldots, n$),

(a) $|J_{Y \rightarrow X}| = \prod_{i=1}^{n} \prod_{j=i+1}^{n} \left\{ \frac{f(\lambda_i) - f(\lambda_j)}{\lambda_i - \lambda_j} \right\}^2 \prod_{i=1}^{n} \frac{df(\lambda_i)}{d\lambda_i} |$.

(b) For example, if $Y = X^k$, $k$ a positive integer, then with $f(\lambda) = \lambda^k$,

$$X^k = (RD_{\lambda}R^{-1})(RD_{\lambda}R^{-1}) \cdots (RD_{\lambda}R^{-1}) = RD_{\lambda^k}R^{-1} (= RD_{f(\lambda)}R^{-1}).$$

Hence

$$|J_{Y \rightarrow X}| = \prod_{i=1}^{n} \prod_{j=i+1}^{n} \left\{ \frac{\lambda_i^k - \lambda_j^k}{\lambda_i - \lambda_j} \right\}^2 \prod_{i=1}^{n} k\lambda_i^{k-1}$$

$$= \prod_{i=1}^{n} \prod_{j=1}^{n} (\lambda_i^{k-1} + \lambda_i^{k-2}\lambda_j + \ldots + \lambda_j^{k-1})$$

$$= \prod_{i=1}^{n} \prod_{j=1}^{n} \sum_{r=1}^{k} \lambda_i^{k-r}\lambda_j^{r-1}.$$
The reader is also referred to (18.15a).

(c) In some applications, \( Y \) is a random matrix whose eigenvalues are distinct with probability 1. The Jacobian \( |J_{X-Y}| \) is then given by \( |J_{Y-X}|^{-1} \), but it is expressed in terms of the eigenvalues of \( X \) rather than \( Y \), which is not so convenient in applications.

(d) If \( X \) is symmetric, then

\[
|J_{Y-X}| = \prod_{i=1}^{n} \prod_{j=i+1}^{n} \left\{ \frac{f(\lambda_i) - f(\lambda_j)}{\lambda_i - \lambda_j} \right\} \prod_{i=1}^{n} \frac{df(\lambda_i)}{d\lambda_i}.
\]

Proofs. Section 18.13.


18.56b. Henderson and Searle [1979: 73].


18.14 PAIRS OF MATRICES

18.57. Let \( Y_1 \) and \( Y_2 \) be positive definite \( n \times n \) matrices. If \( \det(Y_1 - \lambda Y_2) = 0 \) has \( n \) distinct roots \( \lambda_1 > \lambda_2 > \ldots > \lambda_n > 0 \), there exists a unique matrix \( W = (w_{ij}) \), with \( w_{ii} > 0 \) (\( i = 1, 2, \ldots, n \)), such that \( Y_1 = W D_1 W' \), \( Y_2 = W W' \), and \( D_1 = \text{diag}(\lambda_1, \ldots, \lambda_n) \) (cf. 16.51c). Then

\[
|J_{Y_1, Y_2 \rightarrow W, D_1}| = 2^n |\det W|^{n+2} \prod_{i=1}^{n} \prod_{j=i+1}^{n} (\lambda_i - \lambda_j).
\]

18.58. Let \( X_1 \) and \( X_2 \) be positive definite.

(a) If \( Y_1 = X_2^{-1/2} X_1 X_2^{-1/2} \) and \( Y_2 = X_2 \), then \( Y_1 \) and \( Y_2 \) are positive definite and

\[
|J_{Y_1, Y_2 \rightarrow X_1, X_2}| = |\det X_2|^{-(n+1)/2}.
\]

(b) If \( Y_1 = (X_1 + X_2)^{-1/2} X_1 (X_1 + X_2)^{-1/2} \) and \( Y_2 = X_1 + X_2 \), then \( Y_1 \) and \( Y_2 \) are positive definite and

\[
|J_{Y_1, Y_2 \rightarrow X_1, X_2}| = |\det(X_1 + X_2)|^{-(n+1)/2}.
\]

18.59. Let \( X_1 \) and \( X_2 \) be \( n \times n \) positive definite matrices. If \( Y_1 = X_1 \) and \( Y_2 = X_1 + X_2 \), then \( Y_1 \) and \( Y_2 \) are positive definite and there exists a nonsingular \( V \) such that \( Y_1 = V D_1 V' \), \( Y_2 = V V' \), and \( D_1 = \text{diag}(\phi_1, \ldots, \phi_n) \), where \( 1 > \phi_1 > \phi_2 > \ldots > \phi_n > 0 \) are the roots of \( \det(X_1 - \phi(X_1 + X_2)) = 0 \). Then (cf. 18.57)

\[
|J_{Y_1, Y_2 \rightarrow V, D_1}| = 2^n |\det V|^{n+2} \prod_{i=1}^{n} \prod_{j=i+1}^{n} (\phi_i - \phi_j)|.

18.57. Deemer and Olkin [1951: 350].


Asymptotic theory and large sample approximations play a key role in statistical distribution theory. In this chapter we apply some of the theory of limits to vectors and matrices.

19.1 LIMITS

**Definition 19.1.** Let \( A(t) = (a_{ij}(t)) \). We say that \( \lim_{t \to t_0} A(t) = A \) if \( a_{ij}(t) \to a_{ij} \) for all \( i, j \). Of particular interest is the case when \( t = \epsilon \) and \( t_0 = 0 \), as in the following result.

19.1. Suppose \( A = (a_{ij}) \) is nonsingular,

(a) The elements of \( A^{-1} \) are continuous functions of the \( a_{ij} \).

(b) If \( \lim_{\epsilon \to 0} A(\epsilon) = A \), then \( \lim_{\epsilon \to 0}[A(\epsilon)]^{-1} = A^{-1} \).

(c) \( \lim_{\epsilon \to 0}(A - \epsilon I)^{-1} = A^{-1} \).

(d) If \( A \) is \( m \times n \) and \( B \) is \( n \times m \), both independent of \( \epsilon \), then

\[
\lim_{\epsilon \to 0} \left( \begin{array}{cc} I_m & \epsilon A \\ \epsilon B & I_n \end{array} \right)^{-1} = I_{m+n}.
\]
19.2. (Continuity Argument) A number of matrix results can be proved by taking limits when continuity can be assumed, as was the case in (19.1) above. For example, a particular result may be true for a nonsingular matrix $A$. If $A$ is singular, we can choose $\epsilon > 0$ such that $A + \epsilon I$ is nonsingular (Abadir and Magnus [2005: 165]), set up the appropriate equation, and then let $\epsilon \to 0$. We may find that the result is then true for singular matrices. For an example of this technique see Zhang [1999: 56].

Proofs. Section 19.1.


19.2 SEQUENCES

Sequences of vectors and matrices occur in many parts of statistics, especially in the development of asymptotic results. In particular, we are often interested in the limit of powers of matrices, as in stochastic processes where the focus is on transition matrices. We first of all consider convergence of a sequence of vectors with respect to a norm.

**Definition 19.2.** Let $V$ be a vector space over $F$, and let $\| \cdot \|$ be a norm on $V$. We say that the sequence of vectors $\{x^{(k)}\}$ in $V$ converges with respect to the norm to a vector $x \in V$ if and only if $\|x^{(k)} - x\| \to 0$ as $k \to \infty$. It should be noted that $x$ is just an element of a vector space so that it can be regarded as either a real or complex vector or matrix, with an appropriate norm.

19.3. From (4.54) we see that if the sequence $\{x^{(k)}\}$ converges to a vector $x$ for one vector norm, it converges to $x$ for any vector norm. Choosing the $L_\infty$ norm we see that, for all vector norms on $\mathbb{R}^n$ or $\mathbb{C}^n$, $\lim_{k \to \infty} x^{(k)} = x$ with respect to any vector norm if and only if

$$\lim_{k \to \infty} x^{(k)}_i = x_i, \text{ for all } i = 1, 2, \ldots, n.$$  

The extension from vectors to matrices is straightforward.

**Definition 19.3.** Let $\{A_k\}$ ($k = 1, 2, \ldots$) be a sequence of $m \times n$ matrices, and let $a_{ij}^{(k)}$ denote the $(i, j)$th element of $A_k$. The sequence $\{A_k\}$ converges to $A = (a_{ij})$, that is $\lim_{k \to \infty} A_k = A$, if

$$\lim_{k \to \infty} a_{ij}^{(k)} = a_{ij} \quad \text{for all } i, j.$$  

A sequence that does not converge is said to diverge. The same definitions obviously apply to vectors as well. We shall assume that $m = n$, unless otherwise stated. If $A$ is a square matrix and $\lim_{k \to \infty} A^k = 0$, then we say that $A$ is convergent.

19.4. Using the above notation, suppose $\lim_{k \to \infty} A_k = A$ and $\lim_{k \to \infty} B_k = B$. Let $\alpha$ and $\beta$ be any constants, and let $P$ and $Q$ be any $n \times n$ matrices. From the limiting properties of scalars, the following results are straightforward.

(a) $\lim_{k \to \infty} (\alpha A_k + \beta B_k) = \alpha A + \beta B$. 


(b) \( \lim_{k \to \infty} A_k B_k = AB \).

(c) \( \lim_{k \to \infty} PA_k Q = PAQ \).

19.5. The sequence \( \{A^k\} \) converges if and only if the following hold.

1. Each eigenvalue \( \lambda \) of \( A \) satisfies either \( |\lambda| < 1 \) or \( \lambda = 1 \).

2. When \( \lambda = 1 \) occurs, the algebraic and geometric multiplicities of the eigenvalue 1 are the same.

19.6. If there is a matrix norm \( \|\cdot\| \) such that \( \|A\| < 1 \), then \( A \) is convergent.

19.7. \( A \) is convergent if and only if all the eigenvalues \( \lambda \) are less than 1 in modulus (i.e., \( \rho(A) < 1 \), where \( \rho(A) \) is the spectral radius of \( A \)).

19.8. If the eigenvalue 1 occurs with algebraic and geometric multiplicity \( t \) (i.e., is semisimple), and all other eigenvalues are less than 1 in modulus, then

\[
\lim_{k \to \infty} A^k = X(Y'X)^{-1}Y',
\]

where \( X \) and \( Y \) are the \( n \times t \) matrices of \( t \) linearly independent right, respectively, left eigenvectors associated with the eigenvalue 1.

19.9. Let \( A \) be \( n \times n \), let \( \{A_k\} \) \( (k = 1, 2, \ldots) \) be a sequence of real \( n \times n \) matrices, and let \( \|\cdot\|_{p, in} \) be an matrix norm induced by the \( L_p \) vector norm. If \( p = 1, 2, \) or \( \infty \) (cf. 4.74), then

(a) \( \lim_{k \to \infty} A_k = 0 \) if and only if \( \lim_{k \to \infty} \|A_k\|_{p, in} = 0 \).

(b) \( \lim_{k \to \infty} A_k = A \) if and only if \( \lim_{k \to \infty} \|A_k - A\|_{p, in} = 0 \). If we use \( \|A_k - A\|_F \), then this result also applies to \( m \times n \) matrices; cf. Harville [1997: 431].

(c) If \( \lim_{k \to \infty} A_k = A \), then \( \lim_{k \to \infty} \|A_k\|_{p, in} = \|A\|_{p, in} \). (The converse may not be true.)

19.10. The following result is useful in the context of limits. Suppose \( C \) is a square matrix and \( (I - C)^{-1} \) exists. If

\[
A = \begin{pmatrix} I & 0 \\ B & C \end{pmatrix}, \quad \text{then} \quad A^k = \begin{pmatrix} I & 0 \\ (I - C)^{-1}(I - C^k)B & C^k \end{pmatrix}.
\]

19.11. If \( \|\cdot\| \) is any matrix norm, then

\[
\rho(A) = \lim_{k \to \infty} \|A^k\|^{1/k},
\]

where \( \rho \) is the spectral radius.

Proofs. Section 19.2.

19.3. Horn and Johnson [1985: 273].


19.10. We use (19.14).


19.3 ASYMPTOTICALLY EQUIVALENT SEQUENCES

There are situations where an $n \times n$ matrix $A$ is difficult to work with, but a related matrix is easier to use that gives approximately the same result when $n$ is large. This idea is made rigorous below.

**Definition 19.4.** Let $\{A(k)\}$ and $\{B(k)\}$ be two sequences of real matrices, where $A(k)$ and $B(k)$ are both $k \times k$, and let $\|\|A\|\|_p$ denote a matrix norm. The two sequences of matrices are defined to be *asymptotically equivalent* if and only if they satisfy the following two conditions (Graybill [1983: 101]).

1. $\|\|A(k)\|\|_2 \leq c < \infty$, $\|\|B(k)\|\|_2 \leq c < \infty$ for $k = 1, 2, \ldots$, where $c$ is a real number that does not depend on $k$.

2. $\lim_{k \to \infty} k^{1/2}\|\|A(k) - B(k)\|\|_F = 0$.

19.12. Let $\{A(k)\}$ and $\{B(k)\}$ be two asymptotically equivalent sequences of $k \times k$ matrices.

(a) Then $\lim_{k \to \infty} k^{-1/2}\|\|A(k)\|\|_F = \lim_{k \to \infty} k^{-1/2}\|\|B(k)\|\|_F$.

(b) Suppose $A^{-1}(k)$ and $B^{-1}(k)$ exist for each $k = 1, 2, \ldots$. If $\|\|A(k)\|\|_2 \leq c < \infty$ and $\|\|B(k)\|\|_2 \leq c < \infty$ for $k = 1, 2, \ldots$, where $c$ is a real number that does not depend on $k$, then $\{A^{-1}(k)\}$ and $\{B^{-1}(k)\}$ are asymptotically equivalent.

19.13. Let $\{A(k)\}$, $\{B(k)\}$, $\{F(k)\}$, and $\{G(k)\}$ be sequences of $k \times k$ matrices.

(a) If $\{A(k)\}$ is asymptotically equivalent to $\{B(k)\}$, and $\{F(k)\}$ is asymptotically equivalent to $\{G(k)\}$, then $\{A(k)F(k)\}$ is asymptotically equivalent to $\{B(k)G(k)\}$.

(b) If, in (a), $\{B(k)\}$ is asymptotically equivalent to $\{C(k)\}$, then $\{A(k)\}$ is asymptotically equivalent to $\{C(k)\}$.

(c) If $\{A(k)B(k)\}$ is asymptotically equivalent to $\{D(k)\}$, and $\|\|A^{-1}(k)\|\|_2 \leq c < \infty$, where $c$ is a constant that does not depend on $k$, then $\{B(k)\}$ is asymptotically equivalent to $\{A^{-1}(k)D(k)\}$.

**Proofs.** Section 19.3.


19.4 SERIES

Definition 19.5. Let \( S_k = A_1 + A_2 + \cdots + A_k \), where the \( A_i \) are \( n \times n \). The series \( S_k \) is said to converge to, or have sum, \( S \) if \( \lim_{k \to \infty} S_k = S \); we write \( S = \sum_{k=1}^{\infty} A_k \).

A series that does not converge is said to diverge. (In what follows we recall that \( \rho(A) \) is the spectral radius of \( A \).)

19.14. If \( S_k = I_n + A + A^2 + \cdots + A^k \), then

\[
S_k = (I_n - A)^{-1}(I_n - A^{k+1}) = (I_n - A^{k+1})(I_n - A)^{-1},
\]

provided \( (I_n - A)^{-1} \) exists.

19.15. The following conditions are equivalent.

1. (Newmann Series) \( I_n + A + A^2 + \cdots \) converges.

2. \( \rho(A) < 1 \).

3. \( \lim_{k \to \infty} A^k = 0 \), that is, \( A \) is convergent.

Moreover, when one (and hence all) of these conditions are satisfied, then

(a) \( I_n - A \) is nonsingular.

(b) \( I_n + A + A^2 + \cdots \) converges to \( (I_n - A)^{-1} \).

19.16. Let \( A \in \mathcal{V} \) be the vector space of \( n \times n \) matrices, and let \( ||| \cdot ||| \) be any matrix norm defined on \( \mathcal{V} \).

(a) If \( |||A||| < 1 \), then \( (I_n - A)^{-1} \) exists and is given by

\[
(I_n - A)^{-1} = \sum_{k=0}^{\infty} A^k.
\]

We can obtain another result by setting \( A = I_n - B \).

(b) Suppose \( B \in \mathcal{V} \) and \( B \) is nonsingular. If \( F = B^{-1}A \), then the infinite series \( B^{-1} + FB^{-1} + F^2B^{-1} + \cdots \) converges if and only if \( \lim_{k \to \infty} F^k = 0 \), in which case \( B - A \) is nonsingular and

\[
(B - A)^{-1} = \sum_{k=0}^{\infty} F^k B^{-1}.
\]

Replacing \( A \) by \( -A \) we get

\[
(A + B)^{-1} = \left( \sum_{k=0}^{\infty} (-B^{-1}A)^k \right) B^{-1}.
\]

If \( A \) is small, we have the approximation \( (A + B)^{-1} \approx B^{-1} - B^{-1}AB^{-1} \).

If \( A \) is the matrix that is nonsingular, we interchange \( A \) and \( B \).

(c) If \( \{a_k\}, k = 0, 1, \ldots \) is a sequence of scalars, then \( \sum_{k=0}^{\infty} a_k A^k \) converges if the series \( \sum_{k=0}^{\infty} |a_k| \cdot |||A|||^k \) of real numbers converges; \( A^0 = I_n \).
(d) \( \sum_{k=0}^{\infty} \alpha_k A^k \) converges absolutely if \( \sum_{k=0}^{\infty} |\alpha_k| \rho^k < \infty \), where \( \rho = \rho(A) \) is the spectral radius of \( A \).

Proofs. Section 19.4.

19.14. Consider \((I_n - A)S_k\) and \(S_k(I_n - A)\) and use Definition 19.3.


19.16. We combine (19.6) with (19.15).


19.5 MATRIX FUNCTIONS

Many functions \( f(t) \), whether polynomial or nonpolynomial like \( \exp(t) \), \( \sin t \), and so on, can be generalized to have a matrix argument. Horn and Johnson [1991: chapter 6] have a good discussion on the meaning of \( f(A) \) and associated properties. They also define a primary matrix function \( f(A) \) associated with the scalar-valued stem function \( f(t) \) using the Jordan canonical form of \( A \), and their book should be consulted for details. We shall only consider some nonpolynomial functions. The following theorem is helpful in this respect.

19.17. Let \( f(t) \) be a scalar-valued function with power series representation \( f(t) = a_0 + a_1 t + a_2 t^2 + \cdots \) that has a radius of convergence \( R > 0 \). If \( A \) is \( n \times n \) and \( \rho(A) < R \), where \( \rho(\cdot) \) is the spectral radius, the matrix power series \( a_0 + a_1 A + a_2 A^2 + \cdots \) converges with respect to every norm on the set of \( n \times n \) matrices, and its sum is denoted by the primary matrix function \( f(A) \).

19.18. Let \( A \) be \( n \times n \) with eigenvalues \( \lambda_i \), and suppose \( f(\lambda) = \sum_{k=1}^{\infty} c_k \lambda^k \) and \( f(A) = \sum_{k=1}^{\infty} c_k A^k \).

(a) Since \( A = RJ_O R^{-1} \), where \( J_O \) is the Jordan canonical form of \( A \), we have \( f(A) = R f(J_O) R^{-1} \).

(b) \( \det f(A) = \det R \cdot \det f(J_O) \cdot (\det R)^{-1} = \det(J_O) = \prod_{i=1}^{n} f(\lambda_i) \).

(c) \( \text{trace } f(A) = \text{trace}(R^{-1} R f(J_O)) = \text{trace}(f(J_O)) = \sum_{i=1}^{n} f(\lambda_i) \).

See also (19.21).

A number of functions with power series expansions fall into the above category, the most common being the exponential function. In fact \( (I_n + A)^\nu \), \( \exp(A) \), \( \log A \), \( \sin A \), and \( \cos A \) can all be defined as primary matrix functions. However, using the Jordan canonical form, we find that all functions \( f \) satisfying certain derivative conditions have the property that \( f(A) \) can be expressed as a polynomial in \( A \) (Meyer [2000a: 603–607]). For further details see Abadir and Magnus [2005: chapter 9] and Meyer [2000a: sections 7.3 and 7.9].
Proofs. Section 19.5.


19.18b. The determinant is the product of its eigenvalues, which are the diagonal elements of the upper-triangular matrix $J_O$.

19.18c. As in (b), except that the trace is the sum of the eigenvalues.

19.6 MATRIX EXPONENTIALS

Matrix exponentials typically arise as solutions of differential equations (cf. Section 17.10).

Definition 19.6. If $A$ is an $n \times n$ matrix, we define

$$\exp(At) = I + tA + \frac{t^2}{2!}A^2 + \cdots + \frac{t^r}{r!}A^r + \cdots, \quad -\infty < t < \infty.$$  

This series converges absolutely for $\rho(A) < \infty$ (by 19.16d).

19.19. Setting $t = 1$, we have the following.

(a) The eigenvalues of $\exp(A)$ are $\exp(\lambda_i)$ ($i = 1, 2, \ldots, n$), where the $\lambda_i$ are the eigenvalues of $A$.

(b) If $A$ is symmetric, then $\exp(A)$ is positive definite as each eigenvalue $\lambda_i$ of $A$ is real and $\exp(\lambda_i)$ is positive.

(c) The matrix $\exp(A)$ is always nonsingular (as from (a) the eigenvalues are nonzero) and

$$[\exp(A)]^{-1} = \exp(-A).$$

(d) $\exp(kA) = [\exp(A)]^k$ for $k$ a positive or negative integer.

(e) $[\exp(A)]^* = \exp(A^*)$.

It then follows that $\exp(A)$ is Hermitian if $A$ is Hermitian, and it is unitary if $A$ is skew-Hermitian.

(f) Every $n \times n$ unitary matrix $U$ can expressed as $\exp(iA)$, where $A$ is some Hermitian $n \times n$ matrix. Note that $iA$ is skew-Hermitian.

(g) If $U$ is an $n \times n$ symmetric unitary matrix, there exists a real symmetric matrix $A$ such that $U = \exp(iA)$.

(h) As the determinant of a matrix is the product of its eigenvalues, it follows from (a) that

$$\det[\exp(A)] = \exp(\text{trace } A).$$

since $\prod_i \exp(\lambda_i) = \exp(\sum_i \lambda_i)$.

(i) If $A$ is real skew-symmetric, then $\exp(A)$ is orthogonal and its determinant is 1.
(j) If \( A \) is skew-Hermitian, then \( C = \exp(A) \) is unitary with \( |\det C| = 1 \).

19.20. Let \( A \) and \( B \) be \( n \times n \) matrices.

(a) If \( AB = BA \), then
\[
\exp(A + B) = \exp(A) \exp(B) = \exp(B) \exp(A).
\]

Although commutativity is a sufficient condition for the above to hold, it is not necessary.

(b) We can have \( \exp(A) \exp(B) = \exp(B) \exp(A) \), but \( AB \neq BA \). For an example see Abadir and Magnus [2005: 256].

(c) \( \det[\exp(A + B)] = \det[\exp(A)] \det[\exp(B)] \).

This follows from (19.19g) above irrespective of whether (a) holds or not.

(d) (Lie Product Formula) \( \lim_{n \to \infty} [\exp(A_n) \exp(B_n)]^n = \exp(A + B) \).

19.21. Let \( A \) be an \( n \times n \) diagonalizable matrix with eigenvalues \( \lambda_i \); that is, there exists a nonsingular matrix \( R \) such that
\[
A = RAR^{-1} = R \text{diag}(\lambda_1, \lambda_2, \ldots, \lambda_n)R^{-1},
\]
\[
A^k = R A^k R^{-1}
\]
and \( \exp(A) = R \text{diag}(e^{\lambda_1}, \ldots, e^{\lambda_n})R^{-1} = Re^A R^{-1} \), say.

(This method avoids using a power series expansion, and it can be generalized to any function \( f(z) \) of a diagonalizable matrix by defining \( f(A) = \text{diag}(f(\lambda_1), f(\lambda_2), \ldots, f(\lambda_n)) \) and setting \( f(A) = R f(A) R^{-1} \). For nondiagonalizable matrices, we can replace \( A \) by its Jordan form \( J_0 \) and use (19.18).

19.22. For general \( t \):

(a) The matrix \( \exp(At) \) is nonsingular for all finite \( t \). Noting that its eigenvalues are \( \exp(t \lambda_i) \), we have from (19.19g),
\[
det(\exp(At)) = \exp(t \text{trace } A), \quad -\infty < t < \infty.
\]

(b) Using power series expansions, \( \exp(At_1) \exp(At_2) = \exp[A(t_1 + t_2)] \) for all \( t_1 \)
and \( t_2 \).

(c) \( \exp(At)^{-1} = \exp(-At) \).

(d) If "\( \otimes \)" is the Kronecker product, we have from (11.9):

(i) \( \exp(I_m \otimes At) = I_m \otimes \exp(At) \).

(ii) \( \exp(At \otimes I_m) = \exp(At) \otimes I_m \).

These results hold for any primary matrix function \( f(\cdot) \) and not just for \( \exp(\cdot) \).

(e) \( \exp(At) \exp(Bt) = \exp[(A + B)t] \) for all finite \( t \in \mathbb{R} \) if and only if \( AB = BA \).

19.23. (Inequalities)
(a) Let $A$ be any $n \times n$ matrix. For any matrix norm $\| \cdot \|$, 
$$\| \exp(A) \| \leq \exp(\|A\|).$$
(b) If $A$ and $B$ are $n \times n$ Hermitian matrices, then 
$$\| \exp(A + B) \|_{ui} \leq \| \exp(A) \exp(B) \|_{ui},$$
for any unitarily invariant norm $\| \cdot \|_{ui}$.

19.24. Let $f$ be a continuous function from the space of $n \times n$ complex matrices to $\mathbb{C}$ with the following properties.

1. $f(XY) = f(YX)$ for all $X$ and $Y$.
2. $|f(X^{2k})| \leq f([XX^*]^k)$ for all $X$ and for all $k = 1, 2, \ldots$.

Then:

(a) $f(XY) \geq 0$ for all Hermitian non-negative definite $X$ and $Y$. In particular, 
$$f(\exp(A)) \geq 0$$
for all Hermitian $A$.
(b) $|f(\exp(A))| \leq f(\Re A)$ for all $A$.
(c) $|f(\exp(A + B))| \leq f(\Re(A + B)) \leq f(\Re A)f(\Re B)$ for all $A, B$.
(d) $0 \leq f(\exp(A + B)) \leq f(\exp(A) \exp(B))$ for all Hermitian $A, B$.

Here $\Re$ means the "real part of." Note that (a) and (d) hold when $f$ is the trace or the determinant. The above inequalities arise in statistical mechanics, population biology, and quantum mechanics.

Proofs. Section 19.6.

19.19a. Follows from the fact that $A^k x = \lambda^k x$ for all $k = 1, 2, \ldots$, and for some $x$. See also Meyer [2000a: 525].
19.19e. Quoted by Horn and Johnson [1991: 439, exercise 9].
19.19f. Quoted by Horn and Johnson [1991: 440, exercise 10].
19.20b. Quoted by Horn and Johnson [1991: 442, exercise 22].
19.22c. Use (e) to verify that exp(−At) is the inverse.
19.22d. Quoted by Horn and Johnson [1991: 440, exercise 13].
19.22e. Abadir and Magnus [2005: 252].
CHAPTER 20

RANDOM VECTORS

20.1 NOTATION

In this chapter we do not use the convention that random variables have capital letters because of the problem of distinguishing between a random matrix and its observed value in the next chapter. As a rough rule, we generally reserve the latter part of the alphabet, \( u, v, \ldots, z \) for random vectors and the rest of the alphabet for constants, including matrices of constants.

20.2 VARIANCES AND COVARIANCES

**Definition 20.1.** If \( \mathbf{x} = (x_i) \) is a vector of random variables, then we define \( E(\mathbf{x}) = (E(x_i)) \), the vector of expected values.

20.1. For conformable vectors and matrices, \( E(A\mathbf{x} + \mathbf{b}) = AE(\mathbf{x}) + \mathbf{b} \).

20.2. Let \( S \) be a convex subset of \( \mathbb{R}^n \) and \( \mathbf{x} \) an \( n \times 1 \) random vector with finite \( E(\mathbf{x}) \). If \( \text{pr}(\mathbf{x} \in S) = 1 \) then \( E(\mathbf{x}) \in S \).

**Definition 20.2.** If \( \mathbf{x} \) and \( \mathbf{y} \) are vectors of random variables, we define the matrix with \((i,j)\)th elements \( \text{cov}(x_i, y_j) \) to be \( \text{cov}(\mathbf{x}, \mathbf{y}) \), the covariance matrix of \( \mathbf{x} \) and \( \mathbf{y} \). When \( \mathbf{x} = \mathbf{y} \), we define \( \text{var}(\mathbf{x}) = \text{cov}(\mathbf{x}, \mathbf{x}) \) to be the variance matrix of \( \mathbf{x} \). (The terms variance-covariance matrix, covariance matrix and dispersion matrix...
are also used in the literature for $\text{var}(x)$. In the following, we recall that $A \succeq B$ implies that $A - B$ is non-negative definite.

20.3. Let $\text{var}(x) = \Sigma$. Since, by (20.6b), $0 \leq \text{var}(a'x) = a'\Sigma a$, we have that $\Sigma$ is non-negative definite. It is nonsingular (i.e., positive definite) if and only if there do not exist constants $a (\neq 0)$ and $b$ such that $a'x = b$ (i.e., $\text{var}(a'x) = 0$).

20.4. If $E(x) = \mu$ and $\text{var}(x) = \Sigma$, then $x - \mu \in C(\Sigma)$ or equivalently $x \in C(\mu, \Sigma)$, with probability 1.

20.5. Let $E(x) = \mu_x$ and $E(y) = \mu_y$.

(a) 

$$\text{cov}(x - a, y - b) = \text{cov}(x, y)$$

$$= E[(x - \mu_x)(y - \mu_y)']$$

$$= E(xy') - \mu_x\mu_y'.$$

(b) The above result also holds if $x = y$ so that:

(i) $\text{var}(x - a) = \text{var}(x)$.

(ii) $\text{var}(x) = E(xx') - \mu_x\mu_x'$.

20.6. The following results are extremely useful.

(a) $\text{cov}(Ax, By) = A\text{cov}(x, y)B'$.

(b) From (a), $\text{var}(Ax) = A\text{var}(x)A'$.

(c) $\text{var}(y - Ax) = \text{var}(y) - A\text{cov}(x, y) - \text{cov}(y, x)A' + A\text{var}(x)A'$.

20.7. If $x$ and $y$ are random vectors with respective means $\mu_x$ and $\mu_y$, then $E((y - Ax - a)(y - Ax - a)') = \text{var}(y - Ax) + (\mu_y - A\mu_x - a)(\mu_y - A\mu_x - a)'$.

20.8. If $a, b, c,$ and $d$ are constants, then

$$\text{cov}(ax + by, cu + dv)$$

$$= ac\text{cov}(x, u) + ad\text{cov}(x, v) + bc\text{cov}(y, u) + bd\text{cov}(y, v).$$

In particular, $\text{var}(u + v) = \text{var}(u) + \text{cov}(u, v) + [\text{cov}(u, v)]' + \text{var}(v)$.

20.9. (Partitioned Vector) Let $z = (x', y')'$ be a random vector with mean $\mu_z = (\mu'_x, \mu'_y)'$, where $x$ is $m \times 1$ and $y$ is $p \times 1$. Then:

(a) $\text{var}(z) = \Sigma_{zz} = \begin{pmatrix} \text{var}(x) & \text{cov}(x, y) \\ \text{cov}(y, x) & \text{var}(y) \end{pmatrix} = \begin{pmatrix} \Sigma_{xx} & \Sigma_{xy} \\ \Sigma_{yx} & \Sigma_{yy} \end{pmatrix}$, say,

where $\Sigma_{yx} = \Sigma_{xy}'$.

(b) $C(\Sigma_{xy}) \subseteq C(\Sigma_{xx})$ and $C(\Sigma_{yx}) \subseteq C(\Sigma_{yy})$.

(c) If $E(x) = 0$, then $\text{cov}(y - Ax, x) = 0$ if and only if $Ax = Bx$ with probability 1, where $B = \Sigma_{yx}\Sigma_{xx}$ and $\Sigma_{xx}$ is any weak inverse of $\Sigma_{xx}$ (i.e., $\Sigma_{xx}\Sigma_{xx} - \Sigma_{xx} = \Sigma_{xx}$).
(d) Using (20.8) and (c),
\[ \text{var}(y - Ax) = \text{var}[(y - Bx) + (B - A)x] \]
\[ = \text{var}(y - Bx) + \text{var}[(B - A)x] \]
\[ \geq \text{var}(y - Bx). \]
for all \( A \).

(e) By (20.6b) we have \( \text{var}(\Sigma_{yx}' \Sigma_{xx}^{-1} x) = \text{var}(Bx) = \Sigma_{yy} - \Sigma_{yx}' \Sigma_{xx}^{-1} \Sigma_{xy}. \) This matrix and the generalized Schur complement \( \Sigma_{yy,x} = \Sigma_{yy} - \Sigma_{yx}' \Sigma_{xx}^{-1} \Sigma_{xy} \) are invariant with respect to the choice of weak inverse \( \Sigma_{xx}^{-1} \) (by (14.8) and (20.9b)).

(f) \( \text{var}(y - Bx) = \Sigma_{yy,x} = \text{var}(y - \mu_y - \Sigma_{yx}'(x - \mu_x)), \) by (20.5b(i)).

(g) (Best Linear Predictor) From (20.7) and (d),
\[ E[(y - Ax - a)(y - Ax - a)'] \succeq \text{var}(y - Ax) \]
\[ \succeq E[(y - \hat{y}_x)(y - \hat{y}_x)'] = \Sigma_{yy,x} \]
for all conformable \( A \) and \( a \), where \( \hat{y}_x = \mu_y + \Sigma_{yx}' \Sigma_{xx}^{-1} (x - \mu_x) \) is called the best linear predictor as it minimizes the left-hand side of the above expression, the so-called mean squared prediction error matrix.

Proofs. Section 20.2.


20.3. Seber and Lee [2003: 8].


20.6a. Seber and Lee [2003: 7].

20.6c. Expand \( \text{cov}(y - Ax, y - Ax) \).

20.7. We use (20.5b(i)) with \( x \) replaced by \( y - Ax \), and then use (20.5b(ii)) with \( x \) replaced by \( y - Ax - a \).

20.8. Seber and Lee [2003: 7].

20.9b. Sengupta and Jammalamadaka [2003: 56, with the roles of \( x \) and \( y \) interchanged].

20.9c. Sengupta and Jammalamadaka [2003: 57].

20.9d. Use (20.9c) to prove that the covariance term is zero.

20.9e. \( \text{var}(Bx) = BS_{xx}B' = \Sigma_{yx} \Sigma_{xx}^{-1} (\Sigma_{xx}') \Sigma_{xy} = \Sigma_{yx} (\Sigma_{xx}^{-1} \Sigma_{xx} \Sigma_{xx}'(1)) \Sigma_{xy}, \) where \( (\Sigma_{xx}') = \Sigma_{xx}'(1) \), say, for some weak inverse \( \Sigma_{xx}'(1) \) of \( \Sigma_{xx} \), as \( \Sigma_{xx} \) is symmetric. Then \( C = \Sigma_{xx} \Sigma_{xx}^{-1} \Sigma_{xx}'(1) \) is a weak inverse of \( \Sigma_{xx} \) as \( \Sigma_{xx} C \Sigma_{xx} = \Sigma_{xx} \).

20.9f. Using (c) and \( B = \Sigma_{yx} \Sigma_{xx}^{-1} \), we obtain
\[ \text{cov}(y - Bx, y - Bx) = \text{cov}(y - Bx, y) = \text{var}(y - Bx) = \Sigma_{yy,x}. \]

20.9g. \( E[(y - Ax - a)(y - Ax - a)'] \succeq \text{var}(y - Ax), \) by (20.7), and \( \text{var}(y - Ax) \succeq \text{var}(y - Bx), \) from (f).
20.3 CORRELATIONS

20.3.1 Population Correlations

Definition 20.3. If $x$ and $y$ are random variables, then their population correlation coefficient is defined to be $\rho(x, y) = \frac{\text{cov}(x, y)}{\sqrt{\text{var}(x)\text{var}(y)}} = \frac{\sigma_{xy}}{\sqrt{\sigma_x \sigma_y}}$, say.

20.10. $\rho = \rho(x, y)$ has the following well-known properties.

(a) $-1 \leq \rho \leq +1$.

(b) $\rho^2 = 1$ if and only if $x$ and $y$ are linearly related.

If $\rho = +1$, then $y - \mu_y = \frac{\sigma_x}{\sigma_x}(x - \mu_x)$.

If $\rho = -1$, then $y - \mu_y = -\frac{\sigma_x}{\sigma_x}(x - \mu_x)$.

(c) $\rho(ax, by) = \text{sign}(ab) |ab| \rho(x, y)$.

Definition 20.4. Suppose $x$ has variance matrix $\Sigma = (\sigma_{ij})$. If $\text{corr}(x) = (\rho_{ij})$, where $\rho_{ij} = \sigma_{ij}/(\sigma_{ii}\sigma_{jj})^{1/2}$, then $\text{corr}(x)$ is called the population correlation matrix of $x$.

20.11. Let $C = \text{corr}(x) = (\rho_{ij})$ be an $n \times n$ correlation matrix.

(a) $C = D^{-1/2} \Sigma D^{-1/2}$, where $D$ is a diagonal matrix with positive diagonal elements $\sigma = \text{diag}(\sigma_{11}, \sigma_{22}, \ldots, \sigma_{nn})$.

(b) $C$ is non-negative definite (as $\Sigma$ is).

(c) $\rho_{ii} = 1$ and $|\rho_{ij}| < 1$ (for all $i, j, j \neq i$).

(d) The largest eigenvalue of $C$ is less than $n$.

(e) $0 < \det C \leq 1$.

(f) A well-known correlation matrix is of the form $C = (1 - \rho)I_n + \rho J_n$, where $J_n$ is an $n \times n$ matrix with all its elements equal to 1. For $C$ to be positive definite we must have $-1/(n - 1) < \rho < 1$. For further details about this matrix see (15.18a).

Definition 20.5. Let $x$ be a $d$-dimensional random vector with $E(x) = \mu$ and $\text{var}(x) = \Sigma$, where $\Sigma$ is positive definite. Consider the partitions

$x = \begin{pmatrix} x_1^T \\ x_2^T \end{pmatrix}$, $\mu = \begin{pmatrix} \mu_1^T \\ \mu_2^T \end{pmatrix}$, and $\Sigma = \begin{pmatrix} \Sigma_{11} & \Sigma_{12} \\ \Sigma_{12}^T & \Sigma_{22} \end{pmatrix}$,

where $x_2 = (x_2, \ldots, x_d)'$, $\mu_2 = (\mu_2, \ldots, \mu_d)'$ and $\Sigma_{22}$ is $(d - 1) \times (d - 1)$. Here $\text{var}(x_1) = \Sigma_{11}$, $\Sigma_{12}$ is the vector of covariances between $x_1$ and each of the variables in $x_2$, and $\text{var}(x_2) = \Sigma_{22}$. The (population) multiple correlation coefficient between $x_1$ and $x_2$, denoted by $\rho_{1.23\ldots,d}$, is the maximum correlation between $x_1$ and any linear function $a'x_2$ of $x_2, \ldots, x_d$. Thus

$R = \rho_{1.23\ldots,d} = \max_a \frac{\text{cov}(x_1, a'x_2)}{\sqrt{\text{var}(x_1)\text{var}(a'x_2)}}^{1/2} = \max_a \frac{a'\Sigma_{12}}{(\sigma_{11} a'\Sigma_{22} a)^{1/2}}$.
Also, $R^2$ is sometimes called the \textit{(population) coefficient of multiple determination}, and $R$ is the positive square root (Muirhead [1982: section 5.2] and Anderson [2003: section 2.5]).

\textbf{20.12.} $R$ has the following properties.

(a) $R = (\sigma'_{12} \Sigma^{-1}_{22} \sigma_{12}/\sigma_{11})^{1/2}$.

(b) $0 \leq R \leq 1$.

(c) If $\sigma_{11}$ is the first diagonal element of $\Sigma^{-1}$, then, from (14.11),

$$\sigma_{11} = (\sigma_{11} - \sigma'_{12} \Sigma^{-1}_{22} \sigma_{12})^{-1}$$

and $1 - R^2 = 1/(\sigma_{11}^2)$.\[1200]

(d) When $x$ has a nonsingular multivariate normal distribution $N_d(\mu, \Sigma)$ we have from (20.23f) that

$$E(x_1 \mid x_2) = \mu_1 + \sigma'_{12} \Sigma^{-1}_{22} (x_2 - \mu_2)$$

and

$$\text{var}(x_1 \mid x_2) = \sigma_{11} \cdots \sigma_{d} = \sigma_{11} - \sigma'_{12} \Sigma^{-1}_{22} \sigma_{12}.$$\[1200]

Then:

(i) $1 - R^2 = \sigma_{11} \cdots \sigma_d / \sigma_{11}$.

(ii) $\sigma_{11} \cdots \sigma_d \leq \sigma_{11}$.

(iii) $R$ is the correlation between $x_1$ and $E(x_1 \mid x_2)$.

(e) When $d = 2$, $R = |\rho_{12}| = |\rho(x_1, x_2)|$.

\textbf{Definition 20.6.} The previous Definition 20.5 can be readily generalized. Let $x$ be a $d$-dimensional random vector with $E(x) = \mu$ and positive definite variance matrix $\Sigma$. Consider the partitions

$$x = \left(\begin{array}{c} x_1 \\ x_2 \end{array}\right), \quad \mu = \left(\begin{array}{c} \mu_1 \\ \mu_2 \end{array}\right), \quad \Sigma = \left(\begin{array}{cc} \Sigma_{11} & \Sigma_{12} \\ \Sigma_{21} & \Sigma_{22} \end{array}\right),$$

where $x_1$ is $k \times 1$, $x_2$ is $(d - k) \times 1$, and so on, and let $x_i$ be a variable in $x_1$ ($i = 1, 2, \ldots, k$). The (population) multiple correlation coefficient between $x_i$ and the variables $x_{k+1}, \ldots, x_d$ in $x_2$, denoted by $R_{i \cdot k+1, k+2, \ldots, d}$, is the maximum correlation between $x_i$ and any linear function $a'x_2$ of $x_{k+1}, \ldots, x_d$. Note that $R_{1 \cdot 2, \ldots, d} = R$.

\textbf{Definition 20.7.} Using the notation of the previous definition, let $\Sigma_{11, 2} \equiv \Sigma_{11} - \Sigma_{12} \Sigma^{-1}_{22} \Sigma_{21} = (\sigma_{ij, k+1, k+2, \ldots, d}$, say). Given $x \sim N_d(\mu, \Sigma)$, then $\Sigma_{11, 2} = \text{var}(x_1 \mid x_2)$ (cf. 20.23f). We define the \textit{(population) partial correlation coefficient} $\rho_{ij \cdot k+1, \ldots, d}$ to be the correlation coefficient between $x_i$ and $x_j$, components of $x_1$, in the conditional distribution of $x_1$ given $x_2$, that is,

$$\rho_{ij \cdot k+1, \ldots, d} = \frac{\sigma_{ij, k+1, \ldots, d}}{(\sigma_{ii, k+1, \ldots, d} \sigma_{jj, k+1, \ldots, d})^{1/2}}.$$\[1200]

This is the correlation between $x_i$ and $x_j$ holding $x_2$ fixed.
20.13. Let $\sigma'_i$ be the $i$th row of $\Sigma_{12}$.

(a) $\sigma_{i,k+1,k+2,\ldots,d} = (\sigma_{ii} - \sigma'_i \Sigma^{-1}_{22} \sigma_i)$.

(b) $\mathcal{R}_{i,k+1,k+2,\ldots,d} = (\sigma'_i \Sigma^{-1}_{22} \sigma_i) / \sigma_{ii}$.

(c) $1 - \mathcal{R}_{i,k+1,k+2,\ldots,d} = (\sigma_{ii} - \sigma'_i \Sigma^{-1}_{22} \sigma_i) / \sigma_{ii}$.

(d) $\mathcal{R}_{i,k+1,\ldots,d} = (\sigma_{ii} - \sigma_{ii,k+1,\ldots,d}) / \sigma_{ii}$.

(e) $1 - \rho^2_{i,k+1,k+2,\ldots,d} = (\sigma_{ii} - \sigma_{ii,k+1,\ldots,d}) / \sigma_{ii,k+1,\ldots,d}$. In particular, with $i = 1$ and $k = 1$, $1 - \rho^2_{12,3,4,\ldots,d} = (\sigma_{11} - \sigma_{11,2,3,4,\ldots,d})$.

(f) $1 - \mathcal{R}^2_{12,3,\ldots,d} = (1 - \rho^2_{12,3,4,\ldots,d}) \cdots (1 - \rho^2_{1,2,\ldots,d-1,2,d}) (1 - \rho^2_{1,2,\ldots,d})$.

(g) $\rho_{ij,k+1,k+2,\ldots,d} = \rho_{ij,k+1,k+2,\ldots,d} - \rho_{i,k+1,k+2,\ldots,d} \rho_{j,k+1,k+2,\ldots,d} / \sqrt{1 - \rho^2_{i,k+1,k+2,\ldots,d} \cdots (1 - \rho^2_{1,2,\ldots,d})} / \sqrt{1 - \rho^2_{j,k+1,k+2,\ldots,d} \cdots (1 - \rho^2_{1,2,\ldots,d})}$.

(h) $\rho_{12,3} = -\rho_{12,3} / [(1 - \rho^2_{12,3}) (1 - \rho^2_{13})]^{1/2}$.

Proofs. Section 20.3.1.

20.11d. The eigenvalues $\lambda_i$ of $C$ are non-negative and $\sum_i \lambda_i = \text{trace } C = n$.

20.11e. Follows from $(\prod_i \lambda_i)^{1/n} \leq \bar{\lambda} = 1$ (as the geometric mean does not exceed the arithmetic mean) and $\det C = \prod_i \lambda_i$.


20.3.2 Sample Correlations

**Definition 20.8.** If $x = (x_i)$ and $y = (y_i)$ are $n \times 1$ vectors representing univariate random samples of size $n$, then their sample correlation coefficient is defined to be

$$r(x, y) = \frac{\sum_{i=1}^n (x_i - \bar{x})(y_i - \bar{y})}{\left[\sum_{i=1}^n (x_i - \bar{x})^2 \sum_{i=1}^n (y_i - \bar{y})^2\right]^{1/2}}.$$  

20.14. $r = r(x, y)$ has the following properties.

(a) $r^2 \leq 1$. When $r^2 = 1$, there is a linear relation between the $y_i$ and the $x_i$ as in (20.10b), but with parameters replaced by their estimates.

(b) $r(ax, by) = \text{sign}(ab) |ab| r(x, y)$.

**Definition 20.9.** Let $x_1, x_2, \ldots, x_n$ be a random sample from a $d$-dimensional distribution with mean $\mu$ and positive definite variance matrix $\Sigma$, and let $S = (s_{ij})$ be the sample covariance matrix given by $S = \sum_{i=1}^{n} (x_i - \bar{x})(x_i - \bar{x})' / (n - 1)$. Let $r_{ij} = s_{ij} / (s_{ii} s_{jj})^{1/2}$, where $r_{ii} = 1$ for $i = 1, 2, \ldots, d$. Then $R = (r_{ij})$ is called the sample correlation matrix. It does not matter if we use $n$ instead of $(n - 1)$, that
is, use $\hat{\Sigma}$, the maximum likelihood estimate of $\Sigma$ under normality, instead of $S$ as $(n - 1)$ cancels out of $R$. Note that $S$ is a random matrix so that it is considered again in the next chapter.

20.15. We now introduce an important device that allows the properties of population parameters to be carried over directly to their sample estimates. Consider the discrete random variable $y$ with probability function

$$\Pr(y = x_i) = \frac{1}{n}, \quad i = 1, 2, \ldots, n.$$  

Then

$$E(y) = \sum_{i=1}^{n} x_i \frac{1}{n} = \bar{x} \quad \text{and} \quad \text{var}(y) = \sum_{i=1}^{n}(x_i - \bar{x})(x_i - \bar{x})' \frac{1}{n} = \hat{\Sigma}.$$  

We can therefore "translate" sample properties into population properties using an appropriate discrete population.

**Definition 20.10.** Using the notation of the previous definition, consider the partition

$$S = \begin{pmatrix} s_{11} & s'_{12} \\ s_{12} & S_{22} \end{pmatrix}.$$  

The sample multiple correlation coefficient between $x_1$ and $x_2, x_3, \ldots, x_d$ is defined to be

$$R = (s'_{12}S^{-1}_{22}s_{12}/s_{11})^{1/2}.$$  

Under normality, $R$ is the maximum likelihood estimate of $\mathcal{R}$, the population multiple correlation. For further details see Anderson [2003: section 4.4].

Sample versions of the other correlations and partial correlations can be defined in a similar manner. One simply replaces $\Sigma$ by $S$ or $\hat{\Sigma}$ in the population definitions. For example, replacing $\Sigma$ by $S$ in Definition 20.7, we have the sample partial correlation

$$r_{i j \cdot k+1, \ldots, d} = \frac{s_{i j \cdot k+1, \ldots, d}}{[s_{ii \cdot k+1, \ldots, d} s_{jj \cdot k+1, \ldots, d}]^{1/2}}.$$  

For further details see Anderson [2003: section 4.3].

20.16. Using the method of (20.15), all the results and optimal properties for population parameters hold for the sample equivalents. For example, from (20.13b),

$$r_{i \cdot k+1, k+2, \ldots, d} = (s'_{i}S^{-1}_{22}s_{i}/s_{ii})^{1/2}.$$  

**Proofs.** Section 20.3.2.

20.14a. Proved using the Cauchy–Schwarz inequality or using (20.15).

20.4 QUADRATICS

20.17. Let \( \mathbf{x} \) be an \( d \)-dimensional random vector with \( \mathbb{E}(\mathbf{x}) = \mu \) and \( \text{var}(\mathbf{x}) = \Sigma \), a non-negative definite matrix of rank \( r \leq d \). Let \( \mathbf{A} \) be a real \( d \times d \) symmetric matrix, and let \( \Sigma = \mathbf{B}\mathbf{B}' \) (cf. 10.10), where \( \mathbf{B} \) is \( d \times r \) and \( \mathbf{B}'\mathbf{A}\mathbf{B} \neq \mathbf{0} \). Then:

(a) With a suitable transformation of the form \( \mathbf{x} = \mathbf{B}\mathbf{P}\mathbf{z} \) we find that

\[
\mathbf{x}'\mathbf{A}\mathbf{x} = a + 2 \sum_{i=1}^{r} b_i z_i + \sum_{i=1}^{r} \lambda_i z_i^2
\]

\[
= \sum_{i=1}^{r} \lambda_i (z_i + \frac{b_i}{\lambda_i})^2 + (a - \sum_{i=1}^{r} \frac{b_i^2}{\lambda_i}), \quad \lambda_i \neq 0, \quad i = 1, 2, \ldots, r
\]

\[
= \sum_{i=1}^{r} \lambda_i z_i^2 \quad \text{for} \quad \mu = 0,
\]

where \( \mathbf{b}' = (b_1, b_2, \ldots, b_r) = \mu'\mathbf{A}\mathbf{B}, \mathbf{z} = (z_1, z_2, \ldots, z_r)', \mathbb{E}(\mathbf{z}) = \mathbf{0}, \text{var}(\mathbf{z}) = \mathbf{I}_r, \mathbf{P}'\mathbf{B}'\mathbf{A}\mathbf{B} = \text{diag}(\lambda_1, \lambda_2, \ldots, \lambda_r) \), the \( \lambda_i \) are the eigenvalues of \( \mathbf{B}'\mathbf{A}\mathbf{B} \) (i.e., of \( \Sigma \mathbf{A} \)), \( \mathbf{P} \) is \( r \times r \) and orthogonal (i.e., \( \mathbf{P}\mathbf{P}' = \mathbf{I}_r \)), and \( a = \mu'\mathbf{A}\mu \).

(b) If \( \Sigma \) is positive definite, we can choose \( \mathbf{B} \) to be triangular (Cholesky decomposition) or \( \Sigma^{1/2} \) (cf. 10.32). In the latter case, we find that

\[
\mathbf{x}'\mathbf{A}\mathbf{x} = \sum_{i=1}^{d} \lambda_i (u_i + c_i)^2,
\]

where the \( \lambda_i \) are the eigenvalues of \( \Sigma^{1/2}\mathbf{A}\Sigma^{1/2} \) (i.e., of \( \Sigma \mathbf{A} \)), \( \mathbb{E}(\mathbf{u}) = \mathbf{0}, \text{var}(\mathbf{u}) = \mathbf{I}_d, \mathbf{c}' = (c_1, c_2, \ldots, c_d) = (\mathbf{P}'\Sigma^{-1/2}\mu)', \) and \( \mathbf{P}\mathbf{P}' = \mathbf{I}_d \).

20.18. Let \( \mathbf{x} \) have mean \( \mu \) and non-negative definite variance matrix \( \Sigma \), and let \( \mathbf{Q} = \mathbb{E}[(\mathbf{x} - \mathbf{a})'\mathbf{A}(\mathbf{x} - \mathbf{a})] \) (= \( \mathbb{E}[\text{trace}\{(\mathbf{x} - \mathbf{a})'\mathbf{A}(\mathbf{x} - \mathbf{a})\}] \)).

(a) Using (20.7),

\[
\mathbb{E}(\mathbf{Q}) = \text{trace}\{\mathbf{A}\mathbb{E}[(\mathbf{x} - \mathbf{a})(\mathbf{x} - \mathbf{a})']\} = \text{trace}(\mathbf{A}\Sigma) + (\mu - \mathbf{a})'\mathbf{A}(\mu - \mathbf{a})'.
\]

(b) If \( \Sigma = \sigma^2 \mathbf{I} \), we have the useful rule \( \mathbb{E}(\mathbf{Q}) = \sigma^2 \text{trace} \mathbf{A} + \mathbf{Q}_{x \rightarrow \mathbb{E}(\mathbf{x})} \).

20.19. Let \( \mathbf{x} \) be a \( d \times 1 \) random vector with mean \( \mu \), variance matrix \( \Sigma \), and finite fourth moments, so that \( \mathbb{E}(\mathbf{xx}') \) and \( \mathbb{E}[(\mathbf{xx}' \otimes \mathbf{xx}')] \) exist, where \( \otimes \) refers to the Kronecker product. If \( \mathbf{A} \) and \( \mathbf{B} \) are real symmetric \( d \times d \) matrices, then

\[
\text{cov}(\mathbf{x}'\mathbf{A}\mathbf{x}, \mathbf{x}'\mathbf{B}\mathbf{x}) = \text{trace}\{(\mathbf{A} \otimes \mathbf{B})\mathbb{E}(\mathbf{xx}' \otimes \mathbf{xx}')\}
-\{\text{trace}(\mathbf{A}\Sigma) + \mu'\mathbf{A}\mu\}{\text{trace}(\mathbf{B}\Sigma) + \mu'\mathbf{B}\mu}\}.
\]

20.20. Let \( \mathbf{x} \) be a random vector with elements \( x_1, x_2, \ldots, x_n \) distributed as independent random variables with means \( \theta_1, \theta_2, \ldots, \theta_n \), common variance \( \mu_2 \), and common third and fourth moments about their means, \( \mu_3 \) and \( \mu_4 \), respectively (i.e., \( \mu_r = \mathbb{E}[(x_i - \theta_i)^r] \)). Let \( \mathbf{A} \) be any symmetric \( n \times n \) matrix, and let \( \mathbf{a} = \text{diag} \mathbf{A} \) be the column vector of the diagonal elements of \( \mathbf{A} \).
(a) We have
\[ \text{var}(x'Ax) = (\mu_4 - 3\mu_2^2)a'a + 2\mu_2^2 \text{trace}(A^2) + 4\mu_2 \theta'A^2\theta + 4\mu_3\theta'Aa. \]

(b) If the \( x_i \) are each normally distributed as \( N(0, \sigma^2) \), then \( \mu_3 = 0, \mu_4 = 3\mu_2^2, \mu_2 = \sigma^2 \), and
\[ \text{var}(x'Ax) = 2\sigma^4 \text{trace}(A^2). \]

If \( B \) is also a symmetric \( n \times n \) matrix, then
\[ \text{cov}(x'Ax, x'Bx) = 2\sigma^2 \text{trace}(AB). \]

These results are generalized in (20.25).

(c) Let \( \gamma_2 = (\mu_4 - 3\mu_2^2)/\mu_2^2 \) be the common kurtosis, and let \( P_i \ (i = 1, 2) \) be symmetric idempotent matrices with \( p_i = \text{diag}(P_i) \), rank \( P_i = f_i (= \text{trace } P_i) \), and \( P_1P_2 = 0 \). If \( P_i\theta = 0 \), then from (a) we have:

(i) \( \text{var}(y'P_1y) = 2\sigma^4 f_i + \gamma_2 p_i^2 p_1 \).

(ii) \( \text{cov}(y'P_1y, y'P_2y) = \sigma^4 \gamma_2 p_1^2 p_2 \).

This result is useful in examining the robustness of the \( F \)-test for a linear hypothesis and a linear model.

Proofs. Section 20.4.


20.20b. Seber and Lee [2003: 16].

20.20c. Atiqullah [1962] and Seber and Lee [2003: 236–237]. Here (ii) is obtained from \( \frac{1}{2} \{ \text{var}((y'(P_1 + P_2)y) - \sum_i \text{var}(y'P_iy)) \}. \)

20.5 MULTIVARIATE NORMAL DISTRIBUTION

20.5.1 Definition and Properties

Definition 20.11. Let \( x \) be a \( d \times 1 \) random vector with mean \( \mu \) and variance matrix \( \Sigma \), which is positive definite. Then \( x \) is said to have a (nonsingular) multivariate normal (or multinormal) distribution if its probability density function is given by

\[
\begin{align*}
    f(x) &= f(x_1, x_2, \ldots, x_d) \\
    &= (2\pi)^{-d/2} (\det \Sigma)^{-1/2} \exp \left\{ \frac{1}{2} (x - \mu)' \Sigma^{-1} (x - \mu) \right\} \\
    &\quad (-\infty < x_i < \infty, \ i = 1, 2, \ldots, d).
\end{align*}
\]
We write \( x \sim N_d(\mu, \Sigma) \). When \( d = 1 \), we replace \( N_1 \) by \( N \), the univariate normal distribution. Note that \( x \sim N_d(0, I_d) \) if and only if the \( x_i \) are independently distributed as \( N(0, 1) \). If \( x \sim N_d(\mu, \Sigma) \), then \( y = \Sigma^{-1/2}(x - \mu) \sim N_d(0, I_d) \). Sampling from a normal distribution is discussed in Section 21.3.

If \( \Sigma \) is positive semi-definite (i.e., singular), then the probability distribution still exists, but not the density function. However, we can extend our definition to include the so-called singular multivariate normal distribution using one of the following equivalent definitions, which includes both the nonsingular and singular cases.

1. The random vector \( x \) is multivariate normal if and only if \( y = a'X \) is univariate normal for all \( a \). If \( y = b \) we define \( y \) to be \( N(b, 0) \).

2. A random \( d \times 1 \) vector \( x \) with mean \( \mu \) and variance matrix \( \Sigma \) has a multivariate normal distribution if it has the same distribution as \( Ax + \mu \), where \( A \) is any \( d \times m \) matrix satisfying \( E = AA' \), and \( z \sim N_m(0, I_m) \).

The singular normal distribution occurs in many places in statistics, for example the distribution of residuals from linear models (Seber and Lee [2003]) and the distribution of the estimated cell proportions from sample survey data (Rao and Scott [1984]). For a general reference on the multivariate normal see Tong [1990].

**20.21.** Adopting the notation of Definition 20.11, suppose that \( \Sigma \) is singular of rank \( r \) (i.e., positive semi-definite). Then, from (20.4), \( x - \mu \in C(\Sigma) \) and we can express \( \Sigma = RR' \), where \( R \) is \( d \times r \) of rank \( r \) (cf. 10.10). Hence if \( P_{\Sigma} \) is the orthogonal projector onto \( C(\Sigma) \) (cf. 2.49d), we have, for \( (I_d - P_{\Sigma})(x - \mu) = 0 \), the density function

\[
 f(x) = (2\pi)^{r/2} [\det(R'R)]^{-1/2} \exp\left[-\frac{1}{2}(x - \mu)\Sigma^-(x - \mu)\right],
\]

and 0 otherwise. Here \( \Sigma^- \) is a weak inverse of \( \Sigma \).

**20.22.** (A Useful Integral) If \( A \) and \( B \) are symmetric \( n \times n \) matrices and \( B \) is positive definite, then using the multivariate normal density function we have

\[
 \int_{-\infty}^{+\infty} \cdots \int_{-\infty}^{+\infty} (x'Ax + a'x + a_0) \exp\left[-(x'Bx + b'x + b_0)\right] dx_1 \cdots dx_n
 = \frac{1}{2} \pi^{n/2} |B|^{-1/2} \exp(\frac{1}{4}b'B^{-1}b - b_0) 
 \times [\text{trace}(AB^{-1}) - a'B^{-1}b + \frac{1}{2}b'B^{-1}AB^{-1}b + 2a_0].
\]

**20.23.** Let \( x \sim N_d(\mu, \Sigma) \), where the distribution may be singular or nonsingular.

(a) The moment generating function of \( x \) is \( E[\exp(t'x)] = \exp(t'\mu + \frac{1}{2}t'\Sigma t) \). This uniquely determines the (nonsingular) distribution when \( \Sigma \) is positive definite.

(b) If \( C \) is \( m \times d \), then \( Cx \sim N_m(C\mu, C\Sigma C') \). The distribution is nonsingular if \( \Sigma \) is positive definite and \( C \) has rank \( m \).

(c) Any subset of a multivariate normal distribution is multivariate normal.

(d) If the covariance of any two vectors that contain disjoint subsets of \( x \) is zero, then the two vectors are statistically independent.
(e) If \( \text{cov}(Ax, Bx) = 0 \), then \( Ax \) and \( Bx \) are statistically independent.

(f) Suppose \( \Sigma \) is positive definite, and let

\[
x = \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}, \quad \mu = \begin{pmatrix} \mu_1 \\ \mu_2 \end{pmatrix}, \quad \text{and} \quad \Sigma = \begin{pmatrix} \Sigma_{11} & \Sigma_{12} \\ \Sigma_{21} & \Sigma_{22} \end{pmatrix},
\]

where \( x_i \) and \( \mu_i \) are \( d_i \times 1 \), \( \Sigma_{ii} \) is \( d_i \times d_i \) \((i = 1, 2)\), and \( d_1 + d_2 = d \). We then have the following conditional distribution

\[
x_2 \mid x_1 \sim N_{d_2}(\mu_{2.1}, \Sigma_{22.1}),
\]

where \( \mu_{2.1} = \mu_2 + \Sigma_{21} \Sigma_{11}^{-1}(x_1 - \mu_1) \) and \( \Sigma_{22.1} = \Sigma_{22} - \Sigma_{21} \Sigma_{11}^{-1} \Sigma_{12} \). Note that \( \Sigma_{22.1} \) is the Schur complement of \( \Sigma_{11} \) in \( \Sigma \), and it is frequently expressed in the form \( (\Sigma/\Sigma_{11}) \) (cf. Section 14.1).

(g) The result (f) still holds if \( \Sigma \) is singular and we replace \( \Sigma_{11}^{-1} \) by \( \Sigma_{11}^{-} \), any weak inverse of \( \Sigma_{11} \).

20.24. (Moments) If \( x \sim N_d(0, \Sigma) \), where \( \Sigma \) is positive definite, and \( P_d = \frac{1}{2}(I_{d^2} + I_{(d,d)}) \) \((= N_d, \text{the symmetrizer of } (11.29h-i))\), then:

(a) \( E(x \otimes x) = \text{vec} \Sigma \).

(b) \( E(xx' \otimes xx') = 2P_d(\Sigma \otimes \Sigma) + (\text{vec} \Sigma)(\text{vec} \Sigma)' \).

If just one of any of the \( x \)'s is replaced by a constant vector, then the answer is \( 0 \).

(c) \( \text{var}(x \otimes x) = 2P_d(\Sigma \otimes \Sigma) \).

(d) Suppose \( x \sim N_d(\mu, \Sigma) \) and \( \Sigma \) is positive definite.

(i) \( E(x \otimes x) = E(z \otimes z) + \mu \otimes \mu = \text{vec} \Sigma + (\mu \otimes \mu) \), where \( z = x - \mu \).

(ii) \( \text{var}(x \otimes x) = 2P_d(\Sigma \otimes \Sigma + \Sigma \otimes \Sigma + \mu \mu' + \mu \mu' \otimes \Sigma) \).

(e) Higher moments are given by Graybill [1983: section 10.91 for the case \( x \sim N_d(0, I_d) \)].

Proofs. Section 20.5.1.


20.5.2 Quadratics in Normal Variables

20.25. Let \( x \sim N_d(\mu, \Sigma) \), where \( \Sigma \) is positive definite.

(a) We have \( (x - \mu)'\Sigma^{-1}(x - \mu) \sim \chi^2_d \) and \( x'\Sigma^{-1}x \sim \chi^2_d(\delta) \), the noncentral chi-squared distribution with noncentrality parameter \( \delta = \mu'\Sigma^{-1}\mu \).

(b) Using the notation of (20.23f), we have the following:

(i) \( Q_1 = (x_1 - \mu_1)'\Sigma_{11}^{-1}(x_1 - \mu_1) \sim \chi^2_d \) (by 20.23c and (a) above).

(ii) Let \( Q_2 = (x - \mu)'\Sigma^{-1}(x - \mu) - (x_1 - \mu_1)'\Sigma_{11}^{-1}(x_1 - \mu_1) \). Then, from (20.23f), \( x_2 | x_1 \sim N_d(\mu_{2.1}, \Sigma_{22.1}) \) and, conditional on \( x_1 \),

\[
Q_2 = (x_2 - \mu_{2.1})'\Sigma_{22.1}^{-1}(x_2 - \mu_{2.1}) \sim \chi^2_{d_2}.
\]

Since this distribution is not a function of \( x_1 \), it is also the unconditional distribution; (iii) below holds for the same reason.

(iii) \( Q_1 \) and \( Q_2 \) are statistically independent.

(c) Let \( A \) and \( B \) be \( d \times d \) matrices.

(i) \[
E(x'Ax \cdot x'Bx) = \text{trace}(A\Sigma)\text{trace}(B\Sigma) + 2\text{trace}(A\Sigma B\Sigma) + \text{trace}(A\Sigma B\Sigma)\mu'\mu + \text{trace}(B\Sigma)\mu'A\mu + 4\mu'\Sigma B\mu + (\mu'\mu)(\mu'B\mu).
\]

(ii) \( \text{cov}(x'Ax, x'Bx) = 2\text{trace}(A\Sigma B\Sigma) + 4\mu'A\Sigma B\mu. \)

(iii) Setting \( A = B \) in (ii), we have

\[
\text{var}(x'Ax) = 2\text{trace}[(A\Sigma)^2] + 4\mu'A\Sigma A\mu.
\]

(d) Let \( x \sim N_d(0, I_d) \), and let \( A, B, \) and \( C \) be all \( d \times d \) symmetric matrices.

(i)

\[
E(x'Ax \cdot x'Bx \cdot x'Cx) = \text{trace} A \text{trace} B \text{trace} C + 2\text{trace} A \text{trace}(BC) + 2\text{trace} B \text{trace}(AC) + 2\text{trace} C \text{trace}(AB) + 8\text{trace}(ABC).
\]

(ii) If \( x \sim N_d(0, \Sigma) \), we replace \( A, B, \) and \( C \) in the right-hand side of (i) by \( A\Sigma, B\Sigma, \) and \( C\Sigma \), respectively.

(e) If \( x \sim N_d(0, \Sigma) \), then:

(i)

\[
\text{cov}[(x'Ax)^2, (x'Bx)] = 4\text{trace}(A\Sigma)\text{trace}(A\Sigma B\Sigma) + 8\text{trace}[(A\Sigma)^2B\Sigma].
\]
(ii) 
\[
E[(x'Ax)^3] = [\text{trace}(A\Sigma)]^3 + 6\text{trace}(A\Sigma)\text{trace}[(A\Sigma)^2] + 8\text{trace}[(A\Sigma)^3].
\]

(f) (Moment Generating Function) If \( Q = x'Ax + a'x + d, \) where \( A \) is real and symmetric, then the moment generating function (m.g.f.) of \( Q \) is

\[
M_Q(t) = E[\exp(Qt)] = \frac{\det(I_d - 2tA\Sigma)^{-1/2}}{\sqrt{\det(I_d - 2tA\Sigma)^{-1}}} \exp\left\{ -\frac{1}{2} (\mu'\Sigma^{-1}\mu - 2td) + \frac{1}{2} (\mu + t\Sigma a)'(I_d - 2tA\Sigma)^{-1}\Sigma^{-1}(\mu + t\Sigma a) \right\}
\]

\[
= \left[ \frac{\det(I_d - 2t\Sigma^{1/2}A\Sigma^{1/2})^{1/2}}{\sqrt{\det(I_d - 2t\Sigma^{1/2}A\Sigma^{1/2})}} \exp\left\{ t(d + \mu'\Lambda\mu + a'\mu) + \frac{t^2}{2} (\Sigma^{1/2}a + 2\Sigma^{1/2}A\mu)'(I_d - 2t\Sigma^{1/2}A\Sigma^{1/2})^{-1} \right\} \right]
\]

\[
= \exp\left\{ t(d + \mu'\Lambda\mu + a'\mu) + \frac{t^2}{2} \sum_{i=1}^d c_i^2 (1 - 2t\lambda_i)^{-1} \right\}
\]

\[
\times \prod_{i=1}^d (1 - 2t\lambda_i)^{-1/2},
\]

where

\[
T'\Sigma^{1/2}A\Sigma^{1/2}T = \text{diag}(\lambda_1, \ldots, \lambda_d),
\]

\( T \) is orthogonal, and

\[
c = (c_1, \ldots, c_d)' = T'(\Sigma^{1/2}a + 2\Sigma^{1/2}A\mu).
\]

Note that

\[
\prod_{i=1}^d (1 - 2t\lambda_i)^{-1/2} = [\det(I_d - 2t\Sigma^{1/2}A\Sigma^{1/2})]^{1/2} = [\det(I_d - 2tA\Sigma)]^{-1/2}.
\]

The m.g.f. can be used to obtain moments of the quadratic form—for example, (c)(iii). Thus if \( Q_0 = x'Ax \) we have:

(i) \( E(Q_0) = \text{trace}(A\Sigma) + \mu'\Lambda\mu. \)

(ii) \( E((Q_0)^2) = 2\text{trace}[(A\Sigma)^2] + 4\mu'(A\Sigma)A\mu + \{\text{trace}(A\Sigma) + \mu'\Lambda\mu\}^2. \)

(iii) \[
E((Q_0)^3) = 8\{\text{trace}[(A\Sigma)^3] + 3\mu'(A\Sigma)^2A\mu\}
\]

\[
+ 6\{\text{trace}[(A\Sigma)^2] + 2\mu'\Lambda\Sigma\mu\}\{\text{trace}(A\Sigma) + \mu'\Lambda\mu\}
\]

\[
+ \{\text{trace}(A\Sigma) + \mu'\Lambda\mu\}^3.
\]

General expressions for \( E(Q_0^h) \) and \( E(Q_0^r) \) are given by Mathai and Provost [1992: 53–54], who also give formulae for \( E(Q_0^{-h}) \), where \( h > 0 \) and can be a fraction (Mathai and Provost [1992: 56–59]).
20.26. Let \( \mathbf{x} \) have the singular normal distribution \( N_d(\mathbf{\mu}, \Sigma) \), where \( \Sigma \) is non-negative definite of rank \( r \) \((r < d)\).

(a) \( \mathbf{x}'\Sigma^+\mathbf{x} \sim \chi^2(\delta) \), the noncentral chi-squared distribution with noncentrality parameter \( \delta = \mathbf{\mu}'\Sigma\mathbf{\mu} \). Here \( \Sigma^+ \) is the Moore–Penrose inverse of \( \Sigma \).

(b) (Moment Generating Function) Let \( \Sigma = \mathbf{B}\mathbf{B}' \) (cf. 10.10), where \( \mathbf{B} \) is \( d \times r \) of rank \( r \) and \( \mathbf{B}'\mathbf{A}\mathbf{B} \neq 0 \). If \( \mathbf{A} \) is a \( d \times d \) real symmetric matrix, then the moment generating function (m.g.f.) of \( Q = \mathbf{x}'\mathbf{A}\mathbf{x} + \mathbf{a}'\mathbf{x} + d \) is

\[
M_Q(t) = \left[ \det(\mathbf{I}_r - 2t\mathbf{B}'\mathbf{A}\mathbf{B}) \right]^{-1/2} \exp \left\{ t(\mathbf{\mu}'\mathbf{A}\mathbf{\mu} + \mathbf{a}'\mathbf{\mu} + d) \right\} \\
+ \frac{t^2}{2} (\mathbf{B}'\mathbf{a} + 2\mathbf{B}'\mathbf{A}\mathbf{\mu})(\mathbf{I}_d - 2t\mathbf{B}'\mathbf{A}\mathbf{B})^{-1}(\mathbf{B}'\mathbf{a} + 2\mathbf{B}'\mathbf{A}\mathbf{\mu}).
\]

An alternative expression in terms of eigenvalues is given by Mathai and Provost [1992: 46–47]. Positive, negative, and fractional moments of \( Q_0 = \mathbf{x}'\mathbf{A}\mathbf{x} \) are given by Mathai and Provost [1992: 54–55, 61–65].

The characteristic function of \( Q \) is obtained from the m.g.f. by replacing \( t \) by \( it \), where \( i = \sqrt{-1} \).

20.27. Let \( \mathbf{Q}_i = \mathbf{x}'\mathbf{A}_i\mathbf{x} + \mathbf{a}_i'\mathbf{x} + d_i \), where \( \mathbf{A}_i \) is a real \( d \times d \) symmetric matrix \((i = 1, 2)\), and suppose \( \mathbf{x} \sim N_d(\mathbf{\mu}, \Sigma) \).

(a) If \( \Sigma \) is positive definite, then the joint moment generating function (m.g.f.) of \( Q_1 \) and \( Q_2 \) is

\[
M_{Q_1,Q_2}(t_1,t_2) = \left[ \det(\mathbf{I}_r - 2t_1\mathbf{A}_1\Sigma - 2t_2\mathbf{A}_2\Sigma) \right]^{-1/2} \\
\times \exp \left\{ -\frac{1}{2}(\mathbf{\mu}'\Sigma^{-1}\mathbf{\mu} - 2t_1d_1 - 2t_2d_2) \right\} \\
+ \frac{1}{2}(t_1\mathbf{a}_1 + t_2\mathbf{a}_2 + \mathbf{\mu})'(\mathbf{I}_d - 2t_1\mathbf{A}_1\Sigma - 2t_2\mathbf{A}_2\Sigma)^{-1} \\
\times \Sigma^{-1}(t_1\mathbf{a}_1 + t_2\mathbf{a}_2 + \mathbf{\mu}).
\]

(b) If \( \Sigma \) is non-negative definite and \( \Sigma = \mathbf{B}\mathbf{B}' \) (cf. 10.10), where \( \mathbf{B} \) is \( d \times r \) of rank \( r \) \((r < d)\), then the joint m.g.f. of \( Q_1 \) and \( Q_2 \) is

\[
M_{Q_1,Q_2}(t_1,t_2) = \left[ \det(\mathbf{I}_r - 2t_1\mathbf{B}'\mathbf{A}_1\mathbf{B} - 2t_2\mathbf{B}'\mathbf{A}_2\mathbf{B}) \right]^{-1/2} \\
\times \exp \left\{ t_1(\mathbf{\mu}'\mathbf{A}_1\mathbf{\mu} + \mathbf{a}_1'\mathbf{\mu} + d_1) + t_2(\mathbf{\mu}'\mathbf{A}_2\mathbf{\mu} + \mathbf{a}_2'\mathbf{\mu} + d_2) \right\} \\
+ \frac{1}{2} \frac{\beta}{t_2}(\mathbf{I}_r - 2t_1\mathbf{B}'\mathbf{A}_1\mathbf{B} - 2t_2\mathbf{B}'\mathbf{A}_2\mathbf{B})^{-1} \\
\times (t_1\mathbf{B}'\mathbf{a}_1 + 2t_2\mathbf{B}'\mathbf{A}_1\mathbf{\mu} + t_2\mathbf{B}'\mathbf{a}_2 + 2t_2\mathbf{B}'\mathbf{A}_2\mathbf{\mu}).
\]

Note that (a) follows from (b) by setting \( \mathbf{B} = \mathbf{B}' = \Sigma^{1/2} \) (cf. 10.32). We can obtain various special cases, for example: (i) if we set \( \mathbf{a}_i = \mathbf{0} \) and \( d_i = 0 \) for \( i = 1, 2 \), and \( \mathbf{\mu} = \mathbf{0} \), we get the joint m.g.f. of \( \mathbf{x}'\mathbf{A}_1\mathbf{x} \) and \( \mathbf{x}'\mathbf{A}_2\mathbf{x} \), or (ii) if we set \( \mathbf{A}_2 = \mathbf{0} \) we get the joint m.g.f. for a quadratic and a linear form.

In (a) and (b), the joint characteristic function is obtained by replacing \( t_1 \) and \( t_2 \) by \( it_1 \) and \( it_2 \), respectively where \( i = \sqrt{-1} \).

The above results were proved by Mathai and Provost [1992: 66, section 3.2] and extended to more than two quadratics. They can also be used to obtain various
product moments, for example if $\Sigma$ is positive definite or non-negative definite we have

(i) $\text{cov}(x'Ax, a'x) = 2\mu'A\Sigma a$.

(ii) $\text{cov}(x'A_1x, x'A_2x) = 2\text{trace}(A_1\Sigma A_2\Sigma) + \mu'A_1\Sigma A_2\mu$.

The m.g.f.s can also be used to obtain cumulants. The reader is referred to Mathai and Provost [1992: sections 3.2d and 3.3] for further details.

20.28. (Distribution of a Quadratic) If $x \sim N_d(\mu, \Sigma)$, where $\Sigma$ is positive definite, and $A$ is a $d \times d$ symmetric matrix, then from (20.17b) we have the representation

$$Q = x'Ax = \sum_{i=1}^{d} \lambda_i(u_i + c_i)^2,$$

where the $\lambda_i$ are the eigenvalues of $\Sigma^{1/2}A\Sigma^{1/2}$ (i.e., of $\Sigma A$), $u = (u_1, u_2, \ldots, u_d)'$ is distributed as $N_d(0, I_d)$, $c = (c_i) = P\Sigma^{-1/2}\mu$, and $P$ is orthogonal. Here the $u_i^2$ are independently and identically distributed as $\chi^2_1$, while the $(u_i + c_i)^2$ are independently distributed as non-central chi-square $\chi^2_1(c_i^2)$ with noncentrality parameter $c_i^2$.

(a) When $\mu = 0$, then $c = 0$ and we find that $Q$ is a linear combination of statistically independent $\chi^2_1$ variables. If the distinct eigenvalues are $\mu_j$ with algebraic multiplicity $m_j$ ($j = 1, 2, \ldots, s$), then $Q \sim \sum_{j=1}^{s} \mu_j \chi^2_{m_j}$.

(b) If $\mu \neq 0$, then $Q$ is a linear combination of statistically independent non-central chi-square variables, each with one degree of freedom.

The above results can be used to find various infinite series expansions, including one in terms of chi-square densities, and some approximations for the distribution of $Q$. If, in (a), $m_j$ is even ($m_j = 2\nu_j$, say), then a finite expression for the distribution of $Q$ is available. Details of all this material including expressions for the case when $\Sigma$ is singular and results on ratios of quadratics are given by Mathai and Provost [1992: chapter 4]. They also give extensive reference lists.

Proofs. Section 20.5.2.


20.26a. Schott [2005: 405, he calls $\delta/2$ the noncentrality parameter].


20.5.3 Quadratics and Chi-Squared

20.29. Suppose \( x \sim N_d(\mu, \Sigma) \) and \( A \) is a \( d \times d \) real symmetric matrix.

(a) If \( \Sigma \) is positive definite, then \( x'Ax \sim \chi^2_r(\delta) \), where \( r = \text{rank} \, A \) (i.e., \( \text{rank}(A\Sigma) \)) and \( \delta = \mu' A \mu \), if and only if \( A\Sigma = \Sigma \) (i.e., \( A\Sigma A = A \)). We get two special cases by setting (i) \( \mu = 0 \) (i.e., \( \delta = 0 \) and the distribution is central chi-square, \( \chi^2_r \)) and (ii) \( \Sigma = I_d \).

(b) If \( \Sigma \) is non-negative definite, then \( x'Ax \sim \chi^2_s(\delta) \), the noncentral chi-square distribution with noncentrality parameter \( \delta = \mu' A \mu \), if and only if:

1. \( \Sigma A\Sigma A = \Sigma A \Sigma \),
2. \( \mu' A\Sigma A \Sigma = \mu' A \Sigma \),
3. \( \mu' A\Sigma A \mu = \mu' A \mu \),
4. \( \text{trace}(A\Sigma) = s \).

Note that when \( \Sigma \) is positive definite, the four conditions reduce to (i) \( A\Sigma A = A \) and (ii) \( \text{trace}(A\Sigma) = r \).

The above results for \( x'Ax \) extend to \( Q = x'Ax + a'x + d \) (Mathai and Provost [1992: 201–214]).

20.30. If \( x \sim N_d(0, I_d) \), then \( x'Ax \) is distributed as the difference of two independently distributed chi-squared variables if and only if \( A^3 = A \) (i.e., \( A \) is tripotent). If \( x \sim N_d(\mu, I_d) \), then the chi-squared distributions are noncentral. This follows from (8.94b) and (20.29a) above.

Proofs. Section 20.5.3.


20.5.4 Independence and Quadratics

20.31. Let \( x \sim N_d(\mu, \Sigma) \), and let \( A_1 \) and \( A_2 \) be \( d \times d \) symmetric matrices.

(a) (Craig–Sakamoto) If \( \Sigma \) is non-negative definite, then \( x'A_1x \) and \( x'A_2x \) are statistically independent if and only if

\[
\begin{pmatrix} \Sigma \\ \mu' \end{pmatrix} A_1 \Sigma A_2 (\Sigma, \mu) = 0,
\]

or, equivalently,

1. \( \Sigma A_1 \Sigma A_2 \Sigma = 0 \),
2. \( \Sigma A_1 \Sigma A_2 \mu = 0 \),
3. \( \Sigma A_2 \Sigma A_1 \mu = 0 \),
4. \( \mu' A_1 \Sigma A_2 \mu = 0 \).
When \( \mu = 0 \), these reduce to \( \Sigma A_1 \Sigma A_2 \Sigma = 0 \), and if \( \Sigma \) is positive definite, the first equation reduces to \( A_1 \Sigma A_2 = 0 \) (or \( A_2 \Sigma A_1 = 0 \)).

(b) We can extend (a) as follows. If \( \Sigma \) is non-negative definite and \( Q_i = x'A_i x + a_i x + d_i \) \((i = 1, 2)\), then \( Q_1 \) and \( Q_2 \) are statistically independent if and only if:

1. \( \Sigma A_1 \Sigma A_2 \Sigma = 0 \),
2. \( \Sigma A_1 \Sigma (2A_2 \mu + a_2) = \Sigma A_2 \Sigma (2A_1 \mu + a_1) = 0 \),
3. \( (a_1 + 2A_1 \mu)' \Sigma (a_2 + 2A_2 \mu) = 0 \).

These are the same as (a) when \( a_1 = a_2 = 0 \). The presence of the constants \( d_1 \) and \( d_2 \) do not affect independence. Note also the following.

(i) If \( \operatorname{rank}(\Sigma A_1) = \operatorname{rank}(A_1) \) or \( \operatorname{rank}(\Sigma A_1 \Sigma) = \operatorname{rank}(\Sigma A_1) \), then \( \Sigma A_1 \Sigma A_2 \Sigma = 0 \) implies that \( A_1 \Sigma A_2 \Sigma = 0 \).

(ii) If \( \operatorname{rank}(\Sigma A_2) = \operatorname{rank}(A_2) \) or \( \operatorname{rank}(\Sigma A_1 \Sigma) = \operatorname{rank}(\Sigma A_2) \), then \( \Sigma A_1 \Sigma A_2 \Sigma = 0 \) implies that \( \Sigma A_1 \Sigma A_2 = 0 \).

(c) If \( \Sigma \) is non-negative definite and \( C \) is a \( p \times d \) matrix, then \( x'A x \) and \( C x \) are statistically independent if

\[ C \Sigma A(\Sigma, \mu) = 0. \]

If \( \Sigma \) is positive definite, then the two conditions reduce to just one condition, namely \( C \Sigma A = 0 \), or \( CA = 0 \) when \( \Sigma = I_d \).

(d) If \( \Sigma \) is non-negative definite, then setting \( A_2 = 0 \) in (b), \( x'A_1 x + a_1 x + d_1 \) and \( a_2' x + d_2 \) are statistically independent if and only if

(i) \( \Sigma A_1 \Sigma a_2 = 0 \),

(ii) \( (a_1 + 2A_1 \mu)' \Sigma a_2 = 0 \).

Setting \( A_1 = 0 \) as well, we see that \( a_1' x + d_1 \) and \( a_2' x + d_2 \) are statistically independent if and only if \( a_1' \Sigma a_2 = 0 \).

20.32. (Bilinear Forms) Suppose \( x_i \sim N_d(0, \Sigma_{ii}) \), where \( \Sigma_{ii} \) is positive definite \((i = 1, 2)\), and \( x_1 \) and \( x_2 \) are statistically independent.

(a) The joint moment generating function of \( Q_A = x_1' A x_2 \) and \( Q_B = x_1' B x_2 \) is

\[ M_{Q_A, Q_B}(t_1, t_2) = \left\{ \det[I_{d_2} - \Sigma^{1/2}_{12} (t_1 A + t_2 B)' \Sigma_{11} (t_1 A + t_2 B) \Sigma^{1/2}_{22}] \right\}^{-1/2}. \]

(b) \( Q_A \) and \( Q_B \) are statistically independent if and only if \( A' \Sigma_1 B = 0 \) and \( B \Sigma_2 A' = 0 \).

20.33. (Hadamard Product) Suppose \( x \sim N_d(\mu, \Sigma) \) and \( A \) and \( B \) are \( m \times d \) matrices. Now \( y = (Ax) \circ (Bx) = \Phi_m(Ax \otimes Bx) \Phi_1 \) (cf. 11.38a) with \( \Phi_1 = 1 \), and we have the following.

(a) \( E(y) = D1_m + (A \mu) \circ (B \mu) \), where \( D \) is the diagonal matrix with diagonal elements equal to those of \( B \Sigma A' \).
Proofs. Section 20.5.4.


20.31c. Quoted by Schott [2005: 413].


20.33a. Quoted by Schott [2005: 439, exercise 10.44]. Using the multiplication rule for the Kronecker product,

\[ \text{var}(Ax \circ Bx) = [A(\mathbf{\Sigma} + \mu'\mu')A'] \circ [B(\mathbf{\Sigma} + \mu'\mu')B'] \]

\[ + [B(\mathbf{\Sigma} + \mu'\mu')A'] \circ [A(\mathbf{\Sigma} + \mu'\mu')B'] \]

\[ - [A\mu\mu'A'] \circ [B\mu\mu'B'] - [A\mu\mu'B'] \circ [B\mu\mu'A']. \]

then use (11.38a(iii)).

20.33b. Using (20.6b), we obtain

\[ \text{var}(y) = \Psi_m(A \otimes B)\text{var}(x \otimes x)(A' \otimes B')\Psi_m. \]

Now substitute for \( \text{var}(x \otimes x) \) using (20.24d(ii)) with \( 2P_d = I_d^2 + I_{(d,d)} \) and \( I_{(d,d)} \) the commutation matrix. We then have \( (A \otimes B)I_{(d,d)} = I_{(d,d)}(B \otimes A) \) and, from (11.38a(iv)), \( \Psi_mI_{(d,d)} = \Psi_m \). Finally, multiply out and reintroduce \( \circ \).

20.5.5 Independence of Several Quadratics

20.34. Suppose \( x \sim N_d(\mu, \Sigma) \), where \( \Sigma \) is positive definite. Let \( A_i \) be a \( d \times d \) symmetric matrix of rank \( r_i \), for \( i = 1, 2, \ldots, k \), and let \( A = A_1 + \cdots + A_k \) be of rank \( r \). Let \( \chi^2_\nu(\delta) \) denote the noncentral chi-square distribution with \( \nu \) degrees of freedom and noncentrality parameter \( \delta \). Consider the following conditions:

1. \( A_i\Sigma \) is idempotent for each \( i \) (i.e., \( A_i\Sigma A_i = A_i \)),
2. \( \mathbf{\Sigma}A \) is idempotent. (i.e., \( A\Sigma A = A \))
3. \( A_i\Sigma A_j = 0 \), for all \( i, j, i \neq j \),
4. \( r = \sum_{i=1}^{k} r_i \),

If any two of (1), (2), and (3) hold, or if (2) and (4) hold, then
(a) $x'A_ix \sim \chi^2_{r_i}(\mu'Ax, \mu)$ for all $i$.
(b) $x'Ax \sim \chi^2_r(\mu'Ax, \mu)$.
(c) $x'A_1x, \ldots, x'A_kx$ are statistically independent.

The extension of the above result to the case when $\Sigma$ is non-negative definite is considered by Mathai and Provost [1992: 239]. When $\mu = 0$ and $\Sigma$ may be singular, further conditions for quadratics to be independently distributed as chi-square variables are given by Rao and Mitra [1971: section 9.3].

Proofs. Section 20.5.5.

20.34. Schott [2005: 413].

\section*{20.6 Complex Random Vectors}

Complex random vectors arise in several places in statistics, the most notable being multivariate time series (cf. Brillinger [1975: 89]) and random matrices (Mehta [2004]).

\textbf{Definition 20.12.} (Complex Random Vectors) Let $x = x_1 + ix_2$ and $y = y_1 + iy_2$ be complex random vectors, where the $x_i$ and $y_i$ are all real random vectors. We then define the following:

\begin{align*}
E(x) & = E(x_1) + iE(x_2), \\
\text{var}(x) & = E[(x - Ex)(x - Ex)^*], \quad \text{and} \\
\text{cov}(x, y) & = E[(x - Ex)(y - Ey)^*],
\end{align*}

where $x^* = x_1' - ix_2'$.

20.35. Using the notation in the above definition, we readily obtain:

(a) $\text{var}(x) = V_{11} + V_{22} + i(-V_{12} + V_{21})$, where $V_{ij} = \text{cov}(x_i, x_j)$, $i, j = 1, 2$.
(b) $\text{cov}(x, y) = \text{cov}(x_1, y_1) + \text{cov}(x_2, y_2) + i[-\text{cov}(x_1, y_2) + \text{cov}(x_2, y_1)]$.

\textbf{Definition 20.13.} (Complex Normal Distribution) Let $x_1$ and $x_2$ be $d \times 1$ (real) random vectors such that $(x_1', x_2')'$ is $N_{2d}(\mu, \Sigma)$, where $\mu = (\mu_1', \mu_2')'$ and

$$\Sigma = \begin{pmatrix} \Gamma & -\Phi \\ \Phi & \Gamma \end{pmatrix},$$

where $\Gamma$ is non-negative definite, and $\Phi = -\Phi'$ (i.e., real skew-symmetric). Then $x = x_1 + ix_2$ is said to have a complex normal distribution with mean $\mu_x = \mu_1 + i\mu_2$ and variance matrix $E[(x - \mu_x)(x - \mu_x)^*] = \Sigma_x$, where $\Sigma_x = \Sigma_1 + i\Sigma_2$ is Hermitian non-negative definite. Here $\Sigma_1 = 2\Gamma$ and $\Sigma_2 = 2\Phi$ are real matrices. We say that $x \sim N_{2d}(\mu_x, \Sigma_x)$. Thus $x_1 + ix_2$ is complex normal if and only if

$$\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \sim N_{2d} \left[ \begin{pmatrix} \mu_1 \\ \mu_2 \end{pmatrix}, \frac{1}{2} \begin{pmatrix} \Sigma_1 & -\Sigma_2 \\ \Sigma_2 & \Sigma_1 \end{pmatrix} \right].$$
From (20.35) we can identify

\[ \Sigma_1 = \text{var}(x_1) + \text{var}(x_2) \quad \text{and} \quad \Sigma_2 = -\text{cov}(x_1, x_2) + \text{cov}(x_2, x_1). \]


20.36. Using the above notation, and assuming that \( \Sigma_\mathbf{x} \) is Hermitian positive definite (i.e., \( \Sigma_1 \) is positive definite), we have:

(a) \( (\det \Sigma_\mathbf{X})^2 = \det(2\Sigma). \)

(b) \( \Sigma_\mathbf{x}^{-1} = (\Sigma_1 + \Sigma_2 \Sigma_1^{-1} \Sigma_2)^{-1} - i\Sigma_1^{-1} \Sigma_2 (\Sigma_1 + \Sigma_2 \Sigma_1^{-1} \Sigma_2)^{-1}. \)

(c) The probability density function of \( \mathbf{x} \) can be written as

\[
\frac{1}{\pi^d \det \Sigma} \exp[-(\mathbf{x} - \mathbf{\mu}_\mathbf{x})^* \Sigma_\mathbf{x}^{-1} (\mathbf{x} - \mathbf{\mu}_\mathbf{x})].
\]

(d) If \( \mathbf{x} \sim N_q^c(\mathbf{x}_\mathbf{c}, \mathbf{\Sigma}_\mathbf{x}) \) and \( \mathbf{A} \) is \( q \times d \), then \( \mathbf{A} \mathbf{x} \sim N_q^c(A \mathbf{x}_\mathbf{c}, A \Sigma_\mathbf{x} A^*). \) It follows that the marginal distributions of a multivariate complex normal are complex normal.

(e) If \( \Sigma_2 = 0 \), then \( x_1 \) and \( x_2 \) are statistically independent.

(f) The characteristic function of \( \mathbf{x} \) is

\[
E \exp[i \Re(t^* \mathbf{x})] = \exp[i \Re(t^* \mathbf{\mu}_\mathbf{x}) - t^* \Sigma_\mathbf{x} t],
\]

where \( \Re \) is the "real part."


**Proofs.** Section 20.6.


### 20.7 REGRESSION MODELS

The study of random vectors would not complete without some discussion of regression models. I shall consider mainly linear models, because matrices play a prominent role in these models. Also, other models can sometimes be transformed into linear ones, or else, with large samples, can be approximated by linear ones. There are many good books on linear regression with several different approaches. I personally prefer a geometrical approach using orthogonal projections as developed by Seber [1977, 1980, 1984] and, to a lesser extent, by Seber and Lee [2003]. This approach is being used a lot more in texts because it avoids some of the algebraic manipulations. For the various kinds of linear model see, for example, Christensen [1997, 2001]. An extensive and detailed theoretical treatment of all aspects of linear models is given by Sengupta and Jammalamadaka [2003]. For results on modifying a linear model by, for example, adding or deleting an observation see Section 15.3.
A typical regression model takes the form $y = \mu + \epsilon$, where $\mu = (\mu_i)$ is an $n \times 1$ vector of unknown parameters, $y = (y_i)$, and $\epsilon = (\epsilon_i)$ are $n \times 1$ random vectors with $E(\epsilon) = 0$ and $\text{var}(\epsilon) = \sigma^2 V$, where $\sigma^2$ is generally unknown and $n \times n$ $V$ may be known. This is usually known as a generalized (weighted) least squares model (cf. Kariya and Kurata [2004], for example). If $\mu_i = f(x_i; \theta)$, where $f$ is a nonlinear function, $x_i$ is a known observation, and $\theta$ is unknown, we have a typical nonlinear regression model. The theory of such models is discussed in detail by, for example, Seber and Wild [1989]. In some models, $V$ is known function of $\mu$, and quasi-likelihood methods can be used (Seber and Wild [1989: section 2.3]). Sometimes $V$ can be a function of other parameters such as autocorrelations in time series models (Seber and Wild [1989: chapter 6]) and variances in components of variance models (Sengupta and Jammalamadaka [2003: section 8.3] and Faraway [2006]). We can also have errors-in-variables models where, for example, the $x_i$s are measured with error (Seber and Wild [1989: chapter 10] and Carroll et al. [2006]). Other models where $\mu$ may contain random components are, for example, mixed models and components of variance models (e.g., P.S.R.S. Rao [1997] and Searle et al. [1992]).

We get another type of nonlinear model when $E(y_i) = \mu_i$, but now $g(\mu_i) = \alpha + \beta' x_i$, and the distribution of $y_i$ belongs to the exponential family. This is called a generalized linear model, and such models are discussed by McCullagh and Nelder [1989] and Dobson [2001]. Other transformation methods are described by Carroll and Ruppert [1988], and another approach is via generalized additive models (Tibshirani and Hastie [1990] and Wood [2006]).

Finally, applying large sample maximum likelihood theory to very general probability distributions, we can prove the asymptotic equivalence of large sample tests for nonlinear hypotheses such as the Likelihood ratio, Wald and Score (Lagrange multiplier) tests by asymptotically linearizing the model and hypothesis. In the linear case, all three test statistics are equivalent (Seber and Wild [1989: section 12.4] and Seber [1980: chapter 11]). Examples using this linearization technique are given by Seber [1967, 1980] and Lee et al. [2002]. We shall now consider the linear regression model.

**Definition 20.14.** We call the above model $y = \theta + \epsilon$ the general linear model if $\theta = X\beta$, where $X$ is a known $n \times p$ matrix of rank $r$ $(r \leq p < n)$, and $\beta$ is a $p \times 1$ vector of unknown parameters. We also assume that $V$ is non-negative definite of rank $v$, and we shall be interested in testing a linear hypothesis $A\beta = c$, where $A$ is $q \times p$ of rank $s$ $(s \leq q < p)$ and $c \in C(A)$. We shall refer to the general linear model as $M = (y, X\beta, \sigma^2 V)$ and the linear hypothesis as $H_0$. For making inferences, we shall also assume that $y$ is multivariate normal, namely $N_n(X\beta, \sigma^2 V)$.

There have been a large number of theoretical results proved for the above general setup and its special cases. However, my approach to linear models when $V$ is a known nonsingular matrix is somewhat pragmatic: Formulate the theoretical model and hypothesis (e.g., Seber and Lee [2003: section 6.4]) and use a statistical computer package such as $R$ to get the required results as well as the diagnostics for validating the model.

If $V$ is a known positive definite matrix, there exists a unique positive definite square root (cf. 10.32) $V^{1/2}$ so that making the transformation $V^{-1/2}y = V^{-1/2}X\beta + V^{-1/2}\epsilon$ we get the model

$$z = W\beta + \eta, \text{ where } \text{var}(\eta) = V^{-1/2}VV^{-1/2} = I_n.$$
We therefore begin with the model \((y, X\beta, \sigma^2 I_n)\).

With regard to \(H_0\), we frequently have \(c = 0\). If not we can “remove” \(c\) as follows. Let \(P_0\) satisfy \(A\beta_0 = c\) and consider the model \(z = X\gamma + \epsilon\), where \(z = y - X\beta_0\) and \(\gamma = \beta - \beta_0\). Then \(H_0\) becomes \(A\gamma = 0\), so for the moment we assume \(c = 0\), which fits in with the method of least squares described below. It should be noted that we can incorporate \(c\) if we use a different method of estimation, namely we find affine unbiased estimators that satisfy a minimum trace criterion (Magnus and Neudecker [1999: chapter 13]).

20.7.1 \(V\) Is the Identity Matrix

20.37. (Estimation) Consider the model \((y, X\beta, \sigma^2 I_n)\), where \(X\) is \(n \times p\) of rank \(r\) and \(\theta = X\beta\).

(a) Assume \(r < p\).

(i) \(\|y - \theta\|_2^2\) is minimized uniquely subject to \(\theta \in \mathcal{C}(X) = \Omega\), say, at \(\hat{\theta}\), the least squares estimate of \(\theta\), where

\[
\hat{\theta} = P_\Omega y, \quad P_\Omega = X(X'X)^{-1}X',
\]

and \(P_\Omega\) is the unique symmetric idempotent matrix representing the orthogonal projection of \(Y\) onto \(\Omega\); \((X'X)^{-1}\) is any weak inverse of \(X'X\).

Note that \(y = \hat{\theta} + (y - \hat{\theta})\) is an orthogonal decomposition of \(y\), and \(P_\Omega X = X\). The matrix \(P_\Omega\) is also referred to as the hat matrix in regression diagnostics (Seber and Lee [2003: section 10.2]).

Other norms and measures can be used for the minimization process to produce alternative estimators to least squares (cf. Groß [2003], Rao and Toutenburg [1999], and Seber and Lee [2003: section 3.13]).

(ii) If \(\hat{\theta} = X\hat{\beta}\), then \(\hat{\beta}\) is not unique. Since \(X'(y - \hat{\theta}) = 0\), \(\hat{\beta}\) satisfies the so-called normal equations \(X'X\hat{\beta} = X'y\), which have a solution \(\hat{\beta} = (X'X)^{-1}X'y = (X'X)^{-1}X'P_\Omega y = (X'X)^{-1}X'\hat{\theta}\).

(iii) \(Q = \|y - \hat{\theta}\|_2^2 = y'(I_n - P_\Omega)y = e'(I_n - P_\Omega)e\), since \((I_n - P_\Omega)\theta = 0\).

(iv) \(\sigma^2\) is usually estimated by its unbiased estimate \(s^2 = Q/(n - r)\), which has certain optimal properties. For example, it is the MINQUE of \(\sigma^2\) (Rao and Rao [1998: section 12.6]).

(v) \(r = y - \hat{\theta} = (I_n - P_\Omega)y\) is called the residual vector and is used for diagnostic purposes.

\(Q = r'r\) is usually called the residual sum of squares and is often denoted by \(RSS\).

(vi) \(E(r) = 0\) and \(\text{var}(r) = \sigma^2(I_n - P_\Omega)\).

(vii) For any \(a\), \(\hat{\phi} = a'\hat{\theta} = a'P_\Omega y\) is a linear estimate of \(\phi = a'\theta\) (i.e., linear in \(y\)) and is unbiased as \(P_\Omega X = X\) implies that \(E(\hat{\phi}) = \phi\).

(viii) (Gauss–Markov) Of all linear unbiased estimates of \(\phi\), \(\hat{\phi}\) is the unique estimate with minimum variance. We refer to \(\phi\) as the BLUE (Best Linear Unbiased Estimate) of \(\phi\).
(ix) If $B\mathbf{y}$ is any unbiased estimate of $\theta$, then

$$D = \text{var}(B\mathbf{y}) - \text{var}(\hat{\theta})$$

is non-negative definite (n.n.d.) and $D = 0$ if and only if $B\mathbf{y} = \hat{\theta}$. We call $\hat{\theta}$ the BLUE of $\theta$.

(x) Let $\mathbf{y} = \mathbf{X}\beta + \sigma \mathbf{u}$, where the elements of $\mathbf{u}$ are i.i.d. with mean zero and variance 1, and density $h(\cdot)$ satisfying $h(-u) = h(u)$ for all $u$. Then, provided it exists, the expected information matrix for the parameter vector $(\beta', \sigma^2)'$ is

$$\left( \begin{array}{cc} c\mathbf{X}'\mathbf{X} & 0 \\ 0 & n\sigma^2 \end{array} \right).$$

When $\mathbf{u}$ is normal, $c = \sigma^{-2}$ and $I_{\sigma^2} = 1/(2\sigma^4)$.

(b) When $\mathbf{X}$ has full rank (i.e., $r = p$) then $(\mathbf{X}'\mathbf{X})^{-1} = (\mathbf{X}'\mathbf{X})^{-1}$ and we have the following:

(i) $\beta = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{y}$.

(ii) $\hat{\beta} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{y}$, $E(\hat{\beta}) = \beta$, and $\text{var}(\hat{\beta}) = \sigma^2(\mathbf{X}'\mathbf{X})^{-1}$.

(iii) From (a) (viii) we find that $b'\hat{\beta}$ is the BLUE of $b'\beta$.

(iv) Suppose the $y_i$ are independent random variables with common variance $\sigma^2$ and common third and fourth moments, $\mu_3$ and $\mu_4$, respectively, about their means. Then $s^2$ is the unique non-negative quadratic unbiased estimate of $\sigma^2$ with minimum variance when $\mu_4 = 3\sigma^4$ or when the diagonal elements of $\mathbf{P}_\Omega = \mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'$ are all equal.

(v) If, as $n \to \infty$, $n^{-1}\mathbf{X}'\mathbf{X}$ converges to a finite positive definite matrix $\mathbf{V}_*$, and the largest diagonal element of $\mathbf{P}_\Omega$ goes to zero, then $\sqrt{n}(\hat{\beta} - \beta)$ converges in distribution to $N_\sigma(0, \sigma^2\mathbf{V}_*)$.

(c) If $\mathbf{X}$ has full rank and $\mathbf{y} \sim \mathcal{N}_n(\mathbf{X}\beta, \sigma^2\mathbf{I}_n)$, then the following hold:

(i) $\hat{\beta} \sim N_p(\beta, \sigma^2(\mathbf{X}'\mathbf{X})^{-1})$.

(ii) $\hat{\beta}$ is statistically independent of $s^2$.

(iii) $Q/\sigma^2 = (n-p)s^2/\sigma^2 \sim \chi^2_{n-p}$.

(iv) $\hat{\beta}$ and $Q/n$ are the maximum likelihood estimates of $\beta$ and $\sigma^2$, respectively, and are also sufficient statistics.

(v) $\hat{\beta}$ is the best unbiased estimate of $\beta$ in the sense that, for any $b$, $b'\hat{\beta}$ is the estimate of $b'\beta$ with minimum variance among all unbiased estimates, and not just among linear ones; that is, it is the MINVUE of $b'\beta$.

(vi) $s^2$ is the MINVUE of $\sigma^2$.

**Definition 20.15.** Let $\mathbf{X}$ be $n \times p$ of rank $r$. The function $b'\beta$ of $\beta$ is said to be *estimable* if it has a linear unbiased estimate, $c'y$, say. Then $b'\beta = E(c'y) = c'\mathbf{X}\beta$ for all $\beta$ so that $b' = c'\mathbf{X}$. Let $\mathbf{A}' = (a_1, a_2, \ldots, a_q)$ be a $q \times p$ matrix. The hypothesis $H_0 : \mathbf{A}\beta = 0$ is said to be testable if each $a_i'\beta$ is estimable for $i = 1, 2, \ldots, q$, that is $\mathbf{A}\beta$ is estimable. If $\mathbf{X}$ has full column rank, then $\mathbf{A}\beta$ is always estimable.
20.38. Suppose that \( r < p \). The following conditions are equivalent.

(1) \( A\beta \) is estimable.

(2) The rows of \( A \) are linearly dependent on the rows of \( X \), that is, there exists a \( q \times n \) matrix \( L \) such that \( A = LX \). If \( \text{rank} A = q \), then \( \text{rank} L = q \) (as \( \text{rank} A \leq \text{rank} L \), by (3.12)). Note that \( Ly \) is a linear unbiased estimator of \( A\beta \).

(3) \( C(A') \subseteq C(X') \).

(4) \( A\hat{\beta} \) is invariant for any choice of \( \hat{\beta} = (X'X)^{-1}X'y \).

(5) \( A(X'X)^{-1}X'X = A \).

20.39. If \( r < p \) and \( A\beta \) is estimable, then from (20.38(2)) above we have:

(a) \( A\hat{\beta} = L\hat{\theta} = LP_\Omega y = LX(X'X)^{-1}X'y = A(X'X)^{-1}X'y \).

(b) \( E(A\hat{\beta}) = E(L\hat{\theta}) = L\theta = A\beta \).

(c) \( \text{var}(A\hat{\beta}) = \text{var}(L\hat{\theta}) = \sigma^2 LP_\Omega L' = \sigma^2 A(X'X)^{-1}A' \). For a single estimable function, \( A \) reduces to \( a' \).

20.40. (Estimation with Constraints) Suppose \( T < p \). We wish to find the least squares estimate of \( \beta \) subject to the \( q \) estimable constraints \( A\beta = 0 \), that is, subject to \( 0 = A\beta = LX\beta = L\theta \), or \( \theta \in N(L) \).

(a) \( \|y - \theta\|_2^2 \) is uniquely minimized subject to \( \theta \in N(L) \cap \Omega = \omega \), say, when \( \theta = \hat{\theta}_H \), where \( \hat{\theta}_H = P_{\omega}y \) and \( P_{\omega} \) represents the orthogonal projection onto \( \omega \).

(b) \( Q_H = \|y - \hat{\theta}_H\|_2^2 = y'(I_n - P_{\omega})y \).

(c) From (2.51b) and (2.51d), \( P_\Omega - P_\omega = P_{\omega_\perp \cap \Omega} \), where \( \omega_\perp \cap \Omega = C(B) \) and \( B = P_\Omega L' \).

(d) From (c),

\[
\hat{\theta}_H = P_{\omega}y \\
= P_\Omega y - P_{\omega_\perp \cap \Omega} y \\
= \hat{\theta} - B(B'B)^{-1}B'y \\
= \hat{\theta} - P_{\Omega} L'(L P_\Omega L')^{-1} L P_\Omega y.
\]

(e) From (d) and \( A = LX \),

\[
P_{\omega_\perp \cap \Omega} = X(X'X)^{-1}A'[A(X'X)^{-1}A']^{-1}A(X'X)^{-1}X'.
\]

(f) If \( \hat{\theta}_H = X\hat{\beta}_H \), we have from (d) and (e)

\[
X\hat{\beta}_H = X\hat{\beta} - X(X'X)^{-1}A'[A(X'X)^{-1}A']^{-1}A\hat{\beta}.
\]
If $A$ has full row rank, $[A(X'X)^{-1}A']^{-1} = [A(X'X)^{-1}A']^{-1}$. If, in addition, $X$ has full column rank, then multiplying by $X'$,

$$
\hat{\beta}_H = \hat{\beta} - (X'X)^{-1}A'[A(X'X)^{-1}A']^{-1}A\hat{\beta}.
$$

We can also obtain this result using Lagrange multipliers (cf. Seber and Lee [2003: 60]).

(g) If we now want to change the constraints to $A\beta = c$, where $c \in \mathcal{C}(A)$, we replace $\hat{\beta}$ by $\hat{\beta} - \beta_0$ (where $A\beta_0 = c$ for some $\beta_0$), $A\hat{\beta}$ by $A\beta - c$, and $y$ by $\hat{y} = y - X\beta_0$. $Q_H$ then becomes $\hat{y}'(I_n - P_\omega)\hat{y}$, and $Q$ remains unchanged as $(I_n - P_\Omega)\hat{y} = (I_n - P_\Omega)y$.

(i) Given the estimable constraints $A\beta = c$, another approach is to note that $A\beta = c$ if and only if $\beta = A^{-}c + (I_p - A^{-}A)\phi$, where (cf. 13.4) $\phi$ is arbitrary, and $A^{-}$ is any weak inverse of $A$. Substituting for $\beta$, the constrained model then becomes

$$
(y - XA^{-}c, X(I_p - A^{-}A)\phi, \sigma^2I_n).
$$

A reasonable choice for $A^{-}$ is $A'(AA')^{-}$.

A second approach is use the model $(y^*, X^*\beta, \sigma^2V)$, where

$$
y^* = \begin{pmatrix} y \\ c \end{pmatrix}, \quad X^* = \begin{pmatrix} X \\ A \end{pmatrix}, \quad V = \begin{pmatrix} I_n & 0 \\ 0 & 0 \end{pmatrix},
$$

and $V$ is singular (Sengupta and Jammalamadaka [2003: 123, 125, 244]).

20.41. (Hypothesis Testing) Suppose we wish to test $H_0 : A\beta = c$ ($c \neq 0$), where $H_0$ is testable, and $A$ is $q \times p$ of rank $s$ ($s \leq q$).

(a) From (20.40g) and (20.40e),

$$
Q_H - Q = \hat{y}'P_{\omega \cap \Omega}\hat{y} = (A\hat{\beta} - c)'[A(X'X)^{-1}A']^{-1}(A\hat{\beta} - c).
$$

(b) $E(Q_H - Q) = \sigma^2s + (A\beta - c)'[A(X'X)^{-1}A']^{-1}(A\beta - c)$.

(c) The test statistic for $H_0$ is

$$
F = \frac{(Q_H - Q)/s}{Q/(n - r)}.
$$

(d) When $H_0$ is true, we have the following.

(i) $P_{\omega \cap \Omega}\hat{y} = P_{\omega \cap \Omega}[y - X\beta - (X\beta - X\beta_0)] = P_{\omega \cap \omega}e$, since from (20.40d) with $B' = LP_\Omega$ we have

$$
LP_\Omega X(\beta - \beta_0) = LX(\beta - \beta_0) = A\beta - c = 0.
$$

(ii) If $y \sim N_n(X\beta, \sigma^2I_n)$, then from (i) the following ratio has an $F$-distribution, that is,

$$
F = \frac{e'P_{\omega \cap \Omega}e/s}{e'(I_n - P_\Omega)e/(n - r)} \sim F_{s,n-r}.
$$


**Definition 20.16.** (Multiple Correlation) Consider the linear model

\[ y_i = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \cdots + \beta_{p-1} x_{i,p-1} + \epsilon_i \]

so that \( X = (1_n, x^{(1)}, \ldots, x^{(p-1)}) \), where \( \text{rank} \, X = p \). If we define \( \hat{\gamma} = \hat{\theta} \), the correlation coefficient of \( y \) and the fitted model \( \hat{y} \) is called the multiple correlation coefficient, and is denoted by \( R \). Its square \( R^2 \), is called the coefficient of (multiple) determination.

20.42. If \( \bar{y} = \sum_{i=1}^{n} y_i / n \), then:

(a) \( (y - \hat{\gamma})' 1_n = 0 \).

(b) \( \sum_{i=1}^{n} (y_i - \bar{y})^2 = \sum_{i=1}^{n} (y_i - \hat{\gamma}_i)^2 + \sum_{i=1}^{n} (\hat{\gamma}_i - \bar{y})^2 \).

(c) \( R^2 = \frac{\sum_{i=1}^{n} (\hat{\gamma}_i - \bar{y})^2}{\sum_{i=1}^{n} (y_i - \bar{y})^2} \).

(d) \( RSS = \sum_{i=1}^{n} (y_i - \hat{\gamma}_i)^2 = (1 - R^2) \sum_{i=1}^{n} (y_i - \bar{y})^2 \).

**Proofs.** Section 20.7.1.


20.37a(ix). \( P_{\Omega} \) is symmetric and idempotent. Because \( By \) is unbiased, \( (I_n - B)\theta = 0 \), so that \( C[(I_n - B)'] \perp \Omega \) and \( P_{\Omega} = P_{\Omega}B' = BP_{\Omega} \). This leads to \( D = B(I_n - P_{\Omega})B' \), which is non-negative definite (n.n.d.) as \( I_n - P_{\Omega} \) is n.n.d. Finally, \( D = 0 \) if and only if \( (I_n - P_{\Omega})B' = 0 \) or \( B = P_{\Omega} \).


20.37c. Seber and Lee [2003: 47–48 for (i)–(iii); section 3.5 for (iv); 50 for (v)] and Rao [1973a: 319 for (vi)].

20.38. Searle [1971].

20.41b. Use (20.18b) with \( E(A\hat{\beta}) = A\beta \) and \( P_{\omega \perp \Omega} = s \).


20.7.2 V Is Positive Definite

The results for $V$, a known positive definite matrix, follow directly from the results for $V = I_n$ by replacing $y$ by $V^{-1/2}y$, $\theta$ by $V^{-1/2}\theta$, and $X$ by $V^{-1/2}X$ through all the previous theory. For example, we now minimize $(y - \theta)'V^{-1}(y - \theta)$ subject to $\theta \in \Omega$ to obtain $\hat{\theta}$, say. We can do this by changing the inner product space or, more simply, by using the transformation $V^{-1/2}$ so that $X'X$ becomes $X'V^{-1}X$ and $X'y$ becomes $X'V^{-1}y$, giving us

$$V^{-1/2}\hat{\theta} = V^{-1/2}X(X'V^{-1}X)^{-1}X'V^{-1}y.$$  

Assuming $\text{rank } X = p$, and setting $\hat{\theta} = X\hat{\beta}$, we now have two unbiased estimates of $\beta$, namely

$$\hat{\beta} = (X'X)^{-1}X'y \quad \text{and} \quad \hat{\beta} = (X'V^{-1}X)^{-1}X'V^{-1}y.$$  

Then using (20.6b),

$$\text{var}(\hat{\beta}) = \sigma^2(X'X)^{-1}X'VVX(X'X)^{-1} \quad \text{and} \quad \text{var}(\hat{\beta}) = \sigma^2(X'VVX)^{-1}.$$  

The above estimators are often called the ordinary least squares estimate $\text{OLSE}(\beta) = \hat{\beta}$ and the generalized least squares estimate $\text{GLSE}(\beta) = \hat{\beta}$. As $\hat{\beta}$ is the BLUE of $\beta$, we can expect this estimator to be more efficient in some sense than $\hat{\beta}$. Various measures of efficiency are given in (12.6), and a popular one is the Watson efficiency $\phi = 1/E_1$, where

$$\phi = \frac{\det[\text{var}(\hat{\beta}_{GLS})]}{\det[\text{var}(\hat{\beta}_{OLS})]} = \frac{[\det(X'X)]^2}{\det(X'VVX) \cdot \det(X'V^{-1}X)}.$$  

From (12.6a),

$$1 \geq \phi \geq \prod_{i=1}^{m} \frac{4\lambda_i\lambda_{n-i+1}}{\lambda_i + \lambda_{n-i+1}} = \prod_{i=1}^{m} (1 - \rho_i^2),$$  

where $m = \min\{p, n - p\}$ and $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n > 0$ are the eigenvalues of $V$. $E_1 = 1$ if and only if the two estimators are the same. The ratios $4\lambda_i\lambda_{n-i+1}/(\lambda_i + \lambda_{n-i+1})^2$ are the squared antieigenvalues of $V$ (cf. Section 6.7), and the $\rho_i$ can be taken as the canonical correlations between the OLSE $\hat{\theta}$ and its residual $r = y - \hat{\theta}$. For references on the topic see Drury et al. [2002] and the survey by Chu et al. [2005b].

The Watson efficiency has also been applied to partitioned regression models

$$X\beta = (X_1, X_2)\beta = X_1\beta_1 + X_2\beta_2,$$  

where $X$ and $V$ have full rank. A subset Watson efficiency can be defined for the estimate of $\beta_1$, and the overall efficiency factorized into components. For details and examples see Chu et al. [2004; 2005a,b].
20.7.3 V Is Non-negative Definite

We now assume that \( V \) is a known singular matrix of rank \( v \) \((v < n)\) and that \( \text{rank} \, X < \text{rank} \, V \). For a thorough review and historical summary of the topic see Puntanen and Styan [1989]. Theoretical details are given by Sengupta and Jammalamadaka [2003: chapter 7], Baksalary et al. [1990], and, more briefly, by Christensen [2002]. Singular models arise, for example, in finite population sampling, in some experimental designs, in some state-space models, and in models where some of the \( y \)-variables are virtually error-free and are effectively constants.

20.44. Consider the model \((y, X\beta, \sigma^2V)\), where \( V \) is singular and \( \text{rank} \, X = r \) \((r \leq p)\). Let \( H = P_\Omega \) and \( M = I_n - P_\Omega = I_n - H \), so that from (20.37a(i)) \( \theta = Hy \).

(a) The model is consistent (i.e., the inference base is not self-contradictory) if \( y \in C(X, V) \) with probability 1. This follows from the fact that \( y - X\beta \in C(V) \) with probability 1.

(b) One expression for the best linear unbiased estimate (BLUE) \( \theta^\dagger \) of \( \theta \) takes the form \( \theta^\dagger = Gy \) if and only if \( G(X, VM) = (X, 0) \) (Puntanen et al. [2000]). The numerical value of \( \theta^\dagger \) is unique with probability 1, but \( G \) is unique if and only if \( C(X, V) = \mathbb{R}^n \).

When \( V \) is nonsingular, \( \theta^\dagger = \hat{\theta} \) (cf. 20.43).

(c) One general solution to \( G(X, VM) = (X, 0) \) is

\[
G = I_n - VM(MVM)^{-1}M + F[I_n - MVM(MVM)^{-1}M],
\]

where \( F \) is arbitrary.

(d) (i) Some representations of \( \theta^\dagger \) are

\[
\theta^\dagger = \hat{\theta} - HVM(MVM)^{-1}My \\
= \hat{\theta} - HVM(MVM)^{+}My \\
= \hat{\theta} - HVM(MVM)^{+}y \\
= y - VM(MVM)^{-1}My.
\]

(ii) Also

\[
\theta^\dagger = X(X'W^{-1}X)^{-1}X'W^{-1}y,
\]

where \( W = V + XUX' \) and \( U \) is an arbitrary matrix such that \( C(W) = C(X, V) \).

(e) If \( X \) has full column rank and \( \theta^\dagger = X\beta^\dagger \), then \( \beta^\dagger = (X'X)^{-1}X'\theta^\dagger \).

(f) \( \theta^\dagger \) is invariant to the choice of \( (MVM)^{-} \).

(g) Asymptotic theory for \( \theta^\dagger \) is given by Sengupta and Jammalamadaka [2003: 522].

(h) (Mean and Variance)

(i) Since \( E(My) = MX\theta = 0 \), it follows from (d) that \( E(\theta^\dagger) = \theta \).
(ii) From (d) and $\mathbf{HM} = \mathbf{0}$,

\[
\text{var}(\theta^\dagger) = \sigma^2[H\mathbf{V}H - H\mathbf{V}(\mathbf{M}\mathbf{V})^{-1}\mathbf{M}\mathbf{V}H]
= \sigma^2[V - \mathbf{V}(\mathbf{M}\mathbf{V})^{-1}\mathbf{M}\mathbf{V}]
= \sigma^2[X(X'W^{-1}X' - \mathbf{X}\mathbf{U}\mathbf{X}')].
\]

(iii) If $\mathbf{X}$ has full column rank and $\theta^\dagger = \mathbf{X}\beta^\dagger$, then

\[
\text{var}(\beta^\dagger) = \text{var}(\hat{\beta}) - (X'X)^{-1}X'\mathbf{V}(\mathbf{M}\mathbf{V})^{-1}\mathbf{M}\mathbf{V}X(X'X)^{-1},
\]

where $\text{var}(\hat{\beta}) = (X'X)^{-1}X'\mathbf{V}X(X'X)^{-1}$.

(i) The residual is

\[
r = y - \theta^\dagger
= \mathbf{M}y + H\mathbf{V}(\mathbf{M}\mathbf{V})^{-1}\mathbf{M}\mathbf{V}X(X'X)^{-1}Y,
\]

and

\[
\text{var}(r) = \sigma^2 \mathbf{V}(\mathbf{M}\mathbf{V})^{-1}\mathbf{M}\mathbf{V}.
\]

(j) Let $f = \text{rank} (\mathbf{V}, \mathbf{X}) - \text{rank} \mathbf{X}$. The weighted residual sum of squares is

\[
Q^\dagger = (y - \theta^\dagger)'\mathbf{V}^{-1}(y - \theta^\dagger) = y'\mathbf{M}(\mathbf{M}\mathbf{V})^{-1}\mathbf{M}\mathbf{V}X(X'X)^{-1}Y,
\]

and

\[
\mathbb{E}(Q^\dagger/f) = \sigma^2.
\]

(k) If $\mathbf{A}{\beta}$ is estimable, then the BLUE of $\mathbf{A}{\beta}$ is

\[
(\mathbf{A}{\beta})^\dagger = \mathbf{A}\mathbf{X}^{-1}[\mathbf{I}_n - \mathbf{V}(\mathbf{M}\mathbf{V})^{-1}\mathbf{M}]{\gamma}.
\]

Furthermore,

\[
\text{var}[(\mathbf{A}{\beta})^\dagger] = \sigma^2 \mathbf{A}\mathbf{X}^{-1}[\mathbf{V} - \mathbf{V}(\mathbf{M}\mathbf{V})^{-1}\mathbf{M}](\mathbf{A}\mathbf{X}^{-1})'.
\]

(l) (Inverse Partitioned Matrix Approach) Let

\[
\begin{pmatrix} \mathbf{V} & \mathbf{X} \\ \mathbf{X}' & \mathbf{0} \end{pmatrix}^{-1} = \begin{pmatrix} \mathbf{C}_1 & \mathbf{C}_2 \\ \mathbf{C}_3 & -\mathbf{C}_4 \end{pmatrix}.
\]

(i) $\theta^\dagger = \mathbf{X}\mathbf{C}_2{\gamma} = \mathbf{X}\mathbf{C}_3{\gamma}$.

(ii) $\text{var}(\theta^\dagger) = \sigma^2 \mathbf{X}\mathbf{C}_4X'$.

(iii) $r = \mathbf{V}\mathbf{C}_1{\gamma}$.

(iv) Referring to (j), $Q^\dagger = {\gamma}'\mathbf{C}_1{\gamma}$.

(m) $\theta^\dagger = \hat{\theta}$ if and only any one of the following conditions hold.

(1) $HV = VH$.

(2) $VV = HVH$. 
(3) \( \text{HVM} = 0 \).

(4) \( \mathcal{C}(VX) \subseteq \mathcal{C}(X) \).

For these and further conditions see Puntanen and Styan [1989, 2006] and Isotalo et al. [2005b: chapter 6].

20.45. If \( X \) has full column rank \( p \) and \( \mathcal{C}(X) \subseteq \mathcal{C}(V) \), the so-called weakly singular model, then the Watson efficiency is

\[
\phi = \frac{[\text{det}(X'X)]^2}{\text{det}(X'VX) \cdot \text{det}(X'V+X)}.
\]

If rank \( V = v \ (p + 1 \leq v \leq n) \),

\[
1 \geq \phi \geq \prod_{i=1}^{m} \frac{4\lambda_i\lambda_{v-i+1}}{\left(\lambda_i + \lambda_{v-i+1}\right)^2} = \prod_{i=1}^{h} (1 - \rho_i^2),
\]

where \( m = \min\{p, v - p\} \) and \( h \) is the number of nonzero canonical correlations between the ordinary least squares estimate and its residual (Chu et al. [2004, 2005a]). These authors have also applied the Watson efficiency to partitioned regression models for the case when \( V \) is positive definite. The result about the canonical correlations still applies. For other bounds on the efficiency for the singular model see Sengupta and Jammalamadaka [2003: 316–318].

20.46. Let \( \mathcal{U} = \{ U : 0 \preceq U \preceq V, \mathcal{C}(U) \subseteq \mathcal{C}(X) \} \), where \( A \preceq B \) means that \( B - A \) is non-negative definite. The maximal element \( U \) in \( \mathcal{U} \) is called the shorted matrix (operator) with respect to \( X \), and is denoted by \( S(V | X) \). Then

\[
\text{var}(\theta^\dagger) = S(V | X).
\]

For further references relating to shorted matrices see Mitra and Puntanen [1991], Mitra and Puri [1979], and Mitra et al. [1995].

20.47. (Linear Restrictions) Suppose that we are interested in the linear (estimable) restrictions \( A\beta = c \). Let \( Q_H^\dagger \) be the residual sum of squares after fitting the model subject to the constraints.

(a) \( Q_H^\dagger - Q^\dagger = \left[(A\beta)^\dagger - c\right][\sigma^{-2}\text{var}(A\beta)^\dagger]^{-1}\left[(A\beta)^\dagger - c\right] \).

(b) \( \frac{Q_H^\dagger - Q^\dagger}{Q^\dagger} \cdot \frac{f}{m} \sim F_{m,f} \),

the \( F \)-distribution, where \( f = \text{rank}(V, X) - \text{rank} X \), \( m = \text{rank}[\text{var}(A\beta)^\dagger] \), and \( Q^\dagger \) is given in (20.44j).

Proofs. Section 20.7.3.

20.44d. See Rao [1973b]. The last expression for \( \theta^\dagger \) is derived by Sengupta and Jammalamadaka [2003: 252, with \( L = I \)].
We use the fact that $(MA)^+M = (MA)^+$ for any $A$ such that $(MA)^+$ exists, since $(MA)^+M$ satisfies the four conditions for it to be the Moore–Penrose inverse of $MA$, and $M$ is idempotent.


20.44h(iii). Isotalo et al. [2005b: 11].

20.44i. Sengupta and Jammalamadaka [2003: 253–255].


20.47. Sengupta and Jammalamadaka [2003: 277, 288].

20.8 OTHER MULTIVARIATE DISTRIBUTIONS

In this section we consider a number of continuous multivariate distributions. These distributions can be regarded as special cases of matrix variate distributions (cf. Section 21.9).

20.8.1 Multivariate $t$-Distribution

**Definition 20.17.** A $d \times 1$ random vector $\mathbf{x} = x_1, x_2, \ldots, x_d)'$ has a multivariate $t$-distribution if its probability density function is given by

$$f(\mathbf{x}) = \frac{\Gamma\left(\frac{\nu + d}{2}\right)}{(\pi \nu)^{d/2} \Gamma\left(\frac{\nu}{2}\right) (\det \Sigma)^{1/2}} \left[1 + \nu^{-1}(\mathbf{x} - \mu)'\Sigma^{-1}(\mathbf{x} - \mu)\right]^{-(\nu + d)/2},$$

$$(-\infty < x_i < \infty, \ i = 1, 2, \ldots, d),$$

where $\Sigma = (\sigma_{ij})$ is positive definite and $\Gamma(\cdot)$ is the Gamma function. We write $\mathbf{x} \sim t_d(\nu, \mu, \Sigma)$. The distribution $t_d(1, 0, I_d)$ is called the multivariate Cauchy distribution.

20.48. Suppose $\mathbf{x} \sim t_d(\nu, \mu, \Sigma)$, then:

(a) $E(\mathbf{x}) = \mu$ and $\text{var}(\mathbf{x}) = \nu \Sigma/(\nu - 2)$ ($\nu > 2$).

(b) $(x_i - \mu_i)/\sqrt{\sigma_{ii}} \sim t_\nu$, where $t_\nu$ is the univariate $t$-distribution with $\nu$ degrees of freedom.

(c) $(\mathbf{x} - \mu)'\Sigma^{-1}(\mathbf{x} - \mu)/d \sim F_{d, \nu}$, where $F_{d, \nu}$ is the univariate $F$-distribution with $d$ and $\nu$ degrees of freedom, respectively.

(d) Any subset of $\mathbf{x}$ has a multivariate $t$-distribution.

For further details see Kotz and Nadarajah [2004]. They also give a number of probability integrals and discuss the noncentral $t$-distribution.
20.8.2 Elliptical and Spherical Distributions

**Definition 20.18.** A \( d \times 1 \) random vector \( x \) is said to have an *elliptical distribution* with parameters \( \mu \) (\( d \times 1 \)) and \( V \) (\( d \times d \)) positive definite if its density function is of the form

\[
c_d(\det V)^{-1/2} h[(x - \mu)'V^{-1}(x - \mu)]
\]

for some function \( h \). We will write \( x \sim E_d(\mu, V) \) to denote that the distribution belongs to the class of elliptical distributions. The name comes from the fact that the above probability density function is constant on concentric ellipsoids

\[
(x - \mu)'V^{-1}(x - \mu) = c,
\]

and an alternative name is *elliptically contoured distribution*. The multivariate \( t \), multivariate normal, the contaminated normal, and a mixture of normal distributions are examples of elliptical distributions. Fang et al. [1990], Gupta and Varga [1993], and Kollo and von Rosen [2005: section 2.3] discuss these and other examples of elliptical distributions. The kurtosis for elliptical distributions need not be zero, so that its typical bell-shaped surface can be more or less peaked than the multivariate normal. This flexibility allows one to study the robustness of statistical inference based on the normal distribution. For the theory and statistical inference based on samples from elliptical distributions see Anderson [1993; 2003, section 3.6], Fang and Anderson [1990], and Kariya and Sinha [1989]. For some asymptotic theory see Anderson [2003: 102, 158]. Matrix versions of the elliptical distribution are also available (Anderson [2003] and Girko and Gupta [1996]).

20.49. Let \( x \sim E_d(\mu, V) \).

(a) For some function \( \psi \), the characteristic function of \( x \) is

\[
\phi(t) = E(e^{i't'x}) = e^{i't'\mu \psi(t'Vt)}.
\]

(b) From (a) we have that any subset of \( x \) has an elliptical distribution of the same form. For example, if \( x_1 \) and \( \mu_1 \) are the first \( k \) elements of \( x \) and \( \mu \) respectively, and \( V_{11} \) is the leading principal \( k \times k \) submatrix of \( \Sigma \), then \( x_1 \sim E_k(\mu_1, V_{11}) \).

(c) Provided they exist, \( E(x) = \mu \) and \( \text{var}(x) = aV \) for some constant \( a \). In terms of the characteristic function \( a = -2\psi'(0) \).

(d) It follows from (c) that all distributions in the class \( E_d(\mu, V) \) have the same mean \( \mu \) and the same correlation matrix \( \text{corr}(x) = (\rho_{ij}) \). Since \( a \) cancels out, we have \( \rho_{ij} = v_{ij} / (v_{ii}v_{jj})^{1/2} \).

(e) Let \( \Sigma = -2\psi'(0)V = (\sigma_{ij}) \) be the variance matrix of \( x \), and suppose that \( x \) has finite fourth moments. Then:

(i) The marginal distributions of the \( x_i \) all have zero skewness and the same kurtosis

\[
\gamma_2 = \frac{\kappa_4}{(\kappa_2)^2} = \frac{3[\psi''(0) - \psi'(0)^2]}{\psi'(0)^2} = 3\kappa, \quad \text{say},
\]

where \( \kappa_r \) is the \( r \)th cumulant.
(ii) All fourth-order cumulants are determined by $\kappa$, namely

$$\kappa_{ijkl} = \kappa(\sigma_{ij}\sigma_{kl} + \sigma_{ik}\sigma_{jl} + \sigma_{il}\sigma_{jk}).$$

This result is useful in asymptotic theory relating to smooth functions of elements of the sample variance matrix.

20.50. Let $x \sim E_d(\mu, V)$, where $V$ is diagonal. If $x_1, x_2, \ldots, x_n$ are mutually independent, then $x$ is multivariate normal.

20.51. Suppose $x \sim E_d(\mu, V)$ and $\mu$, $\mu_1$, and $V$ are partitioned as follows:

$$x = \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}, \quad \mu = \begin{pmatrix} \mu_1 \\ \mu_2 \end{pmatrix}, \quad \text{and} \quad V = \begin{pmatrix} V_{11} & V_{12} \\ V_{21} & V_{22} \end{pmatrix},$$

where $x_1$ and $\mu_1$ are $k \times 1$ and $V_{11}$ is $k \times k$. Provided the following exist, then:

(a) $E(x_1 \mid x_2) = \mu_1 + V_{12}V_{22}^{-1}(x_2 - \mu_2)$.

(b) $\text{var}(x_1 \mid x_2) = g(x_2)(V_{11} - V_{12}V_{22}^{-1}V_{21})$

for some function $g$. Moreover, the conditional distribution of $x_1$ given $x_2$ is $k$-variate elliptical. If $g(x_2)$ is a constant so that $\text{var}(x_1 \mid x_2)$ does not depend on $x_2$, then $x$ must be normal.

**Definition 20.19.** A $d \times 1$ random vector $x$ is said to have a spherical distribution if $x$ and $Tx$ have the same distribution for all $d \times d$ orthogonal matrices $T$. If $x$ has a density function, then this function depends on $x$ only through $x'x$. The multivariate normal $N_d(0, \sigma^2I_d)$ and the multivariate $t, t_d(\nu, 0, \sigma^2I_d)$, are spherical distributions.

20.52. If $x \sim E_d(0, I_d)$, then $x$ has a spherical distribution with a density function of the form $c_d h(x'x)$. Let

$$x_1 = r \sin \theta_1 \sin \theta_2 \cdots \sin \theta_{d-2} \sin \theta_{d-1}$$

$$x_2 = r \sin \theta_1 \sin \theta_2 \cdots \sin \theta_{d-2} \cos \theta_{d-1}$$

$$x_3 = r \sin \theta_1 \sin \theta_2 \cdots \cos \theta_{d-2}$$

$$\cdots$$

$$x_{d-1} = r \sin \theta_1 \cos \theta_2$$

$$x_d = r \cos \theta_1,$$

where $r > 0$, $0 < \theta_i \leq \pi$ ($i = 1, 2, \ldots, d - 2$), and $0 < \theta_{d-1} \leq 2\pi$. Then $r$, $\theta_1, \theta_2, \ldots, \theta_{d-1}$ are independent, and the distributions of $\theta_1, \ldots, \theta_{d-1}$ are the same for all $x$, with $\theta_k$ having a probability density function proportional to $\sin^{d-1-k} \theta_k$ (so that $\theta_{d-1}$ is uniformly distributed on $(0, 2\pi)$). Also $y = x'x = r^2$ has probability density function

$$f_y(y) = \frac{c_d \pi^{d/2}}{\Gamma(\frac{1}{2}d)} y^{(d/2)-1} h(y), \quad (y > 0).$$

In particular, if $x \sim N_d(0, I_d)$, we have $h(y) = e^{-y/2}$ leading to the familiar result that $y \sim \chi^2_d$. 
20.53. Let $x$ have a $d$-dimensional spherical distribution with $\Pr(x = 0) = 0$.

(a) If $u = \|x\|_2 = (x'x)^{1/2}$ and $y = \|x\|_2^{-1}x$, then $y$ is uniformly distributed over a $d$-dimensional sphere located at the origin with unit radius, and $y$ and $u$ are independent.

(b) If $v = a'x/\|x\|_2$, where $a \in \mathbb{R}^d$ and $a'a = 1$, then
$$w = (d - 1)^{1/2} \frac{v}{(1 - v^2)^{1/2}} \sim t_{d-1},$$
the $t$-distribution.

(c) If $A$ is a $d \times d$ symmetric idempotent matrix of rank $k$, then $z = x'Ax/x'x$ has a beta distribution with parameters $\frac{1}{2}k$ and $\frac{1}{2}(d - k)$.

Proofs. Section 20.8.2.

20.49. Muirhead [1982: 34–42].

20.50. Muirhead [1982: 35].


20.8.3 Dirichlet Distributions

Definition 20.20. Let $x = (x_1, x_2, \ldots, x_d)'$ be a $d \times 1$ random vector. Then $x$ is said to have a Type-1 Dirichlet distribution if its density function is given by
$$f(x) = \frac{\Gamma(\alpha_1 + \cdots + \alpha_{d+1})}{\Gamma(\alpha_1) \cdots \Gamma(\alpha_{d+1})} x_1^{\alpha_1-1} \cdots x_d^{\alpha_d-1} (1 - x_1 - \cdots - x_d)^{\alpha_{d+1}-1}$$
for $0 < x_i < 1, i = 1, \ldots, d$, $x_1 + \cdots + x_d < 1$, and $\alpha_i > 0$ for $i = 1, \ldots, d + 1$.

We shall write $x \sim D_1(d, \alpha)$, where $\alpha = (\alpha_i)$.

Also $x$ is said to have a Type-2 Dirichlet distribution if its density function is given by
$$f(x) = \frac{\Gamma(\alpha_1 + \cdots + \alpha_{d+1})}{\Gamma(\alpha_1) \cdots \Gamma(\alpha_{d+1})} x_1^{\alpha_1-1} \cdots x_d^{\alpha_d-1} (1 + x_1 + \cdots + x_d)^{-(\alpha_1 + \cdots + \alpha_{d+1})}$$
for $0 < x_i < \infty, i = 1, \ldots, d$ and $\alpha_i > 0$ for $i = 1, 2, \ldots, d + 1$.

We shall write $x \sim D_2(d, \alpha)$. The above are special cases of the matrix versions in Section 21.9.

20.54. Let $y_1, y_2, \ldots, y_m$ be independently distributed as $\chi^2$ variables with degrees of freedom $\alpha_1, \alpha_2, \ldots, \alpha_m$, respectively. If $x_i = y_i/\sum_{j=1}^m y_j$ for $i = 1, 2, \ldots, m - 1$, then $x \sim D_1(m - 1, \alpha/2)$.

Proofs. Section 20.8.3.

CHAPTER 21

RANDOM MATRICES

21.1 INTRODUCTION

Matrices of random variables occur frequently in statistics, especially in the subject of multivariate analysis. Because the latter is a large subject with numerous reference books, I have had to be somewhat selective in my choice of topics. In this chapter, as in the previous one, the upper- and lowercase letters of the alphabet from $a$ to $t$, excluding $Q$, refer to constants, while the remainder generally refer to random variables. Unless otherwise stated, all vectors and matrices are real.

**Definition 21.1.** Let

$$X = (x_{ij}) = \begin{pmatrix} x_1' \\ x_2' \\ \vdots \\ x_n' \end{pmatrix} = (x^{(1)}, x^{(2)}, \ldots, x^{(d)})$$

be an $n \times d$ matrix of random variables with rows that all have the same variance matrix $\Sigma$ and are uncorrelated, that is,

$$\text{cov}(x_r, x_s) = \delta_{rs} \Sigma,$$

where $\delta_{rs} = 1$ for $r = s$ and $\delta_{rs} = 0$ for $r \neq s$. We shall call a matrix with the above properties a **data matrix**.
In practice, the \( x_r \) are usually a random sample, which implies they are independently and identically distributed, that is, i.i.d. However, this won’t be assumed unless indicated.

21.1. If \( x_i \) defined above has mean \( \mu_i \) for each \( i \), then \( E(x_i x'_j) = \delta_{ij} \Sigma + \mu_i \mu'_j \).

21.2. (Some Vec Properties) Let \( X \) be a data matrix as defined above; that is, the columns of \( X' \) are uncorrelated and have the same variance matrix \( \Sigma \). Here “\( \otimes \)” is the Kronecker product.

(a) \( \text{var(vec} X) = \Sigma \otimes I_n \) and \( \text{var(vec} X') = I_n \otimes \Sigma \).

(b) Using \( \text{vec(AXB)} = (B' \otimes A) \text{vec} X \), we have, from (20.6b), (11.1e), and (11.11a),

\[
\text{var[vec(AXB)]} = (B' \otimes A)(\Sigma \otimes I_n)(B' \otimes A)' = (B' \Sigma B) \otimes (AA').
\]

(c) \( \text{var[vec(AX'B)]} = \text{var[(B' \otimes A)vec} X'] = (B' B) \otimes (A \Sigma A') \).

(d) \( \text{cov[vec(AXB), vec(CXD)]} = (B' \Sigma D) \otimes (AC') \).

(e) From (d) we see that if \( U = AXB \) and \( V = CXD \), then \( U \) and \( V \) are pairwise uncorrelated, that is \( \text{cov}(u_{ij}, v_{rs}) = 0 \) for all \( i, j, r, \) and \( s \), if \( AC' = 0 \) and/or \( B' \Sigma D = 0 \).


21.1. Set \( x_i = x_i - \mu_i + \mu_i \) and use (20.5).

21.2. For (a), see Henderson and Searle [1979: 78, with our \( X \) being their \( X' \)]; using (20.6), the proofs of (c) and (d) are similar to (b); and (e) follows from (d).

21.2 GENERALIZED QUADRATIC FORMS

21.2.1 General Results

Definition 21.2. If \( X = (x_1, x_2, \ldots, x_n)' \) is an \( n \times d \) data matrix and \( A = (a_{ij}) \) is a symmetric \( n \times n \) matrix, we shall call the expression \( X'AX = \sum_{i=1}^{n} \sum_{j=1}^{n} a_{ij} x_i x_j' \) a generalized quadratic.

21.3. Using the above notation, let \( \bar{x} = \sum_{i=1}^{n} x_i / n \) and \( \bar{X} = (x_1 - \bar{x}, \ldots, x_n - \bar{x})' \). Then:

(a) \( \bar{X}' \bar{X} = \sum_{i=1}^{n} (x_i - \bar{x})(x_i - \bar{x})' = \sum_{i=1}^{n} x_i x_i' - n \bar{x} \bar{x}' = X'AX \) (\( = Q \), say),

where \( A = (a_{ij}) \) and \( a_{ij} = \delta_{ij} - n^{-1} \). Thus, \( A = I_n - I_n \bar{1}' / n = I_n - P_1 \) is the so-called centering matrix, where \( P_1 \) is the orthogonal projection onto \( \mathcal{C}(I_n) \).

(b) Suppose the \( x_i \) are i.i.d. with mean \( \mu \) and variance matrix \( \Sigma \), and \( S = Q / (n - 1) \). Then

\[
E(S) = \Sigma,
\]
so that $S$, the so-called sample variance matrix, is an unbiased estimator of $\Sigma$. Some writers define $\tilde{S} = (n - 1)S/n$ to be the sample variance matrix; it is the maximum likelihood estimator of $\Sigma$ under normality assumptions.

(c) If diag(s) is the diagonal matrix whose elements are the diagonal elements of $S$, then the sample correlation matrix is given by

$$R = [\text{diag}(s)]^{-1/2}S[\text{diag}(s)]^{-1/2}.$$

(d) The (sample) Mahalanobis distance

$$D_i^2 = (x_i - \bar{x})'S^{-1}(x_i - \bar{x})$$

is the $i$th diagonal element of $(n - 1)\bar{X}(\bar{X}'\bar{X})^{-1}\bar{X}$, and it is often used for diagnostic purposes.

(e) (i) Taking the trace of (a) and using $\text{trace}(cd') = \text{trace}(d'c) = d'c$, we get

$$\sum_{i=1}^{n} (x_i - \bar{x})' (x_i - \bar{x}) = \sum_{i=1}^{n} x_i'(x_i - n\bar{x}'\bar{x}).$$

(ii)

$$\sum_{r=1}^{n} \sum_{s=r+1}^{n} (x_r - x_s)(x_r - x_s)' = \frac{1}{2} \sum_{i \neq j} (x_r - x_s)(x_r - x_s)'$$

$$= n \sum_{i=1}^{n} (x_i - \bar{x})(x_i - \bar{x})'.$$

(iii) Taking traces in (ii),

$$\sum_{r=1}^{n} \sum_{s=r+1}^{n} ||x_r - x_s||^2 = n \sum_{i=1}^{n} ||x_i - \bar{x}||^2.$$

This result arises in cluster analysis.

We obtain the corresponding univariate cases by taking $d = 1$ in the above results.

21.4. (Asymptotic Sample Theory) Suppose that the $d \times 1$ vectors $x_1, x_2, \ldots, x_n$ are independently and identically distributed (i.i.d.) with mean $\mu$ and variance matrix $\Sigma$.

(a) As $n \to \infty$, $\sqrt{n}(\bar{x} - \mu)$ is asymptotically distributed as $N_d(0, \Sigma)$.

(b) Let $Q = (n - 1)S$.

(i) As $n \to \infty$, $n^{-1/2}(\text{vec} Q - n\text{vec} \Sigma)$ is asymptotically $N_{d^2}(0, V)$, where

$$V = \text{var} \{\text{vec} [(x_i - \mu)(x_i - \mu)']\} = \text{var}[(x_i - \mu) \otimes (x_i - \mu)],$$

by (11.15c).

(ii) In terms of $S$, we have $(n-1)^{1/2}(\text{vec} S - \text{vec} \Sigma)$ is asymptotically $N_{d^2}(0, V)$. 

(c) If $A$ is a real symmetric $n \times n$ matrix, then, under certain conditions, $Q = X'AX$ is asymptotically normal as $n \rightarrow \infty$.

For further details and references see Mathai and Provost [1992: section 4.6b].

21.5. (Asymptotic Theory) Suppose $\sqrt{n}(y - \theta)$ is asymptotically $N_d(0, \Sigma)$, and let $f(u)$ be a $q$-dimensional vector-valued function of $u$ such that each component $f_j(u)$ has a nonzero differential at $u = \theta$. If $F = (f_{ij})$, where $f_{ij} = \partial f_j(u)/\partial u_i$, then

$$\sqrt{n}[f(u) - f(\theta)]$$

is asymptotically $N_q(0, F'\Sigma F)$.

21.6. Suppose $X'$ has columns $x_i$, then

$$E(X'AX) = \sum_{i=1}^{n} \sum_{j=1}^{n} a_{ij} \text{cov}(x_i, x_j) + E(X')AE(X).$$

21.7. Suppose the $x_i$, the columns of $X'$, are statistically independent and $\text{var}(x_i) = \Sigma_i$ for $i = 1, 2, \ldots, n$. Then, from (21.6),

(a) $E(X'AX) = \sum_{i=1}^{n} a_{ii} \Sigma_i + E(X')AE(X)$.

(b) If $\Sigma_i = \Sigma$ for all $i$, then from (a) we have

$$E(X'AX) = (\text{trace } A)\Sigma + E(X')AE(X).$$

(c) Suppose that the $x_i$ are i.i.d. with mean 0 and variance matrix $\Sigma$. If $V = X'X$ and $E(x_i x_i' \otimes x_i x_i') = \Psi$, then

$$\text{var}(\text{vec } V) = n[\Psi - (\text{vec } \Sigma)(\text{vec } \Sigma)'].$$

21.8. (Independence) Let $X' = (x_1, x_2, \ldots, x_n)$, where the $x_i$ are independently distributed as $N_d(\mu_i, \Sigma)$ $(i = 1, 2, \ldots, n)$ and $\Sigma$ is positive definite. Suppose $A$ and $B$ are $n \times n$ symmetric matrices and $C$ is a $k \times n$ matrix. Then:

(a) $X'AX$ and $X'BX$ are statistically independent if and only if $AB = 0$.

(b) $CX$ and $X'AX$ are statistically independent if and only if $CA = 0$.

Setting $C = b'$, we have that $X'b$ and $X'AX$ are statistically independent if and only if $Ab = 0$.

More generally:

(c) Let $Q_i = X'A_i X + \frac{1}{2}(L_i X + X'L_i') + C_i$, where $A_i$ and $C_i$ are real symmetric matrices $(i = 1, 2)$. Then $Q_1$ and $Q_2$ are statistically independent if and only if

$$A_1 A_2 = 0, \quad L_1 A_2 = 0, \quad L_2 A_1 = 0, \quad \text{and} \quad L_1 L_2' = 0.$$ 

We can get various special cases by setting $A_i = 0$ or $L_i = 0$. Mathai and Provost [1992: 286–287] also give results for the case when $\Sigma$ is singular.

Proofs. Section 21.2.1.

21.3a–b. Seber [1984: 8–9].
21.7a. Seber [1984: 6–7].

21.2.2 Wishart Distribution

**Definition 21.3.** Let \( X = (x_1, x_2, \ldots, x_n)' \) be an \( m \times d \) matrix with rows which are independently and identically distributed (i.i.d.) as the multivariate normal distribution \( N_d(0, \Sigma) \), subject to two conditions, namely (i) \( d \leq m \) and (ii) \( \Sigma \) is positive definite. If \( W = X'X \), then \( W \) is said to have a (nonsingular) Wishart distribution with \( m \) degrees of freedom and we write \( W \sim W_d(m, \Sigma) \). The joint probability probability density function of the distinct elements of the symmetric matrix \( W \) (the \( \frac{1}{2}d(d + 1) \) variables in the upper triangle, say) is given in (21.67). This Wishart distribution can, of course, be defined directly in terms of its density function, though the above representation is more convenient for developing the theory, especially in the singular case. If at least one of the two conditions does not hold, then the distribution is said to be singular (cf. Srivastava [2003] for some details). We use \( m \) instead of \( n \) here as \( X \) is used as a "representation" rather than coming from a particular random sample of size \( m \). If \( W \sim W_d(m, \Sigma) \), then we can simply choose any matrix \( X \) with rows which are i.i.d. \( N_d(0, \Sigma) \). Then \( X'X \) has the same distribution as \( W \) and can be used as a "proxy" for the latter. For this reason, most authors simply set \( W = X'X \) (e.g., Seber [1984: 21]). For other general references relating to the Wishart distribution see Anderson [2003] and Muirhead [1982]; in fact most theoretical books on multivariate analysis cover the Wishart distribution in detail.

If the \( x_i \) are independently distributed as \( N_d(\mu_i, \Sigma) \) with \( \Sigma \) positive definite, then \( W = X'X \) has a noncentral Wishart distribution, generally written as \( W_d(m, \Sigma; \Delta) \), where

\[
\Delta = \Sigma^{-1/2}M'M\Sigma^{-1/2}, \quad M = (\mu_1, \mu_2, \ldots, \mu_m)' = E(X),
\]

and \( \Sigma^{1/2} \) is the positive square root of \( \Sigma \) (cf. 10.32). Here \( \Delta \) is called the noncentrality matrix and, since the distribution of \( W \) depends only on the eigenvalues of \( \Delta \), other expressions are used for the noncentrality parameter (Seber [1984: section 2.3.3]). Muirhead [1984: section 10.3] defines \( \Delta = \Sigma^{-1}M'M \) and gives the probability density function of the noncentral distribution and its properties.

When \( W \) has a nonsingular distribution, \( W^{-1} \) is said to have an inverted Wishart. For some details see Anderson [2003: section 7.7] and Muirhead [1982: 113, exercise 3.6]. A generalized version also exists (Brown [2002]).
21.9. An important special case is when the $x_i$ are all $N_d(0,\sigma^2 I_d)$. Then the elements of $X$ are all i.i.d. $N(0,\sigma^2)$ and $X'X \sim W_d(m, I_d)$.

21.10. If the $x_i (i=1,2,\ldots,m)$ are independently distributed as $N_d(\mu_i, \Sigma)$ with $\Sigma$ positive definite, then using (21.2a) we have

$$\text{vec}(X') \sim N_{md}(\text{vec}(M'), I_m \otimes \Sigma),$$

where $M = (\mu_1, \mu_2, \ldots, \mu_m)'$.

21.11. Suppose $W = X'X \sim W_d(m, \Sigma; \Delta)$, where $X$ is defined above. Then:

(a) $\text{E}(W) = m\Sigma + M'M$, where $M$ is defined above. For this reason, some authors define the noncentrality parameter to be $\Phi = M'M$ or even $\frac{1}{2} \Phi$ (e.g., Schott [2005: 422]), which have some advantages, as demonstrated in (21.12) below.

(b) $\text{var}(\text{vec} W) = 2P_m[d(\Sigma \otimes \Sigma) + \Sigma \otimes M'M + M'M \otimes \Sigma]$, where $P_m$ is the symmetrizer matrix defined in Section 11.5.1.

21.12. If we redefine the parameters of a noncentral Wishart and write $W \sim W_d(m, \Sigma; \Phi)$, where $\Sigma$ is positive definite and $\Phi = M'M$, and $C$ is $q \times d$ of rank $q$, then $CWC' \sim W_d(m, C\Sigma C'; C\Phi C')$. In terms of the previous notation, we have $\Delta = (C\Sigma C')^{-1/2}C\Phi C'(C\Sigma C')^{-1/2}$.

21.13. Suppose $W = (w_{ij})$ has a nonsingular Wishart distribution $W_d(m, \Sigma)$.

(a) $W$ is positive definite with probability 1.

(b) The eigenvalues of $W$ are distinct with probability 1.

(c) $\text{E}(W) = m\Sigma$, which still holds if $W$ is singular.

(d) Let $C$ be a $q \times d$ matrix of rank $q$.

(i) $CWC' \sim W_q(m, C\Sigma C')$ and is nonsingular. We have the following special cases.

(ii) Setting $C = a'$ ($a \neq 0$), we have $a'Wa \sim \sigma_n^2 \chi_m^2$, where $\sigma_n^2 = a'\Sigma a$.

(iii) By choosing $C = (I_r, 0) \ (r \leq d)$, or an appropriate permutation of its columns, we see that an $r \times r$ principal submatrix of $W$ has the Wishart distribution $W_r(m, \Sigma_{rr})$, where $\Sigma_{rr}$ is the corresponding $r \times r$ principal submatrix of $\Sigma$.

(iv) If $W$ is singular and rank $C \leq q$, then $CWC'$ has a singular Wishart distribution.

(e) $w_{jj}/\sigma_{jj} \sim \chi_m^2 \ (j=1,2,\ldots,d)$. However, they are not statistically independent. Also $w_{ij}/\sigma_{ij}$ is not chi-square for $i \neq j$.

(f) $\det W/\det \Sigma$ is distributed as a product of $d$ independent chi-square variables with respective degrees of freedom $m, m-1, \ldots, m-d+1$. 

(g) The moment generating function (m.g.f.) of $W = (w_{ij})$ is

$$M(T) = E \left[ \exp \left( \sum_{j=1}^{k} \sum_{k=1}^{d} t_{jk} w_{jk} \right) \right]$$

$$= E \{ \exp[\text{trace}(UW)] \}$$

$$= [\det(I_d - 2U\Sigma)]^{-m/2},$$

where $U = U'$, $u_{jj} = t_{jj}$ and $u_{jk} = u_{kj} = \frac{1}{2} t_{jk}$ ($j < k$). Since this moment generating function exists in a neighborhood of $T = 0$, it uniquely determines the (nonsingular) probability density function of $W$ and can therefore be used for deriving a number of results given below. The characteristic function is derived by Muirhead [1982: 87].

We have essentially found the m.g.f. of $X'X$ when the columns of $X'$ are i.i.d. $N_d(0, \Sigma)$, where $\Sigma$ is positive definite. The m.g.f. of $X'AX + \frac{1}{2}(LX+X'L') + C$ when the columns of $X'$ are i.i.d. $N_d(\mu, \Sigma)$ is given by Mathai and Provost [1992: section 6.4]. They also give results for the cases when the $x_i$ are correlated and $\Sigma$ is singular.

21.14. Let $W \sim W_d(m, \Sigma)$, where $\Sigma$ is possibly singular, and let $A$ be a $d \times d$ (not necessarily symmetric) matrix. Then:

(a) $E(WAW) = m[\Sigma A \Sigma + \text{trace}(A^2)A] + m^2 \Sigma A \Sigma.$

(b) If $m > d + 1$, and $\Sigma$ is nonsingular, then

(i) $E(WAW^{-1}) = \frac{1}{m-d-1} [m \Sigma A \Sigma^{-1} - A' - (\text{trace} A)I_d].$

(ii) $E(W^{-1}AW) = \frac{1}{m-d-1} [m \Sigma^{-1} A \Sigma - A' - (\text{trace} A)I_d].$

(c) If $m > d + 3$, and $\Sigma$ is nonsingular, then

$$E(W^{-1}AW^{-1}) = \frac{(m-d-2)\Sigma^{-1}A\Sigma^{-1} + \Sigma^{-1}A\Sigma^{-1} - \text{trace}(A\Sigma^{-1})\Sigma^{-1}}{(m-d)(m-d-1)(m-d-3)}.$$

21.15. Suppose that the columns $x_i$ ($i = 1, \ldots, m$) of $X'$ are independently distributed as $N_d(\mu_i, \Sigma)$ with $\Sigma$ positive definite, and $A$ is a symmetric $d \times d$ matrix of rank $r$. Then, if $A$ is idempotent, we have

$$X'AX \sim W_d(m, \Sigma; \Delta),$$

the noncentral Wishart distribution with

$$\Delta = \Sigma^{-1/2}M'AM\Sigma^{-1/2} \quad \text{and} \quad M = (\mu_1, \mu_2, \ldots, \mu_m).$$

The case when the $x_i$ are not independent and $\Sigma$ is non-negative definite is considered by Vaish and Chaganty [2004: 382].

21.16. Suppose that $m$ columns of $X'$ are i.i.d. as $N_d(0, \Sigma)$, where $\Sigma$ is positive definite, and let $A$ and $B$ be $m \times m$ symmetric matrices.
(a) Let $X'AX$ and $X'BX$ have Wishart distributions. They are statistically independent if and only if $AB = 0$. (This result is generalized in (21.17).)

(b) Let $X'AX$ have a Wishart distribution. Then $X'b$ is statistically independent of $X'AX$ if and only if $Ab = 0$.

21.17. Suppose that the columns $x_i$ $(i = 1, \ldots, m)$ of $X'$ are independently distributed as $N_d(\mu_i, \Sigma)$, and let $A_1, A_2, \ldots, A_t$ be a sequence of $n \times n$ symmetric matrices with ranks $r_1, r_2, \ldots, r_t$ such that $\sum_{i=1}^t A_i = I_n$. If one (and therefore all) of the conditions of (8.78) hold, then the $X'A_iX$ $(i = 1, 2, \ldots, t)$ are independently distributed as the noncentral Wishart, $W_d(r_i, \Sigma; \Delta_i)$, where $\Delta_i = \Sigma^{-1/2}M'A_iM\Sigma^{-1/2}$ is the noncentrality parameter and $M = (\mu_1, \mu_2, \ldots, \mu_m)'$. An extension of this result to the case when the $x_i$ are not independent and $\Sigma$ is non-negative definite is given by Vaish and Chaganty [2004: 383] and Tian and Styan [2005: 391].

21.18. If $W_i \sim W_d(m_i, \Sigma)$ $(i = 1, 2)$, and $W_1$ and $W_2$ are statistically independent, then $W_1 + W_2 \sim W_d(m_1 + m_2, \Sigma)$.

21.19. Let

$$W = \begin{pmatrix} W_{11} & W_{12} \\ W_{12} & W_{22} \end{pmatrix} \sim W_d(m, \Sigma), \quad m \leq d,$$

where $\Sigma$ is positive definite, $W_{ii}$ is $d_i \times d_i$ $(i = 1, 2)$, and $d_1 + d_2 = d$. Suppose $\Sigma$ is partitioned in the same way as $W$ and $\Sigma_{22.1} = \Sigma_{22} - \Sigma_{21}\Sigma_{11}^{-1}\Sigma_{12}$.

(a) We have $W_{22.1} = W_{22} - W_{21}W_{11}^{-1}W_{12} \sim W_d(m - d_1, \Sigma_{22.1})$, and $W_{22.1}$ is statistically independent of $(W_{11}, W_{12})$. Note that $W_{12} = W_{21}$.

(b) If $\Sigma_{12} = 0$, then $Y = W_{21}W_{11}^{-1}W_{12} \sim W_d(d_1, \Sigma_{22})$ and $Y$ is statistically independent of $W_{22.1}$.

Definition 21.4. (Hotelling’s Distribution) Suppose $y \sim N_d(0, \Sigma)$, $W \sim W_d(m, \Sigma)$, $y$ is statistically independent of $W$, and both distributions are nonsingular. Then

$$T^2 = my'W^{-1}y$$

is said to have a Hotelling’s distribution, and we write $T^2 \sim T_{d,m}^2$.

21.20. Referring to the above definition, $F = \frac{T_{d,m}^2}{m - d + 1} \sim F_{d,m - d + 1}$, the $F$-distribution with $d$ and $m - d + 1$ degrees of freedom, respectively.

If, instead, $y \sim N_d(\theta, \Sigma)$, then $F \sim F_{d,m - d + 1, \delta}$, the noncentral $F$-distribution with noncentrality parameter $\delta = \theta'\Sigma\theta$.

21.21. (Eigenvalues)

(a) If the probability density function of the $m \times d$ matrix $Y$ is $f(Y'Y)$, then the probability density of $B = Y'Y$ is

$$\frac{\pi^{dm/2}}{\Gamma_d(\frac{1}{2}m)}(\det B)^{(m-d-1)/2}f(B),$$

where $\Gamma_d(\cdot)$ is given by (21.67).
(b) If the real symmetric $d \times d$ matrix $C$ has a probability density function of the form $g(\lambda_1, \lambda_2, \ldots, \lambda_d)$, where $\lambda_1 > \lambda_2 > \cdots > \lambda_d$ are the eigenvalues of $C$, then the probability density function of the eigenvalues is

$$\frac{\pi^{d^2/2}}{\Gamma_d(d/2)} g(\lambda_1, \ldots, \lambda_d) \prod_{i<j} (\lambda_i - \lambda_j).$$

(c) Suppose $W \sim W_d(m, I_d)$. Using (a) and (b), the probability density function of the eigenvalues of $W$ is

$$\frac{\pi^{d^2/2}}{2^{dm/2} \Gamma_d(d/2) \Gamma_d((d-1)/2)} \exp(-\frac{1}{2} \sum_{i=1}^{d} \lambda_i) \prod_{i<j} (\lambda_i - \lambda_j).$$

(d) Suppose $W \sim W_d(m, \Sigma)$, where $m \geq d$ and $\Sigma$ is positive definite. Then the probability density function of the eigenvalues of $W$ is

$$\frac{\pi^{d^2/2}}{2^{dm/2} \Gamma_d(d/2) \Gamma_d((d-1)/2)} \prod_{i<j} (\lambda_i - \lambda_j) \ _0F_0^d(-\frac{1}{2} \Lambda, \Sigma^{-1}), \quad (\lambda_1 > \cdots > \lambda_d > 0),$$

where $\Lambda = \text{diag}(\lambda_1, \ldots, \lambda_d)$ and $\ _0F_0^d$ is a two-matrix hypergeometric function. When $\Sigma = I_n$, we have

$$\ _0F_0^1(-\frac{1}{2} \Lambda, I_d) = \ _0F_0^1(-\frac{1}{2} \Lambda, I_d) = \exp(-\frac{1}{2} \text{trace} \Lambda),$$

which gives us (c).

21.22. (Generalized Eigenvalues) Let $W_i$ ($i = 1, 2$) be independently distributed as nonsingular $W_d(m_i, \Sigma)$ (i.e., $m_1, m_2 \geq d$ and $\Sigma$ positive definite). The probability density function of the generalized eigenvalues, namely the roots of

$$\det(W_1 - \lambda W_2) = 0,$$

is

$$\frac{\pi^{d^2/2}}{\Gamma_d(d/2 \Gamma_d((m_1 + m_2)/2))} \prod_{i=1}^{d} \lambda_i^{(m_1 - d)/2} \prod_{i=1}^{d} (\lambda_i + 1)^{-(m_1 + m_2)/2} \prod_{i<j} (\lambda_i - \lambda_j),$$

for $\lambda_1 \geq \cdots \geq \lambda_d \geq 0$.

Definition 21.5. (Complex Wishart Distribution) Suppose $x_1, x_2, \ldots, x_m$ are independently and identically distributed as the complex multivariate normal distribution $N_d^c(0, \Sigma_x)$ (cf. Section 20.6), then $W = \sum_{i=1}^{m} x_i x_i^*$ is said to have a complex Wishart distribution denoted by $W_d^c(m, \Sigma_x)$. It is used in approximating the distributions of estimates of spectral density matrices in multivariate time series and in random normal (Gaussian) processes generally. Some of the properties of the (real) Wishart distribution carry over into the complex case. For a number of references see Brillinger [1975: 90].

21.23. Suppose $W = (w_{ij}) \sim W_d^c(m, \Sigma_x)$, where $m \geq d$ and $\Sigma_x$ is Hermitian positive definite. Then:
(a) The probability density function of the distinct elements of $W$ is
\[
\frac{(\det W)^{m-d} \exp\left[ -\frac{1}{2} \text{trace}(\Sigma_x^{-1} W) \right]}{\pi^{d(d-1)/2}(\det \Sigma_x)^m \prod_{j=1}^d \Gamma(m-j+1)}.
\]

(b) $E(W) = m\Sigma_x$.

Proofs. Section 21.2.2.

21.11a. Follows from (21.7b) with $A = I_m$.
21.18. This can be readily proved using moment generating functions (cf. 21.13g).
21.21a. Anderson [2003: 539, with $Y \rightarrow Y'$ and $p \rightarrow d$].
21.21c. Anderson [2003: 539] and Muirhead [1982: 389, with $\lambda = 1, n\lambda_i = \lambda_i$].
21.21d. For details see Muirhead [1982: 388–389, with $\lambda_i = n\lambda_i$].

21.3 RANDOM SAMPLES

21.3.1 One Sample

21.24. Let $x_i, i = 1, 2, \ldots, n$, be a random sample from a $d$-dimensional distribution with mean $\mu$ and variance matrix $\Sigma$. Let $X = (x_1, x_2, \ldots, x_n)'$ be the data matrix and let $z_i = x_i - \mu$ ($i = 1, 2, \ldots, n$). Suppose that the following third and fourth moment matrices exist, namely
\[
\Phi = E(z_i \otimes z_i z_i') \quad \text{and} \quad \Psi = E(z_i z_i' \otimes z_i z_i'),
\]
where "⊗" is the Kronecker product. Let \( z = (z_1', z_2', \ldots, z_n')' = \text{vec}(X') - I_n \otimes \mu \) so that \( E(z) = 0 \) and \( E(zz') = \text{var}(\text{vec} X') = I_n \otimes \Sigma \) (by (21.2a)). Define \( \Phi_* = E(z \otimes zz') \) and \( \Psi_* = E(zz' \otimes zz') \). Then:

(a) If \( K_{dn} \) (I_{(n,d)}) is the commutation (vec-permutation) matrix, \( E_{ii} = e_i e_i' \) is an \( n \times n \) matrix with 1 in the \((i,i)\)th position and zeros elsewhere, and \( G = (E_{11}, E_{22}, \ldots, E_{nn})' \), then

\[
\Phi_* = (I_n \otimes K_{dn} \otimes I_d)(G \otimes \Phi).
\]

(b) If \( K_{nn} = \sum_{i=1}^n (E_{ii} \otimes E_{ii}) \), then

\[
\Psi_* = (I_{n^2d^2} + K_{nd,nd})(I_n \otimes \Sigma \otimes I_n \otimes \Sigma) + [\text{vec}(I_n \otimes \Sigma)][\text{vec}(I_n \otimes \Sigma)']' + (I_n \otimes K_{dn} \otimes I_d)(K_{nn} \otimes [\Psi - (I_{d^2} + K_{dd})(\Sigma \otimes \Sigma)] - (\text{vec} \Sigma)(\text{vec} \Sigma')'(I_n \otimes K_{nd} \otimes I_d).
\]

(c) Under normality we have the following results.

(i) \( \Phi = \Phi_* = 0 \).

(ii) If \( P_d = \frac{1}{2}(I_{d^2} + K_{dd}) \) (the symmetrizer matrix), then, from (20.24b),

\[
\Psi = 2P_d(\Sigma \otimes \Sigma) + (\text{vec} \Sigma)(\text{vec} \Sigma')'.
\]

(iii) \( \Psi_* = 2P_{nd}(I_n \otimes \Sigma \otimes I_n \otimes \Sigma) + [\text{vec}(I_n \otimes \Sigma)][\text{vec}(I_n \otimes \Sigma)']' \).

Methods for finding \( E(x \otimes x \otimes x), E(x \otimes x \otimes x \otimes x) \), and higher moments are given by Meijer [2005].

21.25. Let \( x_i, i = 1, 2, \ldots, n \), be a random sample from a nonsingular normal distribution \( N_d(\mu, \Sigma) \). Then:

(a) \( \bar{x} \sim N_d(\mu, \Sigma/n) \).

(b) \( Q = (n - 1)S \sim W_d(n - 1, \Sigma) \).

(c) From (b) we can obtain the probability density function of the eigenvalues of \( Q \), and therefore those of \( S \). As this joint distribution is rather intractable, asymptotic theory has been developed for large \( n \) for both the eigenvalues and eigenvectors of \( S \), especially as related to providing approximate inferential procedures for principal component analysis. The reader is referred to Seber [1984: 197-199] for a summary of the results, and to Anderson [2003: section 13.5], Muirhead [1982: chapter 9], and Schott [2005: 427-429] for further details and some derivations.

(d) We consider some properties of \( S \). Here \( P_d \) is the symmetrizer matrix (cf. 20.24b) and \( G_d \) is the duplication matrix.

(i) \( \text{var}(\text{vec} S) = (n - 1)^{-1}2P_d(\Sigma \otimes \Sigma) = (n - 1)^{-1}2P_d(\Sigma \otimes \Sigma)P_d \).

(ii) We note that the above matrix in (i) is singular as \( S \) is symmetric, which implies that \( \text{vec} S \) has repeated elements. We can get round this by using the vector \( \text{vech} S \). Then

\[
\text{var}(\text{vech} S) = \frac{2}{n - 1}G_d^+P_d(\Sigma \otimes \Sigma)P_dG_d^+. \]
(iii) As \( n \to \infty \), \((n - 1)^{1/2}(\text{vec}\, S - \text{vec}\, \Sigma)\) is asymptotically distributed as \( N_{d^2}(0, V) \), where \( V = 2P_d(\Sigma \otimes \Sigma) \).

(iv) From vech\, S = \( G^+_d \text{vec}\, S \), (20.6b), and (iii), \((n - 1)^{1/2}(\text{vech}\, S - \text{vech}\, \Sigma)\) is asymptotically distributed as \( N_k(0, G^+_d V G^+_d) \), where \( k = d(d+1)/2 \).

(v) If \( s = \text{diag}\, S \) and \( \sigma = \text{diag}\, \Sigma \), then

\[
E(s) = \sigma \quad \text{and} \quad \text{var}(s) = \frac{2}{n - 1}(\Sigma \circ \Sigma),
\]

where "\( \circ \)" is the Hadamard product. Also, as \( n \to \infty \), \((n - 1)^{1/2}(s - \sigma)\) is asymptotically distributed as \( N_d(0, 2\Sigma \circ \Sigma) \).


e) \( \bar{x} \) and S are statistically independent.

(f) \( \bar{x} \) and S are jointly sufficient and complete for \( \mu \) and \( \Sigma \).

(g) A useful statistic is

\[(i) \quad T^2 = n(\bar{x} - \mu)S^{-1}(\bar{x} - \mu) \sim T^2_{d,n-1} \text{ (cf. 21.20). This statistic can be used for testing the null hypothesis } H_0 : \mu = \mu_0.\]

(ii) When the underlying data come from an elliptical distribution, \( T^2 \) is asymptotically \( \chi^2_d \).

(h) If \( H_0 : \mu \in V \), where \( V \) is a \( p \)-dimensional vector subspace of \( \mathbb{R}^d \), then we have the following.

\[(i) \quad T^2_{\min} = \min_{\mu \in V} T^2 \sim T^2_{d-p,n-1}.\]

(ii) If we have \( H_0 : \mu = K\beta \), where \( K \) is a known \( d \times p \) matrix of rank \( p \) and \( \beta \) is a vector of \( p \) unknown parameters, then \( V = \mathcal{C}(K) \) and

\[
T^2_{\min} = n(\bar{x}'S^{-1}\bar{x} - \bar{x}'S^{-1}K\beta^*),
\]

where \( \beta^* = (K'S^{-1}K)^{-1}K'S^{-1}\bar{x} \).

(iii) Suppose we have \( H_0 : A\mu = 0 \), where \( A \) is \( d - p \times d \) of rank \( d - p \), so that \( V = \mathcal{N}(A) \), the null space of \( A \). Then

\[
T^2_{\min} = n(A\bar{x})'(ASA')^{-1}A\bar{x}.
\]

A slight generalization of this is given in (i) below.

(i) Let \( A \) be a \( q \times d \) matrix of rank \( q \). Then:

\[(i) \quad n(A\bar{x} - A\mu)'(ASA')^{-1}(A\bar{x} - A\mu) \sim T^2_{q,n-1}. \text{ This can be used for testing } H_0 : A\mu = c.\]

(ii) If \( A \) is a matrix of contrasts so that \( A1_d = 0 \), then

\[
n\bar{x}'A'(ASA')^{-1}A\bar{x} = n\bar{x}'S^{-1}\bar{x} - \frac{n(\bar{x}'S^{-1}1_d)^2}{1_d'S^{-1}1_d}.
\]
21.3.2 Two Samples

21.26. Let $v_1, v_2, \ldots, v_{n_1}$ be a random sample from $N_d(\mu_1, \Sigma)$, $w_1, w_2, \ldots, w_{n_2}$ be an independent random sample from $N_d(\mu_2, \Sigma)$, and $\theta = \mu_1 - \mu_2$. Also define $Q_1 = \sum_{i=1}^{n_1} (v_i - \bar{v})(v_i - \bar{v})'$ and $Q_2 = \sum_{i=1}^{n_2} (w_i - \bar{w})(w_i - \bar{w})'$. Then:

(a) $\bar{v} - \bar{w} \sim N_d(\theta, (n_1^{-1} + n_2^{-1})\Sigma)$.

(b) $Q = Q_1 + Q_2 \sim W_d(n_1 + n_2 - 2, \Sigma)$.

(c) $n_1 n_2 (n_1 + n_2)^{-1} (\bar{v} - \bar{w} - \theta)' S_p^{-1} (\bar{v} - \bar{w} - \theta) \sim T^2_{d, n_1 + n_2 - 2}$, the $T^2$ distribution (cf. 21.20), where $S_p = Q / (n_1 + n_2 - 2)$.

We can use this statistic to test $H_0 : \theta = c$.

(d) If $C$ is a $q \times d$ matrix of rank $q$ ($q \leq d$), then

$$\frac{n_1 n_2}{(n_1 + n_2)} [C(\bar{v} - \bar{w}) - C\theta]' (CS_p C')^{-1} [C(\bar{v} - \bar{w}) - C\theta] \sim T^2_{q, n_1 + n_2 - 2}.$$ 

This can be used to test $H_0 : C\theta = 0$. When $C$ is an appropriate $d - 1 \times d$ contrast matrix then the methodology relating to $H_0$ is referred to as profile analysis.

The topic of more than two samples is best handled as a special case of the multivariate linear model described in the next section.

Proofs. Section 21.3.2.

21.4 MULTIVARIATE LINEAR MODEL

21.4.1 Least Squares Estimation

**Definition 21.6.** Let \( \mathbf{Y} = \mathbf{\Theta} + \mathbf{U} \), where \( \mathbf{\Theta} = \mathbf{XB} \), \( \mathbf{B} \) is a \( p \times d \) matrix of unknown parameters, \( \mathbf{X} \) is an \( n \times p \) known matrix of constants of rank \( r \) (\( r \leq p \)), \( \mathbf{U} = (u_1, \ldots, u_n)' = (u^{(1)}, \ldots, u^{(d)}) \), and the \( u_i \) are a random sample from a distribution with mean 0 and variance matrix \( \Sigma \). Then \( \mathbf{Y} = \mathbf{XB} + \mathbf{U} \) is called a multivariate linear model. When \( d = 1 \), this reduces to the univariate linear model of Section 20.7.

We have introduced a change in notation in this section. Up till now, \( \mathbf{X} \) has represented a matrix of random variables, whereas now we assume it to be a matrix of constants. This will be the case if we can carry out any analysis conditional on the observed value of \( \mathbf{X} \). However, the use of \( \mathbf{X} \) is traditional for linear models, and in some cases the elements of \( \mathbf{X} \) take only values 0 or 1, thus representing qualitative variables. In this case, \( \mathbf{X} \) is sometimes referred to as the design matrix, though, as Kempthorne [1980: 249] argues, a better term is perhaps model matrix.

The matrix \( \mathbf{Y} \) now takes over the role of a data matrix. In what follows we let \( R = C(\mathbf{X}) \).

**Definition 21.7.** If we partition \( \mathbf{Y}, \mathbf{\Theta}, \) and \( \mathbf{B} \) in the same way that we partitioned \( \mathbf{U} \), then the \( j \)th column of the multivariate linear model is the univariate model \( y^{(j)} = \theta^{(j)} = \mathbf{X}\beta^{(j)} + u^{(j)} \), where \( u^{(j)} \) has mean 0 and variance matrix \( \sigma_{jj}\mathbf{I}_n \). If \( \mathbf{P}_\Omega \mathbf{y}^{(j)} \) is the (ordinary) least squares estimate of \( \theta^{(j)} \) (cf. 20.37a), where \( \mathbf{P}_\Omega = \mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}' \), we say that \( \hat{\mathbf{\Theta}} = \mathbf{P}_\Omega \mathbf{Y} \) is the least squares estimate of \( \mathbf{\Theta} \). When \( r = p \), then setting \( \hat{\mathbf{\Theta}} = \mathbf{Y}\hat{\mathbf{B}} \) we have \( \hat{\mathbf{B}} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\hat{\mathbf{\Theta}} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{Y} \), called the least squares estimate of \( \mathbf{B} \). If \( r < p \), then \( \hat{\mathbf{B}} \) is not unique and we can use (as in the univariate case) \( \hat{\mathbf{B}} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{Y} \), where \( (\mathbf{X}'\mathbf{X})^{-1} \) is any weak inverse of \( (\mathbf{X}'\mathbf{X}) \).

21.27. \( y_i = \hat{\mathbf{B}}'\mathbf{x}_i + u_i \), where \( \mathbf{x}_i \) is the \( i \)th row of \( \mathbf{X} \).

21.28. If \( \mathbf{X} \) has full rank, then \( \mathbf{E}(\hat{\mathbf{B}}) = \mathbf{B} \).

21.29. We have the following covariance properties.

(a) \( \text{cov}(y_r, y_s) = \text{cov}(u_r, u_s) = \delta_{rs}\Sigma \), where \( \delta_{rs} = 1 \) when \( r = s \) and 0 otherwise.

(b) \( \text{cov}(y^{(j)}, y^{(k)}) = \text{cov}(u^{(j)}, u^{(k)}) = \sigma_{jk}\mathbf{I}_d \) for all \( j, k = 1, \ldots, d \).

(c) If \( \mathbf{X} \) has full rank \( p \), then \( \hat{\beta}^{(j)} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'y^{(j)} \) and

\[
\text{cov}(\hat{\beta}^{(j)}, \hat{\beta}^{(k)}) = \sigma_{jk}(\mathbf{X}'\mathbf{X})^{-1} \quad (\text{all } j, k = 1, \ldots, d).
\]

21.30. Let \( \mathbf{G}(\mathbf{\Theta}) = (\mathbf{Y} - \mathbf{\Theta})'(\mathbf{Y} - \mathbf{\Theta}) \).

(a) (i) \( \mathbf{E} = \mathbf{G}(\hat{\mathbf{\Theta}}) = \mathbf{Y}'(\mathbf{I}_n - \mathbf{P}_\Omega)\mathbf{Y} = \mathbf{U}'(\mathbf{I}_n - \mathbf{P}_\Omega)\mathbf{U} \).

(ii) \( \mathbf{E}(\mathbf{E}) = (n - r)\Sigma \).

(iii) \( \mathbf{E} \) is positive definite with probability 1.

Here \( \mathbf{E} \) is sometimes referred to as the error matrix or residual matrix.

(b) \( \mathbf{G}(\mathbf{\Theta}) - \mathbf{G}(\hat{\mathbf{\Theta}}) = (\hat{\mathbf{\Theta}} - \mathbf{\Theta})'(\hat{\mathbf{\Theta}} - \mathbf{\Theta}) \) is positive semidefinite for all \( \mathbf{\Theta} = \mathbf{XB} \), and equal to \( 0 \) if and only if \( \mathbf{\Theta} = \hat{\mathbf{\Theta}} \). We can say that \( \hat{\mathbf{\Theta}} \) is the minimum of the
matrix $G(\Theta)$. As a consequence we have the following properties of the least squares estimate from (10.48b,d) and (10.47a(iii)).

(i) $\text{trace } G(\Theta) \geq \text{trace } G(\hat{\Theta})$.

(ii) $\det G(\Theta) \geq \det G(\hat{\Theta})$.

(iii) $\|G(\Theta)\|_F \geq \|G(\hat{\Theta})\|_F$, where $\|A\|_F = \{\text{trace}(A'A)\}^{1/2}$ and $\|\cdot\|_F$ is the Frobenius norm.

Any of these three results could be used as a definition of $\hat{\Theta}$.

21.31. (Generalized Gauss–Markov Theorem) If $\phi = \sum_{j=1}^{d} h_j^{(j)} \theta^{(j)}$, a linear combination of all the elements of $\Theta$, then $\hat{\phi} = \sum_{j=1}^{d} h_j^{(j)} \hat{\theta}^{(j)}$ is the BLUE of $\phi$ (i.e., the linear unbiased estimate with minimum variance).

21.32. (Two-Sample Case) Setting $V' = (v_1, v_2, \ldots, v_{n_1})$, $W' = (w_1, w_2, \ldots, w_{n_2})$, and $Y = (V', W')'$ we see that the two-sample problem (cf. 21.26) is a special case of the multivariate model with

$$X_B = \begin{pmatrix} 1_{n_1} & 0 \\ 0 & 1_{n_2} \end{pmatrix} \begin{pmatrix} \mu_1' \\ \mu_2' \end{pmatrix}.$$

The extension to $n$ samples is straightforward.

**Definition 21.8.** If $X$ has less than full rank, then each univariate model also has less than full rank. From (20.38(2)), $a'_i\beta^{(j)}$ is estimable for each $i = 1, 2, \ldots, q$ and each model $j = 1, 2, \ldots, d$ if $a_i \in C(X')$. Let $A' = (a_1, a_2, \ldots, a_q)$. Combining these linear combinations, we say that $AB$ is estimable if $A' = X'L'$ or $A = LX$ for some $q \times n$ matrix $L$.

21.33. Suppose $AB$ is estimable.

(a) If $A$ is $q \times p$ of rank $q$, then $L$ has rank $q$ by (20.38(2)).

(b) $A_B = LX(X'X)^{-}X'Y = LP_{\Omega}Y = (P_{\Omega}L')'Y$ is invariant for any choice of weak inverse $(XX')^{-}$ as $P_{\Omega}$ is invariant. Here $P_{\Omega}L'$ is unique (but not $L$, unless $X$ has rank $p$) and has full row rank.

(c) $\hat{\phi} = a'A_Bb = a'L\hat{\Theta}b$ is the BLUE of $\phi = a'A_Bb = a'L\Theta b$.

(d) $A(X'X)^{-}A = LP_{\Omega}L' = (P_{\Omega}L')P_{\Omega}L'$ is invariant and nonsingular by (b).

(e) $E(A_B) = LP_{\Omega}XB = LX_B = AB$, since $P_{\Omega}X = X$.

**Proofs.** Section 21.4.1.


21.32. Seber [1984: section 8.6.4].
21.33b. \( E(\hat{A}\hat{B}) = (P_\Omega M')' \Theta. \) If \( (P_\Omega M')' Y \) is another estimate, then \( [P_\Omega M' - P_\Omega L']' \Theta = 0 \) and \( C[P_\Omega(M' - L')] \perp C(X) \) as the columns of \( \Theta \) are in \( C(X) \). Thus, \( P_\Omega M' - P_\Omega L' = \Theta \) as \( C[P_\Omega(M' - L')] \subseteq C(X) \).

21.33c. The result follows from (21.31) by relabeling.

### 21.4.2 Statistical Inference

Let \( Y = \Theta + U \). In this section we now assume that the underlying distribution of the columns \( \mathbf{u}_i \) of \( U' \) is a (nonsingular) multivariate normal distribution \( N_d(0, \Sigma) \).

The case when \( \Sigma \) is singular is considered by, for example, Srivastava and von Rosen [2002]. The multivariate model can be expressed in terms of the univariate model \( \text{vec}(Y) = \text{vec}(XB) + \text{vec}U \), where from (21.2a) \( \text{vec}(XB) = (I_d \otimes X) \text{vec} \mathbf{B} \) and \( \text{var}(\text{vec}U) = \Sigma \otimes I_n \) (cf. Searle [1978]). A more general model in which \( \text{var}(\text{vec}U) = \Sigma \otimes V \), with \( V \) and \( \Sigma \) possibly singular, is considered by Sengupta and Jammalamakada [2003: chapter 10].

21.34. The likelihood function for \( Y \), the density function of \( \text{vec}(Y) \) (or, more conveniently, \( \text{vec}(Y') \)) is the joint distribution of the independent \( y_i \), and it can be expressed in the form

\[
(2\pi)^{-nd/2}(\det \Sigma)^{-n/2} \exp\{\text{trace}\left[-\frac{1}{2}(Y - \Theta)'\Sigma^{-1}(Y - \Theta)\right]\}.
\]

21.35. Suppose \( \Theta = XB \), where \( X \) has rank \( r \), and let \( E \) be given by (21.30a). We assume \( n - r \geq d \). Then:

(a) \( E \sim W_d(n - r, \Sigma) \).

(b) \( E \) is statistically independent of \( \Theta \) (and of \( \hat{B} \) if \( X \) has full rank \( p \)).

(c) The maximum likelihood estimates of \( \Sigma \), \( \Theta \), and \( B \) (if \( X \) has full rank), are \( \hat{\Sigma} = E/n, \hat{\Theta} \), and \( \hat{B} \). The maximum value of the likelihood function is \( (2\pi)^{-nd/2}(\det \hat{\Sigma})^{-n/2}e^{-nd/2} \). (This corrects a typo in Seber [1984: 407].)

(d) If \( X \) has full rank, then \( (\hat{B}, \hat{\Sigma}) \) is sufficient for \( (B, \Sigma) \).

(e) Referring to the \( j \)th column of \( \hat{B} \), if \( X \) has full rank (cf. 21.29c),

\[
\hat{b}^{(j)} \sim N_n(\beta^{(j)}, \sigma_{jj}(X'X)^{-1}).
\]

21.36. Suppose that \( \Theta = XB \), where \( X \) has rank \( r \). Let \( A \) be a known \( q \times p \) matrix of rank \( q \), and let \( AB \) be estimable. We are interested in testing \( H_0 : AB = C \), where \( C \) is a constant matrix. Then:

(a) Referring to (21.30), the minimum \( E_H \), say, of \( G(XB) \) subject to \( AB = C \) occurs when \( \hat{B} \) equals

\[
\hat{B}_H = \hat{B} - (X'X)^{-1}A'[A(X'X)^{-1}A']^{-1}(AB - C).
\]

Although \( \hat{B} \) and \( \hat{B}_H \) are not unique when \( r < p \), \( \hat{\Theta} = X\hat{B} \) and \( \hat{\Theta}_H = X\hat{B}_H \) are unique. Also \( E_H \) is positive definite with probability one.
(b) \( H = E_H - E = (A\bar{B} - C)'[A(X'X)^{-1}A']^{-1}(A\bar{B} - C) \).

\( H \) is positive definite with probability one.

(c) \( E(H) = q\Sigma + (A\bar{B} - C)'[A(X'X)^{-1}A']^{-1}(A\bar{B} - C) = q\Sigma + D, \) say, and \( D \) is positive definite.

(d) \( H \) and \( E \) are statistically independent.

(e) When \( H_0 \) is true, \( H \sim W_d(q, \Sigma) \). When \( H_0 \) is false, \( H \) has a noncentral Wishart distribution \( W_d(q, \Sigma; \Delta) \), with noncentrality matrix given by \( \Delta = \Sigma^{-1/2}D\Sigma^{-1/2} \).

(f) Let \( E_H^{1/2} \) be the positive definite square root of \( E_H \) (cf. 10.32). Then, when \( H_0 \) is true, \( V = E_H^{-1/2}HE_H^{-1/2} \) has a \( d \)-dimensional matrix variate Type-1 beta distribution with degrees of freedom \( q \) and \( n - r \) (cf. Section 21.9)

21.37. Four different criterion are usually computed for testing \( H_0 \), and are expressed as functions of eigenvalues of \( V \) given in (21.36(f)) above.

1. Roy’s maximum root test \( \phi_{\text{max}} \), the maximum eigenvalue of \( HE^{-1} \), based on the so-called union–intersection principle.

2. Likelihood ratio test \( (\det E / \det E_H)^{n/2} \).

3. The Lawley–Hotelling trace \( (n - r) \text{trace}(HE^{-1}) \).

4. Pillai’s trace \( \text{trace}(HE_H^{-1}) \).

These tests are summarised by Seber [1984: chapter 8], but for further details and distribution theory see Muirhead [1982: chapter 10].

Proofs. Section 21.4.2.

21.34. Seber [1984: 406].

21.35. Seber [1984: section 8.4].

21.36. Seber [1984: section 8.6].

21.4.3 Two Extensions

We give two extensions to the theory, which demonstrate how matrix theory can be applied.

21.38. (Generalized Hypothesis) Suppose we want to test \( H_0 : ABD = 0 \), where \( A \) is \( q \times p \) of rank \( q \) \( (q \leq p) \) and \( D \) is a known \( d \times v \) matrix of rank \( v \) \( (v \leq d) \). To do this, let \( Y_D = YD \) so that the linear model \( Y = XB + U \) is transformed to

\[ Y_D = XBD + UD = XL + U_0, \]

say, where the columns of \( U_0 \) are i.i.d. \( N_v(0, D'\Sigma D) \). Then \( H_0 \) becomes \( A\Lambda = 0 \) and we can apply the previous theory of (21.36) to this transformed model.
(a) $H$ now becomes $H_D = D'HD = (A^T D)[A(X'X)^{-1}A']^{-1}A^T D$ and $E$ becomes $E_D = D'ED \sim W_v(n - r, D'\Sigma D)$.

(b) When $A^T D = 0$ is true, $H_D \sim W_v(q, D'\Sigma D)$. The only change to the previous theory is to replace $Y$ by $Y_D$ and $d$ by $v$.

(c) The above theory reduces to that of Section 21.4.2 if we set $D = I_d$ and $v = d$.

This hypothesis is used for carrying out a profile analysis of more than two populations (Seber [1984: section 8.7]).

21.39. (Generalized Model and Hypothesis) Consider the model

$$Y = X\Delta K' + U,$$

where $X$ is a known $n \times p$ of rank $p$, $\Delta$ is $p \times k$ matrix of unknown parameters, $K'$ is a known $k \times d$ of rank $k$ ($k < d$), and the rows of $U$ are independently and identically distributed (i.i.d.) as $N_d(0, \Sigma)$. We wish to test the hypothesis

$$H_0 : \Delta \Delta D = 0,$$

where $\Delta$ is $q \times d$ of rank $q$ and $D$ is $k \times v$ of rank $v$. This model is usually called the growth curve model and it is considered, along with extensions, by Pan and Fang [2002] and Kollo and van Rosen [2005: chapter 41]. A brief discussion is given by Seber [1984: section 9.7].

One simple approach to the above model when there are appropriate rank conditions is to transform the model to remove $K'$ using a right inverse of $K'$. One method, suggested by (Potthoff and Roy [1964] and described in detail by Seber [1984: 479], is to choose a nonsingular $d \times d$ matrix $G$ (usually positive definite) such that the $k \times k$ matrix $K'G^{-1}K$ is nonsingular, and transform $y_i$ to $C_1y_i$, where $C_1 = G^{-1}K(K'G^{-1}K)^{-1}$ is $d \times k$ of rank $k$. Then $K'C_1 = I_k$ so that

$$Y_1 = YC_1 = X\Delta K'C_1 + UC_1 = X\Delta + U_1,$$

where the columns of $U_1$, namely $C_1u_i$, are i.i.d. $N_k(0, \Sigma_1)$ with $\Sigma_1 = C_1'\Sigma C_1$. We have now reduced the model to the previous case, and the theory used there for testing $H_0$ can be applied here with $Y$ replaced by $Y_1$ and $d$ by $k$.

21.5 DIMENSION REDUCTION TECHNIQUES

21.5.1 Principal Component Analysis (PCA)

Given a data set of interrelated variables represented by an $n \times d$ data matrix $X = (x_1, x_2, \ldots, x_n)'$, the aim of principal component analysis (PCA) is to reduce the dimensionality $d$ of the data set, while still retaining as much of the variation present in the data set as possible. This is achieved by transforming to a new set of variables, called the principal components, which are uncorrelated and are ordered so that the first few retain most of the variation present in all of the original variables. Also, we would hope that the components may have some physical interpretation.

We shall first look at the underlying population model that generates the data, and then consider the sample estimates of various quantities. There are numerous
books on multivariate analysis that contain chapters or sections on principal components, e.g., Anderson [2003], Krzanowski [1988], Muirhead [1982], and Seber [1984] (which happen to be in my office when writing this). However, more specialized books are available such as Flury [1988] and Jolliffe [2002].

**Definition 21.9.** Let \( x \) be a random \( d \)-dimensional vector with mean \( \mu \) and variance matrix \( \Sigma \). Let \( T = (t_1, t_2, \ldots, t_d) \) be an orthogonal matrix such that, by the spectral theorem (cf. 16.44), we have

\[
\Sigma t_j = \lambda_j t_j \quad \text{and} \quad T^\top \Sigma T = \Lambda = \text{diag}(\lambda_1, \lambda_2, \ldots, \lambda_d),
\]

where \( \lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_d \) are the ordered eigenvalues of \( \Sigma \). The sum trace \( \Sigma \) is sometimes called the total variance. If \( y = (y_j) = T^\top (x - \mu) \), then \( y_j = t_j^\top (x - \mu) \) \((j = 1, 2, \ldots, d)\) is called the \( j \)th population principal component of \( x \). In developing the population theory there is no loss of generality in assuming \( \mu = 0 \).

A major drawback to the above approach is that it can be sensitive to the units of measurement used for each \( z_i \). For this and other reasons some authors work with the population correlation matrix \( \text{corr}(x) \) rather than the variance matrix \( \Sigma \). For a discussion of the relative merits of the two approaches see Jolliffe [2002: section 2.3]. The optimal properties described below for \( \Sigma \) also apply to \( \text{corr}(x) \) if we use the standardized vector \( z = (z_i) \), where \( z_i = (x_i - \mu_i)/\sigma_{ii} \), instead of \( x \).


(a) \( \Sigma = T \Lambda T^\top = \sum_{i=1}^d \lambda_i t_i t_i^\top \).

(b) The principal components define the principal axes of the family of ellipsoids \((x - \mu)' \Sigma^{-1} (x - \mu) = \text{const}\). 

(c) Since \( t_j \) has unit length, \( y_j \) is the length of the orthogonal projection of \( x - \mu \) in direction \( t_j \).

(d) As var(\( y \)) = \( \Lambda \), the \( y_j \) are uncorrelated and var(\( y_j \)) = \( \lambda_j \).

(e) \( \sum_{j=1}^d \text{var}(y_j) = \sum_{j=1}^d \text{var}(x_j) = \text{trace} \Sigma, \) the total variance. We can use \( \lambda_j / \text{trace} \Sigma \) to measure the relative magnitude of \( \lambda_j \). If the \( \lambda_i \) \((i = k + 1, \ldots, d)\) are relatively small so that the corresponding \( y_i \) are “small” (with zero means and small variances), then \( y_{(k)} = (y_1, y_2, \ldots, y_k)' \) can be regarded as a \( k \) dimensional approximation for \( y \). Thus \( y_{(k)} \) can be used as a “proxy” for \( x \) in terms of explaining a major part of the total variance.

It should be noted that the last few components are likely to be more useful than the first few in detecting outliers that are not apparent from the original variables (Jolliffe [2002: 237]).

(f) Let \( T_{(k)} = (t_1, \ldots, t_k) \). Then:

(i) \( \max_{a'a=1} \text{var}(a'x) = \text{var}(t_1'x) = \text{var}[t_1' (x - \mu)] = \text{var}(y_1) = \lambda_1 \),

so that \( y_1 \) is the normalized linear combination of the elements of \( x - \mu \) with maximum variance \( \lambda_1 \).

(ii) \( \max_{a'a=1, T_{(k-1)}a=0} \text{var}(a'x) = \text{var}(t_k'x) = \text{var}(y_k) = \lambda_k \), so that \( t_k' (x - \mu) \) is the normalized linear combination of the elements \( x - \mu \) uncorrelated with \( y_1, y_2, \ldots, y_{k-1} \) with maximum variance \( \lambda_k \).
The above results can be expressed in several different ways (e.g., Jolliffe [2002: 11-12]).

(g) (Predictive Approach) Let $B$ be a $d \times k$ matrix, and consider the “best” linear predictor of $x - \mu$ on the basis of $B(x - \mu)$. The Frobenius norm of the variance matrix of the prediction error is

$$
\| \Sigma - \Sigma B' (B' \Sigma B)^{-1} B' \Sigma \|_F = \| \Sigma^{1/2} (I_d - P_{\Sigma^{1/2} B}) \Sigma^{1/2} \|_F,
$$

where $P_{\Sigma^{1/2} B}$ is a symmetric idempotent matrix representing the orthogonal projection onto $C(\Sigma^{1/2} B)$. The norm is a minimum when $B$ is equivalent to $T(k)$. Moreover, minimizing the trace of the variance matrix of the prediction error—that is, maximizing trace($P_{\Sigma^{1/2} B} \Sigma$)—yields the same result (Jolliffe [2002: 17]).

The results (f) and (g) above are optimal properties shared by principal components, and (e) was used by Hotelling [1933] to define principal components. For further properties see Jolliffe [2002: section 2.1] and Seber [1984: section 5.2]. A key theorem for developing such properties is given next.

21.41. Let $f$ be a function defined on $P$, the set of all $d \times d$ non-negative definite matrices. For any $C \in P$, let $\lambda_1(C) \geq \lambda_2(C) \geq \cdots \geq \lambda_d(C) \geq 0$ be the eigenvalues of $C$. Then $f$ is strictly increasing and invariant under orthogonal transformations if and only if $f(C) = g[\lambda_1(C), \ldots, \lambda_d(C)]$ for some $g$ that is strictly increasing in each argument. This means that minimizing $f(C)$ with respect to $C$ is equivalent to simultaneously minimizing the eigenvalues of $C$. The functions trace $C$, $\|C\|_F = [\text{trace}(CC')]^{1/2}$, and $\det C$ satisfy the conditions on $f$.

21.42. Suppose $f$ satisfies the conditions in (21.41) above and $v_{(k)}$ is a $k$-dimensional vector. Then

$$
f(\text{var}[x - \mu - Aw_{(k)}])
$$

is minimized when $Aw_{(k)} = T(k)y(k) = T(k)T(k)'(x - \mu) = P(x - \mu)$, where $P$ represents the orthogonal projection of $x - \mu$ onto $C(T(k))$.

**Definition 21.10.** (Sample Components) In practice, $\mu$ and $\Sigma$ are unknown and have to be estimated from a sample $x_1, x_2, \ldots, x_n$, that is the $x_i$ are assumed to be independently and identically distributed. We can estimate $\mu$ by $\hat{\mu} = \bar{x}$ and $\Sigma$ by $
\hat{\Sigma} = \bar{X}'\bar{X}/n$, where $\bar{X}$ is the centered matrix $\bar{X} = (x_1 - \bar{x}, \ldots, x_n - \bar{x})'$. Carrying out a similar factorization on $\hat{\Sigma}$ as we did for $\Sigma$, we obtain the eigenvalues $\hat{\lambda}_1 \geq \hat{\lambda}_2 \geq \cdots \geq \hat{\lambda}_d > 0$ and an orthogonal matrix $\hat{T} = (\hat{t}_1, \hat{t}_2, \ldots, \hat{t}_d)$ of corresponding eigenvectors. For each observation $x_i$ we can define a vector of sample (estimated) principal components $\hat{y}_i = \hat{T}'(x_i - \bar{x})$, which gives us

$$
\hat{Y}' = (\hat{y}_1, \hat{y}_2, \ldots, \hat{y}_n) = \hat{T}'\bar{X}'.
$$

Many authors prefer to use the unbiased estimator $S$ of $\Sigma$ instead of $\hat{\Sigma}$ in defining the sample components. In this case

$$
S\hat{t}_j = \frac{n}{n-1} \hat{\Sigma}\hat{t}_j = \left( \frac{n}{n-1} \hat{\lambda}_j \right) \hat{t}_j,
$$

and the eigenvalues of $S$ are $n\hat{\lambda}_j/(n - 1)$. 
The question arises as to whether we should use $S$ or the sample correlation matrix $R$. However, it is much easier to base any inference about the population components on $S$ rather than on $R$ using large sample theory. A key result is that if $x \sim N_d(\mu, \Sigma)$, then from (21.25b), $(n - 1)S \sim W_d(n - 1, \Sigma)$. For aspects of large sample theory see Seber [1984: section 5.2.5] for a brief summary. For further details see Anderson [2003: section 11.6] and Muirhead [1982: chapter 9], and see Kollo and Neudecker [1993, 1997] with regard to elliptical distributions. We note that the theory can be modified to handle dependent data such as a time series (Jolliffe [2002: chapter 12]). Also, PCA can be used in conjunction with other multivariate techniques (Jolliffe [2002: chapter 9]. With some modification, it can be used for discrete data like contingency tables, in which case it is related to the method of correspondence analysis and is mentioned briefly in (21.48) below (cf. Jolliffe [2002: sections 5.4 and 13.1]).

21.43. The score of the $j$th element of the $i$th sample observation, given by $\hat{y}_{ij} = \hat{t}_j(x_i - \bar{x})$, is related to the orthogonal projection of $x_i - \bar{x}$ onto $C(t_j)$, namely (cf. 2.49b)

$$P_{t_j}(x_i - \bar{x}) = \hat{t}_j^T(x_i - \bar{x}) = \hat{y}_{ij}\hat{t}_j.$$  

21.44. Using the result (20.15), we can show that the sample components are the population components for a discrete distribution so that all the optimal properties of population components hold for the sample components. For example, if $v$ is a random vector taking the values $x_i$ ($i = 1, 2, \ldots, n$) with probability $n^{-1}$, then $E(v) = \bar{x}$ and $\text{var}(v) = \hat{\Sigma}$. Applying (20.6b), we have for $a'a = 1$,

$$\text{var}(a'v) = a'\text{var}(v)a = a'\hat{\Sigma}a = \frac{1}{n} \sum_{i=1}^{n} [a'(x_i - \bar{x})]^2,$$

which takes its maximum value of $\lambda_1$ when $a = \hat{t}_1$. For further details see Jolliffe [2002: section 3.7].

21.45. A sample analogue of (21.40g) can be stated as follows. Let $G$ be an $n \times d$ matrix with orthonormal columns. We wish to minimize the sum of the squared distances $x_i - \bar{x}$ from $C(G)$; that is, we wish to minimize $\|X' - P_G\hat{X}'\|_F$, where $\| \cdot \|_F$ is the Frobenius norm and $P_G$ represents the orthogonal projection onto $G$. The minimum is given by $G = \hat{T}(k)$.

21.46. Let $\tilde{X}$ (which has rank $d$ with probability 1) have a singular value decomposition (thin version; cf. Section 16.3) $\tilde{X}_{n \times d} = U_{n \times d}\Delta_{d \times d}V'_{d \times d}$, where $U$ has orthogonal columns and $V$ is an orthogonal matrix. Setting $\hat{T} = V$, we have $\hat{Y} = X\hat{T} = U\Delta$ and

$$\Delta = \text{diag}(\sigma_1, \sigma_2, \ldots, \sigma_d) = \sqrt{n} \text{diag}(\hat{\lambda}_1^{1/2}, \hat{\lambda}_2^{1/2}, \ldots, \hat{\lambda}_d^{1/2}) = \sqrt{n}\hat{\Lambda}^{1/2},$$

the diagonal matrix of singular values of $\tilde{X}$, which are the square roots of the eigenvalues of $\tilde{X}'\tilde{X} (= n\hat{\Sigma})$. For applications see Jolliffe [2002: 45].

21.47. If the $\hat{\lambda}_j$ ($j = k + 1, \ldots, d$) are small relative to trace $\hat{\Sigma}$ (cf. 21.40e), we can approximate $\hat{y}_i$ by its first $k$ elements $\hat{y}_{i(k)}$, say.
21.48. (Contingency Tables) Consider a discrete data set of \( n \) frequency observations arranged in an \( r \times c \) two-way contingency table with \( n_{ij} \) in the \((i,j)\)th cell. Let \( \mathbf{N} = (n_{ij}) \) and define \( \mathbf{P} = n^{-1}\mathbf{N} \), \( \mathbf{D}_r = \text{diag}(\mathbf{r}) \), where \( \mathbf{r} = \mathbf{P}'\mathbf{1}_r \), \( \mathbf{D}_c = \text{diag}(\mathbf{c}) \), where \( \mathbf{c} = \mathbf{P}'\mathbf{1}_c \), and \( \mathbf{X} = \mathbf{P} - \mathbf{r}\mathbf{c}' \). If the variable defining the rows of the contingency table is independent of the variable defining the columns, then the matrix of 'expected counts' is given by \( n\mathbf{r}\mathbf{c}' \). Thus, \( \mathbf{X} \) is a matrix of the residuals that remain when the 'independence' model is fitted to \( \mathbf{P} \). If we apply the singular value decomposition to a redefined \( \tilde{\mathbf{X}} = \mathbf{D}_r^{-1/2}\mathbf{X}\mathbf{D}_c^{-1/2} \) in (21.46), we get the components \( \tilde{\mathbf{Y}} \), which are the same as those obtained by correspondence analysis (Jolliffe [2002: sections 5.4 and 13.1]).

Proofs. Section 21.5.1.

21.40b. This follows from
\[
(x - \mu)'\Sigma^{-1}(x - \mu) = y'T'S^{-1}Ty = y'\Lambda^{-1}y.
\]
See also Jolliffe [2002: 18].

21.40c. We use \( t_j'(x - \mu) = \|t_j\| \cdot \|(x - \mu)\| \cos \theta \).


21.40f. Seber [1984: 181, the inequality should be reversed in line -1].


21.5.2 Discriminant Coordinates

Definition 21.11. Suppose we have \( n \) \( d \)-dimensional observations of which \( n_i \) belong to group \( i \) \((i = 1, 2, \ldots, g; n = \sum_{i=1}^g n_i) \). Let \( x_{ij} \) be the \( j \)th observation in group \( i \), and define
\[
\bar{x}_i = \frac{1}{n_i} \sum_{j=1}^{n_i} x_{ij} \quad \text{and} \quad \bar{x}_r = \frac{1}{n} \sum_{i=1}^g \sum_{j=1}^{n_i} x_{ij}.
\]
Let \( \mathbf{W} = \sum_{i=1}^g \sum_{j=1}^{n_i} (x_{ij} - \bar{x}_i)(x_{ij} - \bar{x}_i)' \), the within-groups matrix, and let \( \mathbf{B} = \sum_{i=1}^g n_i(\bar{x}_i - \bar{x}_r)(\bar{x}_i - \bar{x}_r)' \), the between-groups matrix. Since \( \mathbf{W} \) and \( \mathbf{B} \) are generally positive definite with probability 1, the eigenvalues of \( \mathbf{W}^{-1}\mathbf{B} \) (which are the same as those of \( \mathbf{W}^{-1/2}\mathbf{BW}^{-1/2} \)) are positive and distinct with probability 1, say \( \lambda_1 > \lambda_2 > \cdots > \lambda_d > 0 \). Let \( \mathbf{W}^{-1}\mathbf{Bc}_r = \lambda_r c_r \) \((r = 1, \ldots, d) \), where the \( c_r \) are suitably scaled eigenvectors, and define the \( k \times d \) \((k \leq d)\) matrix \( \mathbf{C} = (c_1, c_2, \ldots, c_k)' \). If we define \( z_{ij} = \mathbf{C}x_{ij} \), then the \( k \) elements of \( z_{ij} \) are called the first \( k \) discriminant coordinates. (Some authors have used the term canonical variates, which I have reserved for Section 21.5.3.) These coordinates are determined so as to emphasize group separation, but with decreasing effectiveness, so that \( k \) has to be found. The coordinates can be computed using an appropriate
transformation combined with a principal component analysis. Typically, the \( c_i \) are scaled so that \( \text{CSC}' = I_r \), where \( S = W/(n - g) \). For further details see Seber [1984: section 5.8].

21.49. The above theory is based on the following results.

(a) Setting \( x_{ij} - \bar{x}_i = x_{ij} - \bar{x}_i + \bar{x}_i - \bar{x}_.. \), squaring, and summing over \( i \) and \( j \), we get

\[
\sum_{i=1}^{g} \sum_{j=1}^{n_i} (x_{ij} - \bar{x}_i)(x_{ij} - \bar{x}_..)' = \sum_{i=1}^{g} n_i (\bar{x}_i - \bar{x}_..)(\bar{x}_i - \bar{x}_..)'
+ \sum_{i=1}^{g} \sum_{j=1}^{n_i} (x_{ij} - \bar{x}_i)'\]

(b) Let \( \lambda = \max_{a,b \neq 0} (a'Ba/a'Wa) \), where the maximum occurs at \( a = c \), say. Differentiating \( a'Ba/a'Wa \) with respect to \( a \) we obtain \( Bc = \lambda Wc \) so that \( W^{-1}Bc = \lambda c \).

21.5.3 Canonical Correlations and Variates

Definition 21.12. Let \( z = (x', y')' \) be a \( d \)-dimensional random vector with mean \( \mu \) and positive definite variance matrix \( \Sigma \). Let \( x \) and \( y \) have dimensions \( d_1 \) and \( d_2 = d - d_1 \), respectively, and consider the partition

\[
\Sigma = \left( \begin{array}{cc}
\Sigma_{11} & \Sigma_{12} \\
\Sigma_{21} & \Sigma_{22}
\end{array} \right),
\]

where \( \Sigma_{ii} \) is \( d_i \times d_i \) and \( \Sigma_{12} = \Sigma_{21}' \). Let \( \rho_1^2 \) be the maximum value of the squared correlation between arbitrary linear combinations \( \alpha'x \) and \( \beta'y \), and let \( \alpha = a_1 \) and \( \beta = b_1 \) be the corresponding maximizing values of \( \alpha \) and \( \beta \). Then the positive square root \( \sqrt{\rho_1^2} \) is called the first (population) canonical correlation between \( x \) and \( y \), and \( u_1 = a_1'x \) and \( v_1 = b_1'y \) are called the first (population) canonical variables. Let \( \rho_2^2 \) be the maximum value of the squared correlation between \( \alpha'x \) and \( \beta'y \), where \( \alpha'x \) is uncorrelated with \( a_1'x \) and \( \beta'y \) is uncorrelated with \( b_1'y \), and let \( u_2 = a_2'x \) and \( v_2 = b_2'y \) be the maximizing values. Then the positive square root \( \sqrt{\rho_2^2} \) is called the second canonical correlation, and \( u_2 \) and \( v_2 \) are called the second canonical variables.

Continuing in this manner, we obtain \( r \) pairs of canonical variables \( u = (u_1, u_2, \ldots, u_r)' \) and \( v = (v_1, v_2, \ldots, v_r)' \). We can then regard \( u \) and \( v \) as lower-dimensional "representations" of \( x \) and \( y \). We shall see below that (i) the elements of \( u \) are uncorrelated, (ii) the elements of \( v \) are uncorrelated, and (iii) the squares of the correlations between \( u_j \) and \( v_j \) (\( j = 1, 2, \ldots, r \)) are collectively maximized in some sense. The mathematics is summarised in the following result.

21.50. Let \( 1 > \rho_1^2 \geq \rho_2^2 \geq \cdots \geq \rho_m^2 > 0 \), where \( m = \text{rank} \Sigma_{12} \), be the \( m \) nonzero eigenvalues of \( \Sigma_{11}^{-1} \Sigma_{12} \Sigma_{22}^{-1} \Sigma_{21} \) (and of \( \Sigma_{22}^{-1} \Sigma_{21} \Sigma_{11}^{-1} \Sigma_{12} \)). Let the vectors \( a_1, a_2, \ldots, a_m \) and \( b_1, b_2, \ldots, b_m \) be the respective corresponding eigenvectors of \( \Sigma_{11}^{-1} \Sigma_{12} \Sigma_{22}^{-1} \Sigma_{21} \) and \( \Sigma_{22}^{-1} \Sigma_{21} \Sigma_{11}^{-1} \Sigma_{12} \). Suppose that \( \alpha \) and \( \beta \) are arbitrary vectors such that for \( r \leq m \), \( \alpha'x \) is uncorrelated with each \( a_j'x \) (\( j = 1, 2, \ldots, r - 1 \)), and \( \beta'y \) is uncorrelated with each \( b_j'y \) (\( j = 1, 2, \ldots, r - 1 \)). Let \( u_j = a_j'x \) and \( v_j = b_j'y \), for \( j = 1, 2, \ldots, r \). Then we have the following results.
(a) The maximum squared correlation between $\alpha'x$ and $\beta'y$ is given by $\rho_r^2$ and it occurs when $\alpha = a_r$ and $\beta = b_r$. 

(b) $\text{cov}(u_j, u_k) = 0$ for $j \neq k$, and $\text{cov}(v_j, v_k) = 0$ for $j \neq k$. 

(c) The squared (population) correlation between $u_j$ and $v_j$ is $\rho_j^2$. 

(d) $\text{cov}(u_i, v_j) = 0$ for $i \neq j$. 

(e) Since $\rho_i^2$ is independent of scale, we can scale $a_j$ and $b_j$ such that $a_j'\Sigma_{11}a_j = 1$ and $b_j'\Sigma_{22}b_j = 1$. The $u_j$ and $v_j$ then have unit variances. Alternatively, we can standardize so that the $a_j$ and $b_j$ all have unit lengths. 

(f) If the $d_1 \times d_2$ matrix $\Sigma_{12}$ has full row rank, and $d_1 < d_2$, then we have $m = d_1$. All the eigenvalues of $\Sigma_{11}^{-1}\Sigma_{12}\Sigma_{22}^{-1}\Sigma_{21}$ are therefore positive, while $\Sigma_{22}^{-1}\Sigma_{21}\Sigma_{11}^{-1}\Sigma_{12}$ has $d_1$ positive eigenvalues and $d_2 - d_1$ zero eigenvalues. However, the rank of $\Sigma_{12}$ can vary as there may be constraints on $\Sigma_{12}$ such as $\Sigma_{12} = 0$ (rank 0) or $\Sigma_{12} = \sigma^2I_d, 1_d$ (rank 1). 

21.51. Given the above notation, suppose that $\Sigma$ is non-negative definite and singular. 

(a) The key matrix is now $A = \Sigma_{11}^{-1}\Sigma_{12}\Sigma_{22}^{-1}\Sigma_{21}$. The nonzero eigenvalues and rank of this matrix are invariant under any choices of the weak inverses $\Sigma_{11}^{-1}$ and $\Sigma_{22}^{-1}$. 

(b) The eigenvalues of $A$ are the squares of the canonical correlations between $x$ and $y$. 

(c) The number of canonical correlations equal to 1 is 

$$k = \text{rank } \Sigma_{11} + \text{rank } \Sigma_{22} - \text{rank } \Sigma.$$ 

(d) If $\Sigma$ is positive definite, then $k = 0$. 

21.52. Suppose $x$ and $y$ have means $\mu_x$ and $\mu_y$, respectively. Let $u = A(x - \mu_x)$ and $v = B(y - \mu_y)$, where $A$ and $B$ are any matrices, each with $r$ rows that are linearly independent, satisfying $A\Sigma_{11}A' = I_r$ and $B\Sigma_{22}B' = I_r$. Then $E[(u - v)'(u - v)]$ is minimized when $u$ and $v$ are vectors of the canonical variables. 

21.53. Suppose $z' = (x', y')'$ has a positive definite variance matrix $\Sigma$. Then $x$ and $y$ have the same canonical correlations as two random vectors $x_0$ and $y_0$ with variance matrix $\Sigma^{-1}$, where $(x_0', y_0')$ is partitioned in the same way as $(x', y')$. This result has been extended to the case of a singular $\Sigma$ using generalized inverses by Latour et al. [1987].

**Definition 21.13. (Sample Estimates)** Let $z_1, z_2, \ldots, z_n$ be a random sample from the distribution described in Definition 21.12. Let $\bar{z} = (\bar{x}', \bar{y}')'$ and $\hat{\Sigma} = \sum_{i=1}^n (z_i - \bar{z})(z_i - \bar{z})'/n$, where $\hat{\Sigma}$ is partitioned in the same way as $\Sigma$, namely

$$n\hat{\Sigma} = \begin{pmatrix} \sum_{i=1}^n (x_i - \bar{x})(x_i - \bar{x})'/n & \sum_{i=1}^n (x_i - \bar{x})(y_i - \bar{y})'/n \\ \sum_{i=1}^n (y_i - \bar{y})(x_i - \bar{x})'/n & \sum_{i=1}^n (y_i - \bar{y})(y_i - \bar{y})'/n \end{pmatrix} \begin{pmatrix} \bar{x}'\bar{x} & \bar{x}'\bar{y} \\ \bar{y}'\bar{x} & \bar{y}'\bar{y} \end{pmatrix} \begin{pmatrix} Q_{11} & Q_{12} \\ Q_{21} & Q_{22} \end{pmatrix}.$$


say, where $Q_{11}$ is $d_1 \times d_1$ and $Q_{12} = Q_{21}'$ is $d_1 \times d_2$. We can assume that $d_1 \leq d_2$. Then given that $\Sigma$ is positive definite and $n - 1 \geq d_1$ we know that, with probability 1, $n\tilde{\Sigma}$ is positive definite and there are no constraints on $Q_{12}$—that is, $\text{rank} Q_{12} = d_1$. Let $r_1^2 > r_2^2 > \cdots > r_{d_1}^2 > 0$ be the eigenvalues of $Q_{11}^{-1}Q_{12}Q_{22}^{-1}Q_{21}$, with corresponding eigenvectors $\hat{a}_1, \hat{a}_2, \ldots, \hat{a}_{d_1}$. We define $u_{ij} = \hat{a}_j'(x_i - \bar{x})$, the $i$th element of $u_j = \tilde{X}\hat{a}_j$, where $\hat{a}_j$ is scaled so that

$$1 = \hat{a}_j'\tilde{\Sigma}_{11}\hat{a}_j = n^{-1}\hat{a}_j'\tilde{X}'\tilde{X}\hat{a}_j = \sum_{i=1}^{n} u_{ij}^2/n = u_j'u_j/n.$$ 

Then $\sqrt{r_j^2}$ is called the $j$th sample canonical correlation and these correlations are distinct with probability 1. We call $u_{ij}$ the $j$th sample canonical variable of $x_i$. In a similar fashion we define $v_{ij} = \hat{b}_j'(y_i - \bar{y})$, the $i$th element of $v_j = \tilde{Y}\hat{b}_j$, to be the $j$th sample canonical variable of $y_i$, where $\hat{b}_1, \hat{b}_2, \ldots, \hat{b}_{d_1}$ are the corresponding eigenvectors of $Q_{22}^{-1}Q_{21}Q_{11}^{-1}Q_{12}$. The $u_{ij}$ and $v_{ij}$ are called the scores of the $i$th observation on the $j$th canonical variables. In computing the sample eigenvalues and eigenvectors we can use $Q_{ab}, \tilde{S}_{ab} = Q_{ab}/n$ or $S_{ab} = Q_{ab}/(n-1)$ ($a,b = 1,2$), as the factors $n$ and $n - 1$ cancel out. Some computer packages use the sample correlation matrix $R$ instead of $\tilde{\Sigma}$. For further details see Seber [1984: section 5.7].

21.54. Using the method of (20.15), the sample canonical variables have the same optimal properties as those described for the population variables, except that population variances and covariances are replaced by their sample counterparts.

21.55. We have the following properties of $r_j$.

(a) The $r_j^2$ are distinct with probability 1.

(b) $r_j^2$ is the square of the sample correlation between the canonical variables whose values are in the vectors $u_j$ and $v_j$.

Proofs. Section 21.5.3.

21.50. Seber [1984: section 5.7; for (d) see 278, solution to exercise 5.28].


21.5.4 Latent Variable Methods

Latent variable methods are similar to PCA in that they endeavor to reduce the dimensionality of the data. However, they do this by imposing a model structure on the data that relates some observed variables to some underlying latent or hidden variables. When the latent variables are continuous or discrete, the method is called factor analysis, while if the latent variables are categorical, the method is usually referred to as latent class analysis. For general references see Bartholomew [1987] and Everitt [1984].
Definition 21.14. (Factor Analysis) Let \( \mathbf{x} = (x_1, x_2, \ldots, x_d)' \) be a random vector with mean \( \mu \) and variance matrix \( \Sigma \). Let \( \mathbf{f} = (f_1, f_2, \ldots, f_m)' \) be an \( m \)-dimensional random vector with mean \( \mathbf{0} \) and variance matrix \( \mathbf{I}_m \). The factor analysis model is defined to be

\[
\mathbf{x} = \mu + \Gamma \mathbf{f} + \epsilon,
\]

where \( \epsilon \) is assumed to be uncorrelated with \( \mathbf{f} \) and has a diagonal variance matrix \( \Psi = \text{diag}(\psi_1^2, \psi_2^2, \ldots, \psi_d^2) \). Here \( \Gamma = (\gamma_{jk}) \) is a \( d \times m \) unknown matrix of constants. The elements of \( \mathbf{f} \) are called (common) factors or latent variables, the elements of \( \epsilon \) are usually called specific or unique factors, and \( \gamma_{jk} \) is called the weight or factor loading of \( x_j \) on the factor \( f_k \).

21.56. \( \Sigma = \Gamma \Gamma' + \Psi \), which leads to

\[
\sigma_{jj} = \sum_{k=1}^{m} \gamma_{jk}^2 + \psi_j^2 = h_{jj}^2 + \psi_j^2,
\]
say, where \( h_j^2 \) is called the communality or common variance and \( \psi_j^2 \) is called the residual variance or unique variance. The aim of factor analysis is to see if \( \Sigma \) can be expressed in the above form for a reasonably small value of \( m \) and to estimate the elements of \( \Gamma \) and \( \Psi \).

21.57. The model is not unique as \( \Gamma \mathbf{f} = (\Gamma \mathbf{L}) \mathbf{L}' \mathbf{f} = \Gamma_0 \mathbf{f}_0 \) for any orthogonal \( \mathbf{L} \) with \( \text{var}(\mathbf{f}_0) = \mathbf{L}' \text{var}(\mathbf{f}) \mathbf{L} = \mathbf{L}' \mathbf{I}_m \mathbf{L} = \mathbf{I}_m \). It is therefore usual to impose the constraint that \( \Gamma' \Psi^{-1} \Gamma \) has positive diagonal elements; under certain conditions this constraint may provide a unique \( \Gamma \). Although factor analysis is very different from PCA, it is often confused with PCA (Jolliffe [2002: chapter 7] and Srivastava [2002: chapter 12]).

21.58. Let \( \hat{\mathbf{f}} = \mathbf{A}(\mathbf{x} - \mu) = \mathbf{A} \mathbf{y} \) be a linear “estimate” of \( \mathbf{f} \). Then the mean square error is

\[
\mathbb{E}(\|\hat{\mathbf{f}} - \mathbf{f}\|_2^2) = \text{trace}(\mathbf{A}' \Sigma \mathbf{A}) - 2 \text{trace}(\mathbf{A} \Gamma) + m.
\]

This is minimized when

\[
\mathbf{A} = \Gamma' \Sigma^{-1} = (\mathbf{I}_m + \Gamma' \Psi^{-1} \Gamma)^{-1} \Gamma' \Psi^{-1}.
\]

Proofs. Section 21.5.4.


21.5.5 Classical (Metric) Scaling

Definition 21.15. Given a set of \( n \) objects, a proximity measure \( \delta_{rs} \) is a measure of the “closeness” of objects \( r \) and \( s \); here closeness does not necessarily refer to physical distance. A proximity \( \delta_{rs} \) is called a dissimilarity if \( \delta_{rr} = 0, \delta_{rs} \geq 0 \), and \( \delta_{rs} = \delta_{sr} \), for all \( r, s = 1, 2, \ldots, n \); the matrix \( \mathbf{D} = (\delta_{rs}) \) is called a dissimilarity matrix. We say that \( \mathbf{D} \) is Euclidean if there exists a \( p \)-dimensional configuration of points \( y_1, y_2, \ldots, y_n \) for some \( p \) such that the interpoint Euclidean distance \( d_{rs} = ||y_r - y_s||_2 = \delta_{rs} \).
21.59. Let \( A = (a_{ij}) \) be a symmetric \( n \times n \) matrix, where \( a_{rs} = \frac{1}{2} \delta_{rs}^2 \). Define \( b_{rs} = a_{rs} - \bar{a}_r - \bar{a}_s + \bar{a} \) so that
\[
B = (b_{rs}) = CAC,
\]
where \( C = (I_n - n^{-1}1_n1_n') \), the usual centering matrix.

(a) \( D \) is Euclidean if and only if \( B \) is non-negative definite.

(b) When \( \delta_{rs}^2 = \|x_r - x_s\|^2 \), \( \bar{X} = (x_1 - \bar{x}, x_2 - \bar{x}, \ldots, x_n - \bar{x})' \), and \( \Delta = (\delta_{rs}^2) \), we find that
\[
\Delta = 1_n1_n' \text{ diag}(\bar{X}X') - 2\bar{X}X' + \text{ diag}(\bar{XX'})1_n1_n'.
\]
Then \( B = -\frac{1}{2}C\Delta C = \bar{X}X' \), where \( \bar{X}'1_n = 0 \). For further details and extensions (e.g., using weights), see Takane [2004]. The next result looks at the reverse of the above process.

21.60. If \( B \) of (21.59) is non-negative definite, then we can find the \( y_i \) as follows. There exists an orthogonal matrix \( V = (v_1, v_2, \ldots, v_n) \) such that
\[
V'BV = \begin{pmatrix}
\Gamma & 0 \\
0 & 0
\end{pmatrix}
\]
(= \( \Lambda \), say),
where \( \Gamma = \text{ diag}(\gamma_1, \gamma_2, \ldots, \gamma_p) \) and \( \gamma_1 \geq \gamma_2 \geq \ldots \geq \gamma_p > 0 \) are the positive eigenvalues of \( B \). Let \( V_1 = (v_1, v_2, \ldots, v_p) \) and
\[
Y = \begin{pmatrix}
\sqrt{\gamma_1}v_1, \\
\sqrt{\gamma_2}v_2, \\
\vdots \\
\sqrt{\gamma_p}v_p
\end{pmatrix} = \begin{pmatrix}
y^{(1)} \\
y^{(2)} \\
\vdots \\
y^{(p)}
\end{pmatrix}
= \begin{pmatrix}
y_1, \\
y_2, \\
\vdots \\
y_n
\end{pmatrix} = \begin{pmatrix}
y(1), \\
y(2), \\
\vdots \\
y(p)
\end{pmatrix}
\]

Then:

(a) \( B1_n = 0 \), since \( C1_n = 0 \).

(b) \( B = V\Lambda V' = YY' \).

(c) \( n^2\bar{Y}'\bar{Y} = (Y'1_n)'(Y'1_n) = 1_n'B1_n = 0 \), so that \( \bar{y} = 0 \).

(d) \( \|y_r - y_s\|^2 = \delta_{rs}^2 \).

21.61. If \( D \) is not Euclidean, then some of the eigenvalues of \( B \) will be negative. However, if the first \( k \) eigenvalues are comparatively large and positive, and the remaining positive or negative eigenvalues are near zero, then the rows of \( Y_k = (y^{(1)}, y^{(2)} \ldots, y^{(k)}) \) will give a reasonable \( k \)-dimensional configuration. If the original objects are \( d \)-dimensional points \( x_i \) \( (i = 1, 2, \ldots, n) \) so that \( \|x_r - x_s\|^2 = \delta_{rs}^2 \), then the \( n \) rows of \( Y_k \) will give an approximate \( k \)-dimensional reduction of a \( d \)-dimensional system of points. The above procedure is often referred to as classical scaling or principal coordinate analysis (Jolliffe [2002: section 5.2] and Seber [1984: section 5.5.1]). Jolliffe [2002: section 5.5] notes that principal coordinate analysis is similar to principal component analysis for certain types of similarity matrix.

Proofs. Section 21.5.5.

21.6 PROCRUSTES ANALYSIS (MATCHING CONFIGURATIONS)

Classical multidimensional scaling of Section 21.5 can be regarded as a technique for trying to match one set of \( n \) points in \( d \)-dimensional space by another set in a lower dimensional space. A related technique, commonly known as procrustes analysis, refers to the problem of matching two configurations of \( n \) points in \( d \)-dimensional space where there is a preassigned correspondence between the points of one configuration and the points of the other.

21.62. Let \( A \) be a real \( d \times d \) matrix with a singular value decomposition \( A = P \Sigma Q' \), where \( P \) and \( Q \) are \( d \times d \) orthogonal matrices and \( \Sigma = \text{diag}(\sigma_1, \sigma_2, \ldots, \sigma_d) \), where the \( \sigma_i \) are the singular values. Then, for all orthogonal \( T \),

\[
\text{trace}(AT) = \text{trace}(TA) \leq \text{trace}[(A'A)^{1/2}],
\]

with equality if \( T = \hat{T} = QP' \). At the maximum,

\[
AT = P \Sigma Q'QP' = P \Sigma P',
\]

which is non-negative definite. In fact \( \text{trace}(AT) \) is maximized if and only if \( AT \) is non-negative definite.

If \( A \) is nonsingular, then \( TA = (A'A)^{1/2} \) has a unique solution

\[
\hat{T} = (A'A)^{-1/2}A'.
\]

21.63. Given two sets of \( d \)-dimensional points \( x_i \) and \( y_i \) \( (i = 1, 2, \ldots, n) \), we wish to move the \( y_i \) relative to the \( x_i \) through rotation, reflection and translation, i.e., by the linear transformation \( Ty_i + c \), where \( T \) is an orthogonal matrix, such that \( \sum_{i=1}^{n} ||x_i - Ty_i - c||^2 \) is minimized. The answer is \( c = \bar{x} - \bar{y} \) together with the minimum of \( \sum_{i=1}^{n} ||x_i - \bar{x} - T'(y_i - \bar{y})||^2 = ||\tilde{X} - \tilde{Y}T||^2_F \) with respect to orthogonal \( T \), where \( \cdot || \cdot ||_F \) is the Frobenius norm. Here

\[
\|\tilde{X} - \tilde{Y}T\|^2_F = \text{trace}[(\tilde{X} - \tilde{Y}T)'(\tilde{X} - \tilde{Y}T)]
= \text{trace}(\tilde{X}'\tilde{X}) + \text{trace}(\tilde{Y}'\tilde{Y}) - 2\text{trace}(\tilde{X}'\tilde{Y}T),
\]

where \( \tilde{X}' = (x_1 - \bar{x}, \ldots, x_n - \bar{x}) \) and \( \tilde{Y} \) is similarly defined. We have to maximize \( \text{trace}(T\tilde{X}'\tilde{Y}) = \text{trace}(TA) \), where \( A = \tilde{X}'\tilde{Y} \), with respect to \( T \). From (21.62) the answer is \( T = QP' \). If \( A \) is nonsingular, we also have that the minimizing \( T \) for our original problem is

\[
T = (\tilde{Y}'\tilde{X}'\tilde{Y})^{-1/2}(\tilde{Y}'\tilde{X}).
\]

For further details concerning various aspects of procrustes analysis such as scaling, rotations and/or reflections, projections, and nonorthogonal transformations, see Gower and Dijksterhuis [2004].

Proofs. Section 21.6.


21.7 SOME SPECIFIC RANDOM MATRICES

21.64. Let \( A(x) \) be a matrix whose elements are function of a random variable \( x \). If \( A \) is positive definite for all \( x \), then, provided that the expectations exist,

\[
E(A^{-1}) - [E(A)]^{-1} \geq 0,
\]

that is, is non-negative definite.

21.65. (Generalized Quadratics)

(a) (Positive Definite) Suppose that the columns of \( X' = (x_1, x_2, \ldots, x_n) \) are statistically independent and \( A \) is an \( n \times n \) non-negative definite matrix of rank \( r \) \((r \geq d)\). If for each \( x_i \) and all \( b \neq 0 \) and \( c \), \( \Pr(b'x_i = c) = 0 \), then

\[
X'AX \text{ is positive definite with probability 1.}
\]

(b) Let \( X' \) be defined as in (a), and let \( A \) be a symmetric matrix of rank \( r \). If the joint distribution of the elements of \( X \) is absolutely continuous with respect to the \( nd\)-dimensional Lebesque measure, then the following statements hold with probability 1:

\[
\text{rank}(X'AX) = \min\{d, r\}
\]

and the nonzero eigenvalues of \( X'AX \) are distinct.

Proofs. Section 21.7.

21.64. Groves and Rothenberg [1969].


21.8 ALLOCATION PROBLEMS

There is a subject area, which is mentioned for completeness, that sometimes uses dimension reducing techniques. This might be described generally as allocation, and includes two topics, discriminant analysis and cluster analysis, for which there are very extensive literatures. The emphasis tends to be on vectors rather than matrices. In essence, discriminant analysis is the problem of allocating an observation to one of two (or more) multivariate distributions, given samples from each distribution. Cluster analysis is a method of partitioning a cluster of observations into “sensible” groupings or classes (e.g., classifying psychiatric illnesses). Both topics are discussed in Seber [1984: chapters 6 and 7]. For further practical overviews of cluster analysis see Everitt [1993], Gordon [1999], and Kaufmann and Rousseeuw [1990]. Discriminant analysis is considered in detail by McLachlan [1992].
21.9 MATRIX-VARIATE DISTRIBUTIONS

In this section we give the density functions of some well known matrix distributions.

**Definition 21.16.** (Matrix-Variate Normal) A random matrix \( p \times n \) matrix \( Y \) with \( E(Y) = M \) is said to have a *matrix-variate normal* distribution if \( y = \text{vec} Y \sim N_{pn}(\text{vec} M, \Psi \otimes \Sigma) \). Following Kollo and von Rosen [2005: section 2.2], we say that \( Y \sim N_{p,n}(M, \Sigma, \Psi) \). These authors show in detail that many of the properties of the multivariate normal carry over to the matrix normal distribution. They also give moments for generalized quadratics and describe matrix-variate elliptical distributions (see also Gupta and Varga [1993]). If \( \mu_i \) is the \( i \)-th column of \( M \) and \( \Psi = I_n \), then the columns of \( Y \) are independently distributed as \( N_{p}(\mu_i, \Sigma) \) and \( Y' \) is now the data matrix. In this case we can identify \( Y = X' \) and \( p = d \), where \( X \) is the data matrix.

21.66. Using the above notation, if \( \Psi \) and \( \Sigma \) are positive definite so that \( \Psi \otimes \Sigma \) is positive definite, and \( m = \text{vec} M \), then the probability density function of \( y = \text{vec} Y \) is

\[
f(y) = (2\pi)^{-pn/2} |\det(\Psi \otimes \Sigma)|^{-1/2} \exp[-\frac{1}{2}(y - m)'(\Psi \otimes \Sigma)^{-1}(y - m)]
\]

\[
= (2\pi)^{-pn/2} |\det(\Psi)|^{-p/2} |\det(\Sigma)|^{-n/2} \text{etr}[-\frac{1}{2} \Sigma^{-1}(Y - M)\Psi^{-1}(Y - M)'],
\]

where \( \text{etr} = e^{\text{trace}} \).

21.67. (Wishart Distribution) In Section 21.2.2 we introduced the random symmetric \( d \times d \) matrix \( W \), which has a distribution \( W_d(m, \Sigma) \). When \( \Sigma \) is positive definite and \( m \geq d \), we can obtain the probability density function of \( \text{vech} W \) (the distinct elements of \( W \)) as

\[
f(\text{vech} W) = c^{-1}(\det W)^{(m-d-1)/2} \text{etr}(-\frac{1}{2} \Sigma^{-1}W),
\]

where \( c = 2^{md/2} |\det(\Sigma)|^{m/2} \Gamma_d(\frac{1}{2}m) \), “etr” is defined in (21.66) above, and

\[
\Gamma_d(a) = \pi^{(d-1)/4} \prod_{j=1}^{d} \Gamma[a - \frac{1}{2}(j - 1)].
\]

**Definition 21.17.** (Matrix-Variate Gamma Distribution) Let \( X \) be a positive definite \( d \times d \) random matrix and \( B \) a positive definite \( d \times d \) matrix of constants. Then \( X \) is said to have a *matrix-variate gamma distribution* if the probability density function of \( x = \text{vech} X \) is

\[
f(x) = \frac{1}{(\det B)^{a/2} \Gamma_d(a)} (\det X)^{a-(d+1)/2} \text{etr}(-BX),
\]

where \( a > (d - 1)/2 \). For some applications see Mathai [1991].

**Definition 21.18.** (Matrix-Variate Beta Distributions) A \( d \times d \) positive definite random matrix \( U \) such that \( V = I_d - U \) is positive definite is said to have a *matrix-variate Type-1 beta distribution* with \( a \) and \( b \) degrees of freedom \( (a, b > (d - 1)/2) \) if the density function of \( u = \text{vech} U \) is

\[
f(u) = \frac{1}{B_d(a, b)} (\det U)^{a-(d+1)/2} (\det[I_d - U])^{b-(d+1)/2},
\]
where
\[ B_d(a, b) = \frac{\Gamma_d(a) \Gamma_d(b)}{\Gamma_d(a + b)}, \quad d \leq 2a, 2b \]
and \( \Gamma_d(a) \) is given in (21.67). Note that \( V = I - U \) also has a matrix-variate beta Type-1 distribution with \( b \) and \( a \) degrees of freedom, respectively. Mathai [1997: 259–260] proves that \( f(u) \) is a density function.

The positive definite random \( d \times d \) matrix \( Y \) is said to have a matrix-variate Type-2 beta distribution with \( a \) and \( b \) degrees of freedom \((a, b \geq (d - 1)/2)\) if the density function of \( y = \text{vech}Y \) is
\[
 f(y) = \frac{1}{B_d(a, b)} (\det Y)^{a - (d + 1)/2} [\det[I_d + Y]^{-(a + b)}. \]

For further details see Mathai [1997: 262–264].

21.68. Suppose, for \( i = 1, 2 \), that \( W_i \) has a nonsingular Wishart distribution \( W_d(m_i, \Sigma) \) (\( \Sigma \) positive definite, \( m_1, m_2 \geq d \)) and \( W_1 \) and \( W_2 \) are statistically independent. Since, by (21.61a), \( W_i \) is positive definite (with probability 1), then so is \( W_1 + W_2 \). Let \( V = (W_1 + W_2)^{-\frac{1}{2}} W_1 (W_1 + W_2)^{-\frac{1}{2}} \), where \((W_1 + W_2)^{1/2}\) is the positive definite square root of \( W_1 + W_2 \) (cf. 10.32). Then:

(a) \( V \) has a matrix-variate Type-1 beta distribution defined above with \( \frac{1}{2} m_1 \) and \( \frac{1}{2} m_2 \) degrees of freedom, respectively.

(b) The eigenvalues \( \lambda_i \) of \( V \) are distinct with probability 1 and can be ordered \( 1 > \lambda_1 > \lambda_2 \cdots > \lambda_d > 0 \) (cf. 21.65b)

(c) The joint probability density function of the \( \lambda_i \) is
\[
 f(\lambda) = c^{-1} \left( \prod_{i=1}^{d} \theta_i \right)^{(m_1 - d - 1)/2} \left[ \prod_{i=1}^{d} (1 - \theta_j) \right]^{(m_2 - d - 1)/2} \prod_{i<j}^{d} (\theta_i - \theta_j),
\]
where \( c = \pi^{-d/2} B_d(\frac{1}{2} m_1, \frac{1}{2} m_2) \Gamma_d(\frac{1}{2} d) \).

(d) \( Y = W_2^{-\frac{1}{2}} W_1 W_2^{-\frac{1}{2}} \) has a matrix-variate Type-2 beta distribution with \( \frac{1}{2} m_1 \) and \( \frac{1}{2} m_2 \) degrees of freedom, respectively.

**Definition 21.19.** (Matrix-Variate Dirichlet Distributions) A set of positive definite \( p \times p \) random matrices \( X_1, X_2, \ldots, X_k \) (i.e., each \( X_i > 0 \)) is said to have a matrix-variate Type-1 Dirichlet distribution with parameter \( \alpha = (\alpha_1, \ldots, \alpha_{k+1})' \), where \( \alpha_i > \frac{p - 1}{2} \) for \( i = 1, 2, \ldots, k + 1 \), if their joint density function is
\[
 f(X_1, \ldots, X_k) = \frac{\Gamma_p(\alpha_1 + \alpha_2 + \cdots + \alpha_{k+1})}{\Gamma_p(\alpha_1) \Gamma_p(\alpha_2) \cdots \Gamma_p(\alpha_{k+1})} \left\{ \prod_{i=1}^{k} (\det X_i)^{\alpha_i - \frac{p + 1}{2}} \right\} \times (\det(I_p - X_1 - \cdots - X_k) ,\alpha_{k+1} - \frac{p + 1}{2} ,
\]
\[
 0 < X_i < I_p, \quad (i = 1, 2, \ldots, k), \quad 0 < \sum_{i=1}^{k} X_i < I_p.
\]
The $X_i$ are said to have a matrix-variate Type-2 Dirichlet distribution with parameter $\alpha$ if their joint density function is

$$f(X_1, \ldots, X_k) = \frac{\Gamma_p(\alpha_1 + \alpha_2 + \cdots + \alpha_{k+1})}{\Gamma_p(\alpha_1)\Gamma_p(\alpha_2)\cdots\Gamma_p(\alpha_{k+1})} \left(\prod_{i=1}^k \det X_i^{\alpha_i - \frac{p+1}{2}}\right) \times \left[\det(I_p + X_1 + \cdots + X_k)\right]^{-\left(\alpha_1 + \cdots + \alpha_{k+1}\right)}, \text{ each } X_i > 0,$$

where $\alpha_i > \frac{p-1}{2}$ for $i = 1, 2, \ldots, k + 1$ (Mathai [1997: section 5.1.8]).

21.69. Let the $p \times p$ random matrices $X_1, \ldots, X_k$ have a joint matrix-variate Type-1 Dirichlet distribution.

(a) Any subset of the $k$ matrices also has a joint matrix-variate Type-1 Dirichlet distribution.

(b) $U = X_1 + \cdots + X_k$ has a matrix-variate Type-1 beta distribution with degrees of freedom $\alpha_1 + \cdots + \alpha_k$ and $\alpha_{k+1}$, respectively.

21.70. Let $X_1, \ldots, X_k$ have a joint matrix-variate Type-2 Dirichlet distribution with parameter $\alpha$, and let $X_0 = X_1 + \cdots + X_k$. Then the $Y_i = (I + X_0)^{-1/2}X_i(I + X_0)^{-1/2}$ ($i = 1, 2, \ldots, k$) are jointly distributed as a matrix-variate Type-1 Dirichlet distribution with parameter $\alpha$.

Proofs. Section 21.9.

21.66. The second equation follows from $(\Psi \otimes \Sigma)^{-1} = \Psi^{-1} \otimes \Sigma^{-1}$ and applying (11.17d(ii)).


21.70. Mathai [1997: 278].

21.10 MATRIX ENSEMBLES

In some situations an $n \times d$ matrix $X$ is simply a matrix of random variables rather than a data matrix involving random vectors. In the former case, some distribution theory for such a random matrix, including $X'X$, is given by Olkin [2002]. However, random matrices have seen an upsurge of interest in nuclear physics and related topics. Random matrix ensembles were first introduced in physics by Wigner to describe the correlations of nuclear spectra. Underlying the subject is the idea that the characteristic energies of chaotic systems behave locally as if they were the eigenvalues of a very large matrix with randomly distributed elements. The dynamical systems considered are characterized by their Hamiltonians, which in turn are represented by Hermitian matrices. There are also some curious links such as that between certain zeros of the Riemann zeta function and eigenvalues of a random matrix. For an introduction to these ideas see Mehta [2004: chapter 1]. The reader should also refer to Section 5.7 for the definition of terms.
**Definition 21.20.** A Gaussian orthogonal ensemble is a set of real symmetric \( n \times n \) matrices of random variables, \( H = (h_{ij}) \) say, where \( H \)

1. has a probability distribution that is invariant under transformations \( T^{-1}HT \)
   where \( T \) is a real orthogonal matrix (i.e., \( T^{-1} = T' \)),

2. and all the \( h_{ij} (i \leq j) \) are statistically independent.

This model applies when the dynamical system is "symmetric under time reversal".

When there is no time reversal symmetry, we can have a Gaussian unitary ensemble with \( H \) a Hermitian matrix and \( T \) replaced by \( U \), a unitary matrix (with \( U^{-1} = U^* \)). There is also a Gaussian symplectic ensemble with \( H \) a self-dual Hermitian matrix and invariance with respect to the transformation \( WRH \), where \( W \) is any symplectic matrix and \( WR \) is its dual (i.e., \( WRW = I \)). This ensemble arises when there is time reversal symmetry and the total spin is a half-integer.

We define \( \beta \) to be the number of variables representing the number of components making up the particular entity under consideration. Thus \( \beta = 1 \) for real numbers, \( \beta = 2 \) for complex numbers and \( \beta = 4 \) for quaternions.

**21.71.** Given any one of the three Gaussian ensembles above, then the probability density function of \( H \) satisfies

\[
f(\text{vech } Z) = \exp(-a \text{trace}(H^2) + b \text{trace } H + c),
\]

where \( a \) is real and positive, \( b \) and \( c \) are real, and \( b \) is usually zero. In each of the three cases, the eigenvalues of \( H \) are real. The total number of real variables in \( H \) consists of \( n \) diagonal elements and \( \frac{1}{2}n(n - 1)\beta \) off-diagonal elements. Also

\[
\text{trace}(H^2) = \sum_{i=1}^{n} \lambda_i^2 \quad \text{and} \quad \text{trace } H = \sum_{i=1}^{n} \lambda_i,
\]

where the \( \lambda_i \) are the eigenvalues of \( H \). By choosing \( \frac{1}{2}n(n - 1)\beta \) certain angular parameters together with the \( \lambda_i \), and making the transformation to these new parameters, the Jacobian can be found. This leads to the density function of the \( \lambda_i \) as

\[
c(\beta, n) \exp(-\sum_{i=1}^{n} \lambda_i^2) \prod_{1 \leq i < j \leq n} |\lambda_j - \lambda_k|^\beta.
\]

It is these eigenvalues that are of interest in nuclear physics (Mehta [2004: 53, 56, 58]).
Inequalities arise in many places in probability and statistics. For example, Tong [1980: chapter 8] gives a number of applications of probability inequalities to simultaneous confidence regions, hypothesis testing and simultaneous comparisons, ranking and selection problems, and reliability and life testing. Some of the results in this chapter can be proved using the concept of majorization and Schur convexity, discussed in Chapter 23.

22.1 GENERAL PROBABILITIES

Let $E_i \ (i = 1, 2, \ldots, n)$ be any events.

22.1. (Boole’s Formula)

$$
\text{pr}(\bigcup_{i=1}^{n} E_i) = \sum_{i=1}^{n} \text{pr}(E_i) - \sum_{i=1}^{n-1} \sum_{j=i+1}^{n} \text{pr}(E_i \cap E_j) \\
+ \sum_{i=1}^{n-2} \sum_{j=i+1}^{n-1} \sum_{k=j+1}^{n} \text{pr}(E_i \cap E_j \cap E_k) - \cdots + (-1)^{n+1} \text{pr}(\bigcap_{i=1}^{n} E_i).
$$

From this we can derive the following inequalities:

$$
\text{pr}(\bigcup_{i=1}^{n} E_i) \leq \sum_{i=1}^{n} \text{pr}(E_i),
$$
inequalities for probabilities and random variables

\[ \Pr(\bigcup_{i=1}^{n} E_i) \geq \sum_{i=1}^{n} \Pr(E_i) - \sum_{i<j} \Pr(E_i \cap E_j), \]
\[ \Pr(\bigcap_{i=1}^{n} E_i) \leq \sum_{i=1}^{n} \Pr(E_i) - \sum_{i<j} \Pr(E_i \cap E_j) + \sum_{i<j<k} \Pr(E_i \cap E_j \cap E_k), \]
and so on.

22.2. Let $\overline{E}_i$ be the complement of $E_i$.

(a) $\Pr(\bigcap_{i=1}^{n} E_i) = \Pr(\bigcap_{i=1}^{n} \overline{E}_i) = 1 - \Pr(\bigcup_{i=1}^{n} E_i)$.

(b) This leads to the Kounias inequality
\[ \Pr(\bigcap_{i=1}^{n} E_i) \geq 1 - \sum_{i=1}^{n} \Pr(\overline{E}_i) + \max_j \sum_{i \neq j} \Pr(\overline{E}_i \cap \overline{E}_j). \]

22.3. Since the probability of the union of disjoint events is the sum of the individual probabilities, we have

(a)
\[ \Pr(\bigcup_{i=1}^{n} \overline{E}_i) = \Pr(\overline{E}_1) + \Pr(\overline{E}_2 \cap E_1) + \cdots + \Pr(\overline{E}_n \cap E_{n-1} \cap \cdots \cap E_1) = \Pr(\overline{E}_1) + \sum_{i=2}^{n} \Pr(\overline{E}_i \cap E_{i-1} \cap \cdots \cap E_1). \]

(b) If $(i)$ denotes an arbitrary index in the set \{1, 2, \ldots, $i-1$\} ($i > 1$), then
\[ \Pr(\bigcup_{i=1}^{n} \overline{E}_i) \leq \Pr(\overline{E}_1) + \sum_{i=2}^{n} \Pr(\overline{E}_i \cap E_{(i)}) = \sum_{i=1}^{n} \Pr(\overline{E}_i) - \sum_{i=2}^{n} \Pr(\overline{E}_i \cap \overline{E}_{(i)}). \]

Since the labeling of the $E_i$ is arbitrary we have the following generalization.

22.4. (Hunter–Worsley Inequality) Let $G$ be a graph representing events $\overline{E}_1, \ldots, \overline{E}_n$ as vertices with $\overline{E}_i$ and $\overline{E}_j$ joined by an edge $e_{ij}$ if and only if $E_i \cap E_j \neq \emptyset$. Then, for any spanning tree $T$ of $G$,
\[ \Pr(\bigcap_{i=1}^{n} E_i) \geq 1 - \sum_{i=1}^{n} \Pr(\overline{E}_i) + \sum_{(i,j) : e_{ij} \in T} \Pr(\overline{E}_i \cap \overline{E}_j). \]

In the class of the above bounds, the sharpest bound is obtained by finding the spanning tree $T^*$ for which the term
\[ \sum_{(i,j) : e_{ij} \in T^*} \Pr(\overline{E}_i \cap \overline{E}_j) \]
is maximum (cf. Hochberg and Tamhane [1987: 364 for further details]). The Kounias inequality (cf. 22.2b) is never sharper as it uses the maximum only over a subset of all spanning trees.

**Proofs.** Section 22.1.

22.1. This result can be readily proved by induction.


22.3a. We take the union of the events on the right-hand side and use results like $\bar{E}_1 \cup (\bar{E}_2 \cap E_1) = \bar{E}_1 \cup \bar{E}_2$ and $E_1 \cap (\bar{E}_2 \cap \bar{E}_1) = \phi$, and so on, to show that the events are disjoint.

22.3b. Follows from $\Pr(\bar{E}_i) = \Pr(\bar{E}_i \cap E_{(i)}) + \Pr(\bar{E}_i \cap \bar{E}_{(i)})$.

### 22.2 BONFERRONI-TYPE INEQUALITIES

22.5. We have the following results.

(a) **(Degree-One Inequality)** If $p_i = \Pr(E_i)$, $i = 1, 2, \ldots, k$, then

$$\Pr(\cap_{i=1}^k E_i) \geq 1 - \sum_{i=1}^k (1 - p_i).$$

(b) **(Degree-Two Inequality)** Let $q_i = \Pr(\bar{E}_i) = 1 - p_i$ and $q_{ij} = q_{ji} = \Pr(\bar{E}_i \cap \bar{E}_j)$ for $i, j = 1, 2, \ldots, k$. Then

(i)

$$1 - Q_1 \leq \Pr(\cap_{i=1}^k E_i) \leq 1 - \frac{Q_1^2}{Q_1 + 2Q_2},$$

where

$$Q_1 = \sum_{i=1}^n q_i \quad \text{and} \quad Q_2 = \sum_{i=2}^n \sum_{j=1}^{i-1} q_{ij} = \sum_{j<i}^n q_{ij}.$$  

Note that $Q_1 + 2Q_2$ is simply $\sum_{i=1}^n \sum_{j=1}^n q_{ij}$, where $q_{ii} = q_i$ for all $i$. Also, from (22.2a), we obtain

$$\Pr(\cup_{i=1}^n \bar{E}_i) \geq \frac{Q_1^2}{Q_1 + 2Q_2}.$$  

(ii) If $q = (q_1, q_2, \ldots, q_n)'$ and $Q = (q_{ij})$ is nonsingular, then

$$\Pr(\cup_{i=1}^n \bar{E}_i) \geq q'Q^{-1}q,$$

by (12.1d). The nonsingularity condition for $Q$ was removed as follows.

(iii) $\Pr(\cup_{i=1}^n \bar{E}_i) \geq q'Q^{-1}q$, where $Q^{-1}$ is a weak inverse of $Q$. 


(iv) The lower bound given in (a) is sharpened in the following result.

\[ 1 - Q_1 + \max_{1 \leq j \leq n} \sum_{i:i \neq j} q_{ij} \leq \Pr(\bigcap_{i=1}^{n} E_i) \leq 1 - Q_1 + Q_2. \]

This is equivalent to

\[ Q_1 - Q_2 \leq \Pr(\bigcup_{i=1}^{n} \overline{E_i}) \leq Q_1 - \max_{1 \leq j \leq n} \sum_{i:i \neq j} q_{ij}. \]

The above results are called second degree because they require only knowledge of pairwise intersections of events. For further information on higher degree inequalities see Tong [1980: 147-148]. Some statistical applications of Bonferroni inequalities to simultaneous confidence intervals are given by Galambos and Simonelli [1996: chapter 8].

**Proofs.** Section 22.1.

22.5a. Tong [1980: 143, theorem 7.1.1]

22.5b(i). Tong [1980: 143, theorem 7.1.2].

22.5b(ii). Tong [1980: 145, lemma 7.1.1].

22.5b(iii). Kounias [1968] and quoted by Tong [1980: 146, theorem 7.1.3].

22.5b(iv). Tong [1980: 147, theorem 7.4.1].

### 22.3 DISTRIBUTION-FREE PROBABILITY INEQUALITIES

#### 22.3.1 Chebyshev-Type Inequalities

If \(x\) is a random variable with mean \(\mu\) and variance \(\sigma^2\), then for \(a > 0\),

\[ \Pr[|x - \mu| \leq a\sigma] \geq 1 - 1/a^2. \]

This is known as the univariate Chebyshev inequality. A one-sided version is given by

\[ \Pr[x - \mu \leq a\sigma] \geq 1 - 1/(1 + a^2), \]

and a multivariate version (with equal variances and common correlation) is considered by Tong [1980: 155, lemma 7.2.1]. We now consider further generalizations of these from Tong [1980: section 7.2].

22.6. Let \(x = (x_1, x_2)'\) be a random vector with mean \(\mu = (\mu_1, \mu_2)\)', variances \(\sigma_1^2\) and \(\sigma_2^2\), and correlation \(\rho\). Then:

(a) For all \(a_i > 0\),

\[ \Pr[\bigcap_{i=1}^{2}(|x_i - \mu_i| \leq a_i\sigma_i)] \geq 1 - [(a_1^2 + a_2^2) + [(a_1^2 + a_2^2)^2 - 4\rho^2 a_1^2 a_2^2)^{1/2}]/(2a_1^2 a_2^2). \]

(b) When \(a_1 = a_2 = a\),

\[ \Pr[\bigcap_{i=1}^{2}(|x_i - \mu_i| \leq a\sigma_i)] \geq 1 - [1 + (1 - \rho^2)^{1/2}]/a^2. \]

The equality is attainable.
22.7. Let \( \mathbf{x} = (x_1, x_2, \ldots, x_n)' \) be a random vector with mean vector \( \mu \) and variance matrix \( \Sigma = (\sigma_{ij}) \). If \( \sigma_i^2 = \sigma_{ii} \) and \( a_i > 0 \) for all \( i \), then

\[
\Pr [ \bigcap_{i=1}^n (|x_i - \mu_i| \leq a_i \sigma_i)] \geq 1 - \sum_{i=1}^n \frac{1}{a_i^2}.
\]

Tong [1980: 153] described a more general result that gives the sharpest lower bound.

22.8. Let \( \mathbf{x} = (x_1, x_2, \ldots, x_n)' \) be a random vector with mean \( \mu \), variances \( \sigma_i^2 \) \( (i = 1, 2, \ldots, n) \), and common correlation \( \rho \), where \( \rho \in [-1/(n-1), 1] \) (to ensure that the variance matrix is positive definite; cf. 15.18a(iv)). Then, for \( a \) satisfying

\[
a > (n-1)(1-\rho)/n^{1/2},
\]

we have

\[
\Pr[\bigcap_{i=1}^n (x_i \leq \mu_i + a\sigma_i)] \geq 1 - \frac{\left(1 + (n-1)\rho + a(n-1)(1-\rho)^{1/2}\right)^2}{n^2 + 1 + (n-1)\rho/n},
\]

where \( u = (n-1)(1-\rho) - 1 \).

22.9. Let \( \mathbf{x} = (x_1, x_2, \ldots, x_n)' \) be a random vector with mean \( \mu \).

(a) Let \( \phi \) be a concave function from \( \mathbb{R}^n \) to \([0, \infty)\). For fixed \( a > 0 \), define \( A = \{ \mathbf{x} | \phi(\mathbf{x}) \leq a \} \). If \( E[\phi(\mathbf{x})] \) exists, then

\[
\Pr(\mathbf{x} \in A) \geq 1 - \frac{\phi(\mu)}{a}.
\]

We now give several applications of the above result.

(b) If \( y \) is a non-negative random variable with \( E(y) < \infty \), then setting \( A = \{ y : y \leq \delta \} \) we have

\[
\Pr(y \geq \delta) \leq \frac{E(y)}{\delta}, \quad \delta > 0.
\]

(c) Suppose that the \( x_i \) are all non-negative, and let \( x_{(1)} \leq \cdots \leq x_{(n)} \) denote the order statistics. Then, for \( c_1 \geq \cdots \geq c_n \geq 0 \), the function \( \phi(\mathbf{x}) = \sum_{i=1}^n c_i x_{(i)} \) is concave in \( \mathbf{x} \). If \( E(x_{(i)}) \) exists, then

\[
\Pr(\sum_{i=1}^n c_i x_{(i)} \leq a) \geq 1 - \sum_{i=1}^n \frac{c_i \mu_{(i)}}{a}, \quad a > 0,
\]

where \( \mu_{(1)} \leq \cdots \leq \mu_{(n)} \) are the ordered means.

For the special case \( c_1 = 1 \) and \( c_2 = \cdots = c_n = 0 \), this reduces to

\[
\Pr(\min_{1 \leq i \leq n} x_i \leq a) \geq 1 - \frac{1}{a} \min_{1 \leq i \leq n} \mu_i,
\]

or equivalently

\[
\Pr[\bigcap_{i=1}^n (x_i > a)] \leq \frac{1}{a} \min_{1 \leq i \leq n} \mu_i.
\]
Proofs. Section 22.3.1.

22.6a. Quoted by Tong [1980: 152].

22.6b. Tong [1980: 150, theorem 7.2.1].

22.8. Tong [1980: 156, theorem 7.2.3].

22.9a. Tong [1980: 157, theorem 7.2.4].

22.9b. Mathai and Provost [1992: 188].

22.9c. Quoted by Tong [1980: 158].

22.3.2 Kolmogorov-Type Inequalities

22.10. Let $y_1, y_2, \ldots, y_n$ be $n$ independent random variables with means $\eta_i$ and variances $\tau_i^2$ ($i = 1, 2, \ldots, n$), and let $\nu_n = (\sum_{i=1}^{n} \tau_i^2)^{1/2}$. Then, for every fixed $a > 0$, we have the following:

(a) $\Pr\left(\bigcap_{r=1}^{n} \left(\bigcup_{i=1}^{r} (y_i - \eta_i) \leq a\nu_n\right)\right) \geq 1 - 1/a^2$.

(b) $\Pr\left(\bigcap_{r=1}^{n} \left(\bigcup_{i=1}^{r} (y_i - \eta_i) \leq a\nu_n\right)\right) \geq a^2/(1 + a^2)$.

Proofs. Section 22.3.2.

22.10a. Tong [1980: 158, theorem 7.3.1].

22.10b. Tong [1980: 159, theorem 7.3.2].

22.3.3 Quadratics and Inequalities

22.11. Let $x$ be a $n \times 1$ random vector with $E(x) = \mu$ and $\text{var}(x) = \Sigma$, and consider the quadratics $Q_i = (x - a)'A_i(x - a)$, where $A_i$ is non-negative definite ($i = 1, 2, \ldots, k$) and $a$ is an arbitrary constant vector.

(a) $\Pr[\bigcap_{i=1}^{k} (Q_i \leq \delta_i)] \geq 1 - \left(\frac{\gamma_1}{\delta_1} + \frac{\gamma_2}{\delta_2} + \cdots + \frac{\gamma_k}{\delta_k}\right)$,

where, for $i = 1, 2, \ldots, k$, we have $\delta_i > 0$ and $\gamma_i = \text{trace}(A_i\Sigma) + (\mu - a)'A_i(\mu - a)$.

(b) $\Pr[\bigcap_{i=1}^{k} (Q_i \geq \delta_i)] \leq \frac{\gamma_1 + \gamma_2 + \cdots + \gamma_k}{\delta_1 + \delta_2 + \cdots + \delta_k}$.

Proofs. Section 22.3.3.

22.4 DATA INEQUALITIES

22.12. The following inequalities hold for any numbers, but the main application is to random observations.

(a) Let $x_1, x_2, \ldots, x_n$ be $n$ observations and define $\bar{x} = \sum_{i=1}^{n} x_i / n$ and $\bar{\sigma}^2 = \sum_{i=1}^{n} (x_i - \bar{x})^2 / n$. Then

$$(x_i - \bar{x})^2 \leq (n - 1)\bar{\sigma}^2, \quad i = 1, 2, \ldots, n.$$ 

Equality holds if all the other $x_j$'s are equal except $x_i$. For an extension of the above see Kabe [1980].

(b) Let $x_1 \geq x_2 \geq \cdots \geq x_n$. Then

$$\bar{x} - \bar{\sigma} \sqrt{(k - 1)/(n - k + 1)} \leq x_k \leq \bar{x} + \bar{\sigma} \sqrt{(n - k)/k}.$$ 

Equality occurs on the left-hand side if and only if

$$x_1 = x_2 = \cdots = x_{k-1} \quad \text{and} \quad x_k = x_{k+1} = \cdots = x_n,$$

and on the right-hand side if and only if

$$x_1 = x_2 = \cdots = x_k \quad \text{and} \quad x_{k+1} = x_{k+2} = \cdots = x_n.$$

(c) Suppose $x_1, x_2, \ldots, x_n$ are $d$-dimensional observations. Let $\bar{x}_n = \sum_{i=1}^{n} x_i / n$ and $S_n = \sum_{i=1}^{n} (x_i - \bar{x}_n)(x_i - \bar{x}_n)' / n$. Then

$$(n - 1)S_n - (x_j - \bar{x}_n)(x_j - \bar{x}_n)' \quad \text{is non-negative definite},$$ 

or equivalently,

$$(x_j - \bar{x}_n)'S_n^{-1}(x_j - \bar{x}_n) \leq n - 1, \quad j = 1, 2, \ldots, n.$$ 

Thus each $x_j$ lies in the interior or on the surface of the ellipsoid $(x - \bar{x}_n)'S_n^{-1}(x - \bar{x}_n) = n - 1$. If $S_n$ is singular, we can replace $S_n^{-1}$ by $S_n^-$, a weak inverse of $S_n$.

(d) If $\bar{x}_{(j)} = \frac{1}{n-1} \sum_{i: i \neq j} x_i$, then

$$\frac{n^2}{n - 1}S_n - (x_j - \bar{x}_{(j)})(x_j - \bar{x}_{(j)})' \quad \text{is non-negative definite},$$ 

or equivalently,

$$(x_j - \bar{x}_{(j)})'S_n^{-1}(x_j - \bar{x}_{(j)}) \leq \frac{n^2}{n - 1}, \quad j = 1, 2, \ldots, n.$$ 

Proofs. Section 22.4.


22.12b. Farnum [1989] and Wolkowicz and Styan [1979].

22.12c. Trenkler and Puntanen [2005]

22.12d. Trenkler and Puntanen [2005].
22.5 INEQUALITIES FOR EXPECTATIONS

22.13. (Multivariate Jensen’s Inequality) Let \( x \) be an \( n \times 1 \) random vector with finite expectation \( E(x) = \mu \).

(a) Let \( \phi \) be a real-valued convex function defined on \( S \), where \( S \) is a convex subset of \( \mathbb{R}^n \). If \( \text{pr}(x \in S) = 1 \), then

\[
E[\phi(x)] \geq \phi(\mu).
\]

(b) If \( \phi \) is a symmetric (cf. Definition 23.6 above (23.14)) and continuous function on \( \mathbb{R}^n \), then

\[
\phi(\mu(1), \mu(2), \ldots, \mu(n)) \leq E[\phi(x(1), x(2), \ldots, x(n))],
\]

where \( \mu(1) \geq \mu(2) \geq \cdots \geq \mu(n) \) and \( x(1) \geq x(2) \geq \cdots \geq x(n) \).

22.14. (Finite Population) Suppose that \( x_1, x_2, \ldots, x_n \) are obtained by sampling without replacement from a finite population, and \( y_1, y_2, \ldots, y_n \) are obtained by sampling with replacement from the same population. Then if \( g \) is continuous and convex,

\[
E \left[ \left( \sum_{i=1}^{n} x_i \right) \right] \leq E \left[ \left( \sum_{i=1}^{n} y_i \right) \right].
\]

Proofs. Section 22.5.


22.6 MULTIVARIATE INEQUALITIES

22.6.1 Convex Subsets

22.15. Let \( x \in \mathbb{R}^d \) be a random vector with symmetric probability density function \( f(x) \), that is, \( f(-x) = f(x) \), such that the set \( \{ x : f(x) \geq \alpha \} \) is convex for all \( \alpha > 0 \). Suppose that \( S \) is a convex subset of \( \mathbb{R}^d \) and is symmetric about \( 0 \) (i.e., if \( x \in S \) then \( -x \in S \) also). Then:

(a) \( \text{pr}(x + cb \in S) \geq \text{pr}(x + b \in S) \) for any constant \( b \in S \) and \( 0 \leq c \leq 1 \).

(b) The result (a) still hold if \( b \) is replaced by \( y \), a random vector distributed independently of \( x \).

(c) If \( x \sim N_d(0, \Sigma) \), then its probability density function satisfies the above conditions.

(d) If \( x \sim N_d(0, \Sigma_1) \) and \( y \sim N_d(0, \Sigma_2) \), where \( \Sigma_1 - \Sigma_2 \) is non-negative definite, then \( \text{pr}(x \in S) \leq \text{pr}(y \in S) \). This type of result has been extended to elliptically contoured distributions by Perlman [1993].

Many of the unimodal symmetric multivariate distributions centered at the origin, like the multivariate normal and multivariate t-distribution, satisfy the conditions of this theorem. For further background see Anderson [1996].
22.6.2 Multivariate Normal

22.16. (Slepian Inequality) Suppose $x \sim N_d(0, \Sigma)$, where $\Sigma = (\sigma_{ij})$ is non-negative definite. Let $y_i = x_i/\sqrt{\sigma_{ii}}$, $i = 1, 2, \ldots, d$ so that $y \sim N_d(0, R)$, where $R = (\rho_{ij})$ is the population correlation matrix. Then, for any constants $c_1, c_2, \ldots, c_d$,

$$\Pr \left[ \cap_{i=1}^{d} (y_i \leq c_i) \right]$$

is an increasing function for each $\rho_{ij}$, $i \neq j$. If $R$ is positive definite, then the above is a strictly increasing function of $\rho_{ij}$, $i \neq j$.

Replacing $c_i$ by $\sqrt{\sigma_{ii}} c_i$, we see that the result still holds if use the $x_i$ instead of the $y_i$.

If all the $\rho_{ij} \geq 0$ ($i \neq j$), then

$$\Pr \left[ \cap_{i=1}^{d} (y_i \leq c_i) \right] \geq \prod_{i=1}^{d} \Pr(y_i \leq c_i).$$

If $\rho_{ij} \leq 0$ for all $i, j, i \neq j$, the above inequality is reversed.

Because we can transform from $x_i$ to $y_i$, researchers have focused, without any loss of generality, on deriving results for $y$, where $y \sim N_d(0, R)$ and $R$ is the correlation matrix.

22.17. (Khatri)

(a) Suppose $x = (x'_1, x'_2)' \sim N_d(0, \Sigma)$, where $x_{(k)}$ is $d_k \times 1$ ($k = 1, 2$) and $d = d_1 + d_2$. Let

$$\Sigma = \begin{pmatrix} \Sigma_{11} & \Sigma_{12} \\ \Sigma_{12} & \Sigma_{22} \end{pmatrix},$$

where $\Sigma_{kk}$ is $d_k \times d_k$. Let $A_1 \subset \mathbb{R}^{d_1}$ and $A_2 \subset \mathbb{R}^{d_2}$ be two convex regions that are symmetric about the origin (cf. 22.15). If $\Sigma_{12}$ has rank zero (i.e., $\Sigma_{12} = 0$) or has rank one, then

$$\Pr \left[ \cap_{k=1}^{2} (x_{(k)} \in A_k) \right] \geq \prod_{k=1}^{2} \Pr(x_{(k)} \in A_k).$$

Setting $x_{(1)} = x_1$, we have

$$\Pr(|x_1| \leq a_1, x_{(2)} \in A_2) \geq \Pr(|x_1| \leq a_1) \Pr(x_{(2)} \in A_2),$$

and repeatedly applying this result to each element of $x_{(2)}$, we obtain

$$\Pr \left[ \cap_{i=1}^{d} (|x_i| \leq a_i) \right] \geq \prod_{i=1}^{d} \Pr(|x_i| \leq a_i).$$

This inequality is strict if $\Sigma$ is positive definite, $\Sigma$ is not a diagonal matrix, and all the $a_i$s are positive.

The above results have been generalized to the case when the mean of $x$ is not necessarily zero. For details see Tong [1980: theorem 2.2.3].

If the correlation matrix $R$ of $x$ has structure $l$ (see (b) below) and is positive definite, then $\Sigma_{12}$ has rank 0 or 1 (quoted by Tong [1980: 33, example 11]).
(b) Suppose \( \mathbf{x} = (x'_1, x'_2, \ldots, x'_r)' \), where \( \mathbf{x} \sim N_d(\mathbf{0}, \mathbf{R}) \) and \( \mathbf{R} = (\rho_{ij}) \) is the correlation matrix. Here \( x(k) \) is \( d_k \times 1 \) \((k = 1, 2, \ldots, r)\), where \( \sum_k d_k = d \). For each \( k \), let \( A_k \subset \mathbb{R}^{d_k} \) be a convex region symmetric about the origin. Suppose we have the product structure \( \rho_{ij} = \lambda_i \lambda_j \), \( \lambda_i \in (-1, 1) \), for all \( i, j \) \((j \neq i)\), called structure 1 by Tong, then the following inequalities hold.

(i) Firstly,

\[
\Pr \left[ \bigcap_{k=1}^r \left( x(k) \in A_k \right) \right] \geq \Pr \left[ \bigcap_{k \in C} \left( x(k) \in A_k \right) \right] \times \Pr \left[ \bigcap_{k \notin C} \left( x(k) \in A_k \right) \right] \\
\geq \prod_{k=1}^r \Pr (x(k) \in A_k)
\]

and

\[
\Pr \left[ \bigcap_{k=1}^r \left( x(k) \notin A_k \right) \right] \geq \Pr \left[ \bigcap_{k \in C} \left( x(k) \notin A_k \right) \right] \times \Pr \left[ \bigcap_{k \notin C} \left( x(k) \notin A_k \right) \right] \\
\geq \prod_{k=1}^r \Pr (x(k) \notin A_k)
\]

holds for every subset \( C \) of the integers \( \{1, 2, \ldots, r\} \). The inequalities are strict if the \( A_i \)'s are bounded sets with positive probabilities and the \( \lambda_i \)'s are nonzero.

(ii) We then have the following special case of the above.

\[
\Pr \left[ \bigcap_{i=1}^d \left( |x_i| \geq a_i \right) \right] \geq \prod_{i=1}^d \Pr (|x_i| \geq a_i).
\]

22.18. (Sidák’s Theorem) Let \( \mathbf{x} \sim N_d(\mathbf{0}, \mathbf{R}(\lambda)) \), where \( \mathbf{R}(\lambda) = (\rho_{ij}(\lambda)) \) is a correlation matrix depending on \( \lambda \in [0, 1] \) in the following way: For a fixed non-negative definite correlation matrix \( \mathbf{T} = (\tau_{ij}) \), we define \( \rho_{ij}(\lambda) = \tau_{ij} \) for all \( i, j = 2, 3, \ldots, d \) and \( \rho_{ij}(\lambda) = \rho_{j1}(\lambda) = \lambda \tau_{1j} \) for \( j = 2, \ldots, d \). Then \( \mathbf{R}(\lambda) \) is non-negative definite for \( \lambda \in [0, 1] \), and

\[
\Pr \left[ \bigcap_{i=1}^d \left( |x_i| \leq a_i \right) \right]
\]

is monotonically nondecreasing in \( \lambda \in [0, 1] \) for every \( a_i \) \((i = 1, 2, \ldots, d)\). If \( \mathbf{T} \) is positive definite (which implies \( \mathbf{R}(\lambda) \) is positive definite), \( \tau_{ij} \neq 0 \) for some \( j > 1 \), and all the \( a_i \)'s are positive, then the above probability is strictly increasing in \( \lambda \).

A consequence of the above result is that if we now have correlation matrix \( \mathbf{R}(\lambda) \), where \( \lambda = (\lambda_1, \lambda_2, \ldots, \lambda_d)' \), \( \rho_{ij}(\lambda) = \lambda_i \lambda_j \tau_{ij} \) for all \( i \neq j \), and each \( \lambda_i \in [0, 1] \), then the above probability is monotonically nondecreasing in each \( \lambda_i \in [0, 1] \). It is strictly increasing in \( \lambda_i \) if \( \mathbf{T} = (\tau_{ij}) \) is positive definite, \( \lambda_i \tau_{ij} \neq 0 \) for some \( j \neq i \), and all the \( a_i \)'s are positive.

22.19. Suppose \( \mathbf{x} \sim N_d(\mathbf{0}, \Sigma) \), where \( \sigma_{ij} = \sigma^2 \) for \( i = j \), \( \sigma_{ij} = \rho \sigma^2 \) for \( i \neq j \), and \( \rho \in [0, 1] \). Define for \( k = 1, 2, \ldots, d \) and \( a > 0 \),

\[
\Pr_1 (k) = \Pr \left[ \bigcap_{i=1}^k (x_i \leq a) \right] \\
\Pr_2 (k) = \Pr \left[ \bigcap_{i=1}^k (|x_i| \leq a) \right]
\]
and
\[ \text{pr}_3(k) = \text{pr} \left[ \cap_{i=1}^k (|x_i| \geq a_i) \right]. \]

Then, for \( m = 1, 2, 3 \), we have
\[ \text{pr}_m(d) \geq [\text{pr}_m(k)]^{d/k} \geq [\text{pr}_m(1)]^d, \quad d > k \geq 2. \]

The inequalities are strict if \( \rho > 0 \).

**Definition 22.1.** Let \( \mathbf{x} = (x_1, x_2, \ldots, x_d)' \) be a random vector. We say that the elements of \( \mathbf{x} \) are **associated random variables** if for any two univariate functions \( g_i(x) \) of \( x \) such that \( \text{E}[g_i(x)] \) exists (\( i = 1, 2 \)) that are nondecreasing in each argument, we have \( \text{cov}[g_1(x), g_2(x)] \geq 0 \). Esary et al. [1967], who introduced the concept, have given a number of results that can be used to readily verify that a given set of random variables is associated.

**22.20.** The following statements are true.

(a) Any subset of associated random variables is a set of associated random variables.

(b) The set consisting of a single random variable is associated.

(c) If two sets of associated random variables are independent, then their union is a set of associated random variables.

(d) Independent random variables are associated.

(e) Nondecreasing functions of associated random variables are associated random variables.

**22.21.** If the elements of the \( d \times 1 \) vector \( \mathbf{x} \) are associated random variables, then
\[ \text{pr} \left[ \cap_{i=1}^d (x_i \leq a_i) \right] \geq \text{pr} \left[ \cap_{i\in C} (x_i \leq a_i) \right] \text{pr} \left[ \cap_{i\notin C} (x_i \leq a_i) \right] \]
\[ \geq \prod_{i=1}^d \text{pr}(x_i \leq a_i) \]
holds for all \( a_i \) and all subsets \( C \) of \( \{1, 2, \ldots, d\} \).

**Proofs.** Section 22.6.2.

22.15. Results quoted by Schott [2005: 83, exercise 2.61] and follow from (2.65e).

22.16. Tong [1980: section 2.1].


22.17b(i). Quoted by Hochberg and Tamhane [1987: 367] and proved by Tong [1980: theorems 2.2.4 and 2.3.2].

22.17b(ii). Tong [1980: 28, theorem 2.3.3].

22.18. Tong [1980: 21, theorem 2.2.5, corollary 1].

22.19. Tong [1980: 30, theorem 2.3.4].

22.20. Tong [1980: 87, theorem 5.2.2].

22.21. Tong [1980: 89, theorem 5.2.4].
22.6.3 Inequalities For Other Distributions

22.22. (Multivariate t-Distribution) Let \( x = (x_1, x_2, \ldots, x_d)' \sim N_d(0, \mathbf{R}) \), where we can assume without loss of generality that \( \mathbf{R} = (\rho_{ij}) \) is the correlation matrix with \( \rho_{ii} = 1 \) (cf. 22.16). Let \( z_i = x_i/u \), where \( u \) is distributed as a \( \sqrt{\chi^2_0/\nu} \) random variable independent of \( x \). Then \( z = (z_1, z_2, \ldots, z_d)' \) has a multivariate \( t \)-distribution with \( \nu \) degrees of freedom and associated correlation matrix \( \mathbf{R} \). In terms of the notation of Section 22.6.2, \( y \sim t_d(\nu, 0, \mathbf{R}) \).

By conditioning on \( u \), the following inequalities from above still hold with \( x_i \) or \( y_i \) replaced by \( z_i \).

(a) If all the \( \rho_{ij} \geq 0 \), then

\[
\Pr\left[ \bigcap_{i=1}^{d} (z_i \leq c_i) \right] \geq \prod_{i=1}^{d} \Pr(z_i \leq c_i).
\]

(b) \( \Pr\left[ \bigcap_{i=1}^{d} (|z_i| \leq a_i) \right] \geq \prod_{i=1}^{d} \Pr(|z_i| \leq a_i) \).

This inequality is strict if \( \mathbf{R} \) is positive definite, \( \mathbf{R} \) is not a diagonal matrix, and all the \( a_i \)'s are positive.

(c) If \( \rho_{ij} = \lambda_i \lambda_j \) (all \( i, j, j \neq i \)), where each \( \lambda_i \in (-1, +1) \), then

\[
\Pr\left[ \bigcap_{i=1}^{d} (|z_i| \geq a_i) \right] \geq \prod_{i=1}^{d} \Pr(|z_i| \geq a_i).
\]

22.23. (Correlated F-ratios) Let \( \chi^2_0, \chi^2_1, \ldots, \chi^2_k \) be independent chi-square variables with degrees of freedom \( \nu_0, \nu_1, \ldots, \nu_k \), and let \( F_i = (\chi^2_i/\nu_i)/(\chi^2_0/\nu_0) \), \( i = 1, 2, \ldots, k \). Then

(a) \( \Pr\left[ \bigcap_{i=1}^{k} (F_i \leq a_i) \right] > \prod_{i=1}^{k} \Pr(F_i \leq a_i) \).

(b) \( \Pr\left[ \bigcap_{i=1}^{k} (F_i > a_i) \right] > \prod_{i=1}^{k} \Pr(F_i > a_i) \).

Proofs. Section 22.6.3.


22.23. Tong [1980: 43, theorem 3.2.2].
Majorization does not seem to be a topic very well known in statistical circles. However, majorization can be used to prove a number of inequalities. A key result is (23.7), from which we may assume without any loss of generality (Tong [1980: 105]) that only two coordinates need be different when proving inequalities. Two applications are, for example, species-diversity indices (Tong [1983]) and optimal design theory (Bhaumik [1995]). The topic is also relevant to the finding of optimal statistical tests (Anderson [2003: section 8.10]).

23.1 GENERAL PROPERTIES

Definition 23.1. Let \( x = (x_1, x_2, \ldots, x_n)' \) and \( y = (y_1, y_2, \ldots, y_n)' \) be vectors in \( \mathbb{R}^n \). Suppose the \( x_i \) are ordered in decreasing order of magnitude as \( x_1 \geq x_2 \geq \cdots \geq x_n \), with the \( y_i \) ordered in a similar fashion. We say that \( x \) is (strongly) majorized by \( y \) (or \( y \) majorizes \( x \)), and use the symbol \( x \ll y \) (or \( y \gg x \)), if

\[
\begin{align*}
  x(1) + x(2) + \cdots + x(i) & \leq y(1) + y(2) + \cdots + y(i), & i = 1, 2, \ldots, n - 1, \\
  x_1 + x_2 + \cdots + x_n & = y_1 + y_2 + \cdots + y_n.
\end{align*}
\]

This definition is given by Marshall and Olkin [1979] and Horn and Johnson [1991], except they use \( x_{[i]} \) instead of \( x(i) \). They and most other authors, except Rao and Rao [1998: chapter 9], use \( x \prec y \) instead of \( x \ll y \); however, I have reserved the
former symbol in the form of \( \mathbf{A} \succ \mathbf{0} \) for positive definite matrices and used \( \mathbf{A} \succ \mathbf{0} \) for matrices with all positive elements.

The above definition has also been extended to infinite sequences (Marshall and Olkin [1979: 16]) and to random vectors (Marshall and Olkin [1979: chapter 11]).

23.1. If the \( x_i \) (and the \( y_i \)) are ordered in increasing magnitude, say \( x_1 \leq x_2 \leq \ldots \leq x_n \), then since \( x_{(i)} = x_{(n-i+1)} \), \( \mathbf{x} \ll \mathbf{y} \) if and only if

\[
x_{(1)} + x_{(2)} + \cdots + x_{(i)} \geq y_{(1)} + y_{(2)} + \cdots + y_{(i)}, \quad i = 1, 2, \ldots, n - 1,
\]

\[
x_1 + x_2 + \cdots + x_n = y_1 + y_2 + \cdots + y_n.
\]

Some authors use this result as their definition, which I find confusing because of the direction of the inequalities. Using the notation \( x_{[i]} \) instead of \( x_{(i)} \), Rao and Rao [1998: 304] proved the equivalence of the two definitions.

23.2. Let \( \pi \) be a permutation of \( \{1, 2, \ldots, n\} \). If \( \mathbf{x} \), \( \mathbf{y} \), and \( \mathbf{z} \) are in \( \mathbb{R}^n \), and \( \mathbf{x}_\pi \) is the vector whose components are a permutation of the elements of \( \mathbf{x} \), then the following hold.

(a) \( \mathbf{x} \ll \mathbf{x} \).

(b) If \( \mathbf{x} = \sum_{i=1}^n x_i / n \), then \( \mathbf{x} \ll \mathbf{x} \).

(c) \( \mathbf{x} \ll \mathbf{x}_\pi \) for every permutation \( \pi \).

(d) If \( \mathbf{x} \ll \mathbf{y} \) and \( \mathbf{y} \ll \mathbf{z} \), then \( \mathbf{x} \ll \mathbf{z} \).

(e) If \( \mathbf{x} \ll \mathbf{z} \), \( \mathbf{y} \ll \mathbf{z} \), and \( 0 \leq \alpha \leq 1 \), then \( \alpha \mathbf{x} + (1 - \alpha) \mathbf{y} \ll \mathbf{z} \).

(f) If \( \mathbf{x} \ll \mathbf{y} \), \( \mathbf{x} \ll \mathbf{z} \), and \( 0 \leq \alpha \leq 1 \), then \( \mathbf{x} \ll \alpha \mathbf{y} + (1 - \alpha) \mathbf{z} \).

(g) If \( \mathbf{z} \) is any vector, then

\[
\begin{pmatrix}
\mathbf{x} \\
\mathbf{z}
\end{pmatrix} \ll \begin{pmatrix}
\mathbf{y} \\
\mathbf{z}
\end{pmatrix}
\text{ if and only if } \mathbf{x} \ll \mathbf{y}.
\]

(h)

\[
\begin{pmatrix}
1/n, 1/n, \ldots, 1/n
\end{pmatrix}' \ll \begin{pmatrix}
1/(n-1), 1/(n-1), \ldots, 1/(n-1), 0
\end{pmatrix}'
\ll \cdots \ll \begin{pmatrix}
1/2, 1/2, 0, \ldots, 0
\end{pmatrix}' \ll (1, 0, \ldots, 0)'.
\]

23.3. The following conditions are equivalent.

(1) \( \mathbf{x} \ll \mathbf{y} \).

(2) \( \mathbf{x} = \mathbf{A} \mathbf{y} \) for some doubly stochastic matrix \( \mathbf{A} \).

(3) \( \mathbf{x} = \mathbf{B} \mathbf{y} \) for some orthostochastic matrix \( \mathbf{B} \).

Note that \( \mathbf{A} \) and \( \mathbf{B} \) are not unique.
23.4. If \( x \geq 0, y \geq 0, \) and \( x \ll y, \) then \( \prod_{i=1}^{n} x_i \geq \prod_{i=1}^{n} y_i. \)

23.5. (Schur) If \( H \) be an \( n \times n \) Hermitian matrix with (real) eigenvalues given by the vector \( \lambda(H) = (\lambda_1, \lambda_2, \ldots, \lambda_n)', \) where \( \lambda_1 \geq \ldots \geq \lambda_n, \) and (real) diagonal elements \( h = (h_{11}, h_{22}, \ldots, h_{nn})', \) then
\[
h \ll \lambda(H)
\]
on \( \mathbb{R}^n. \) This result is an example of a number of inequalities involving the eigenvalues and singular values of a matrix (cf. Marshall and Olkin [1979: chapter 9]), some of which are quoted elsewhere.

23.6. (Fan) If \( A \) and \( B \) are \( n \times n \) Hermitian matrices, then
\[
\lambda(A + B) \ll \lambda(A) + \lambda(B).
\]

**Definition 23.2.** If \( Q \) is a permutation matrix that interchanges just two coordinates of a vector \( x \) (say \( x_j \) and \( x_k \)), then a \( T \)-transform, denoted by \( Tx, \) has \( T \) of the form \( T = \lambda I + (1 - \lambda)Q, \) where \( 0 \leq \lambda \leq 1. \) What \( Tx \) does is transform \( x_j \) into \( \lambda x_j + (1 - \lambda)x_k \) and \( x_k \) into \( \lambda x_k + (1 - \lambda)x_j, \) leaving the other elements of \( x \) unchanged. For example, if \( Q \) interchanges the first two elements of \( x \in \mathbb{R}^n, \) then \( Q = (e_2, e_1, \ldots, e_n) \) is \( I_n \) with its first two columns interchanged.

23.7. We have \( x \ll y \) if and only if there exists a finite number of real vectors \( c_1, c_2, \ldots, c_m \) such that \( x = c_1 \ll c_2 \ll \cdots \ll c_{m-1} \ll c_m = y, \) where, for all \( i, \) \( c_i \) and \( c_{i+1} \) differ in two coordinates only. Thus if \( x \ll y, \) then \( y \) can be derived from \( x \) by successive applications of a finite number of \( T \)-transforms.

**Definition 23.3.** (Weak Majorization) We now generalize the Definition 23.1 above. A vector \( x \) is said to be weakly (sub)majorized by \( y, \) and we denote the relationship by \( x \ll_w y, \) if
\[
x(1) + x(2) + \cdots + x(i) \leq y(1) + y(2) + \cdots + y(i), \quad i = 1, 2, \ldots, n.
\]
Marshall and Olkin [1979] use the notation \( x \prec_w y \) for weak (sub)majorization. Some authors omit the prefix "sub".

We say that \( x \) is weakly (super)majorized by \( y \) and denote the relationship by \( x \ll_w y \) if
\[
x(1) + x(2) + \cdots + x(i) \geq y(1) + y(2) + \cdots + y(i), \quad i = 1, 2, \ldots, n.
\]

23.8. The results below follow directly from the previous definitions.

(a) \( x \ll_w y \) if and only if \( -x \ll_w -y. \)

(b) \( x \ll_w y \) and \( x \ll_w y \) if and only if \( x \ll y. \)

(c) \( x \leq y \) (i.e., \( x_i \leq y_i \) for all \( i \)) implies that \( x \ll_w y \) and \( x \gg_w y. \)

(d) \( x \ll_w y \) if and only if for some \( u, x \leq u \) and \( u \ll y. \)

(e) \( x \ll_w y \) if and only if for some \( v, x \ll v \) and \( v \geq y. \)
23.9. Let $\mathbb{R}_+ = [0, \infty)$. Then $x \ll_w y$ on $\mathbb{R}_+^n$ if and only if there exists a doubly stochastic matrix $A$ such that $x = Ay$.

23.10. $x \ll_w y$ if and only if $\sum_{i=1}^n \phi(x_i) \leq \phi(y_i)$ for all continuous monotonically increasing convex functions $\phi$ (cf. Definition 23.5 below).

23.11. Let $A$ and $B$ be $n \times n$ symmetric matrices, and suppose that $\lambda_1(C) \geq \lambda_2(C) \geq \cdots \geq \lambda_n(C)$ with $\lambda(C)$ the corresponding vector, where $C = A$ or $B$. Then
\[ \lambda(A + B) \ll_w \lambda(A) + \lambda(B). \]

23.12. If $A$ and $B$ are $n \times n$ matrices and $A \leq B$ (i.e., $a_{ij} \leq b_{ij}$ for all $i,j$), then using the notation of (23.11) above we have
\[ \lambda(A) \ll_w \lambda(B). \]

23.13. Let $A$ and $B$ be $n \times n$ real or complex matrices, and let $\sigma_1(C) \geq \sigma_2(C) \geq \cdots \geq \sigma_k(C)$ ($k = \min\{m, n\}$), with $\sigma(C)$ the corresponding vector. Then:

(a) $\sigma(A + B) \ll_w \sigma(A) + \sigma(B)$.

(b) If $m = n$,

(i) $\sigma(AB) \ll_w \sigma(A) \circ \sigma(B)$.

(ii) $\sigma(A \circ B) \ll \sigma(A) \circ \sigma(B)$.

Here "$\circ$" is the Hadamard product.

Proofs. Section 23.1.


23.11. Anderson [2003: 357].


23.2 SCHUR CONVEXITY

**Definition 23.4.** Let \( f \) be a function from \( \mathbb{R}^n \) to \( \mathbb{R}^m \) \((m > 1)\) defined on \( A \subset \mathbb{R}^n \). Then \( f \) is said to be Schur-convex on \( A \) if
\[
x, y \in \mathbb{R}^n \text{ and } x \ll y \text{ on } A \Rightarrow f(x) \ll_w f(y).
\]
Also \( f \) is said to be strongly Schur-convex on \( A \) if
\[
x, y \in \mathbb{R}^n \text{ and } x \ll_w y \text{ on } A \Rightarrow f(x) \ll_w f(y),
\]
and \( f \) is said to be strictly Schur-convex on \( A \) if
\[
x, y \in \mathbb{R}^n \text{ and } x \ll y \text{ on } A \Rightarrow f(x) \ll f(y).
\]

If \( A = \mathbb{R}^n \), we drop the words “on \( A \)”. Note that the label “schur-convex” is a bit misleading as such a function is not necessarily convex.

A function \( f \) is Schur-concave if \((-f)\) is Schur-convex. (The above definitions come from Rao and Rao [1998: 3071, except \( m \) and \( n \) are interchanged.]

The above definitions need to be clarified as follows when \( m = 1 \) and \( f \) is no longer a vector (say \( \phi \)). The function \( \phi \) is Schur-convex (respectively concave) on \( A \) if \( x, y \in \mathbb{R}^n \) and \( x \ll y \) on \( A \Rightarrow \phi(x) \leq \phi(y) \) (respectively \( \phi(x) \geq \phi(y) \)). If \( y \) is not a permutation of \( x \), then \( \phi \) is said to be strictly Schur-convex (respectively concave) on \( A \) if \( x, y \in \mathbb{R}^n \) and \( x \ll y \) on \( A \Rightarrow \phi(x) < \phi(y) \) (respectively \( \phi(x) > \phi(y) \)).

Schur convexity or concavity can be used to prove many inequalities. For example, Marshall and Olkin [1979: chapter 8] list a number of inequalities including those relating to the angles or sides of various geometrical figures such as triangles and polygons. Schur convexity also arises in combinatorial analysis, particularly with respect to graph theory, the theory of network flows, and the study of incidence matrices (Marshall and Olkin [1979: chapter 7]).

**Definition 23.5.** Let \( f \) be a function from \( \mathbb{R}^n \) to \( \mathbb{R}^m \) \((m > 1)\) defined on \( A \subset \mathbb{R}^n \), and let \( x \leq y \) (i.e., \( x_i \leq y_i \) for each \( i \)). Then \( f \) is said to be monotonically increasing on \( A \) if \( x, y \in \mathbb{R}^n \) and \( x \leq y \) on \( A \Rightarrow f(x) \leq f(y) \), monotonically decreasing if \(-f\) is monotonically increasing, and monotone if it is either monotonically increasing or decreasing.

We recall from Section 2.5 that \( f \) is convex if
\[
f(\alpha x + (1 - \alpha)y) \leq \alpha f(x) + (1 - \alpha)f(y),
\]
for every \( 0 \leq \alpha \leq 1 \) and \( x, y \in \mathbb{R}^n \); \( f \) is concave if \(-f\) is convex.

**Definition 23.6.** Let \( f \) be a function from \( \mathbb{R}^n \) to \( \mathbb{R}^m \), and let \( y = f(x) \). Then \( f \) is said to be symmetric if, for every permutation \( \pi \) of \( \{1, 2, \ldots, n\} \), there exists a permutation \( \pi' \) of \( \{1, 2, \ldots, m\} \) such that \( f(x_{\pi}) = y_{\pi'} \) for all \( x \in \mathbb{R}^n \).

If \( m = 1 \), so that \( f = \phi \), say, then \( \phi \) is symmetric if \( \phi(x_{\pi}) = \phi(x) \) for all \( \pi \). Examples of symmetric functions for \( n = 3 \) are \( \phi(x) = x_1 + x_2 + x_3 \), \( \phi(x) = x_1x_2 + x_2x_3 + x_3x_1 \), and \( \phi(x) = x_1x_2x_3 \).

**23.14.** If a function \( f \) from \( \mathbb{R}^n \) to \( \mathbb{R}^m \) is convex and symmetric, then it is Schur-convex. In addition, if \( f \) is monotonically increasing, then \( f \) is strongly Schur-convex.
23.15. Let \( g \) be a function from \( \mathbb{R} \) to \( \mathbb{R} \), and define
\[
  f(x) = (g(x_1), g(x_2), \ldots, g(x_n))^t.
\]
Then, from the previous result, we have the following.

(a) If \( g \) is convex, then \( f \) is Schur-convex.

(b) If \( g \) is a convex monotonically increasing function, then \( f \) is strongly Schur-convex.

(c) Taking \( g(x) = |x| \), \( g(x) = x^2 \), and \( g(x) = \max\{x, 0\} = x^+ \), respectively, we have

\[
  \begin{align*}
  & (i) \ x \ll y \text{ implies that } |x| \llw |y|. \\
  & (ii) \ x \ll y, \ u_i = x_i^2 \text{ and } v_i = y_i^2 \text{ implies that } u \llw v. \\
  & (iii) \ x \ll y \text{ implies that } x^+ \llw y^+.
  \end{align*}
\]

23.16. The following symmetric convex functions are Schur-convex.

(a) \( \phi(x) = \max_i |x_i| \).

(b) \( \phi(x) = (\sum_{i=1}^n |x_i|^r)^{1/r}, \ r \geq 1 \).

23.17. (Sum)

(a) Let \( I \) be an interval of \( \mathbb{R} \), and let \( g \) be a function from \( I \) to \( \mathbb{R} \). If \( g \) is (strictly) convex on \( I \), then \( \phi(x) = \sum_{i=1}^n g(x_i) \) is (strictly) Schur-convex on \( I^n \), as \( \phi \) is symmetric. In this case, \( x \ll y \) on \( I \) implies that \( \phi(x) \leq \phi(y) \) (or \( \phi(x) < \phi(y) \) for strict convexity).

There is also a converse result. Suppose \( g \) is continuous on \( I \). If \( \phi \) is (strictly) Schur-convex on \( I^n \), then \( g \) is (strictly) convex on \( I \).

(b) Combining the above, the inequality
\[
  \sum_{i=1}^n g(x_i) \leq \sum_{i=1}^n g(y_i)
\]
holds for all continuous convex functions \( g \) from \( \mathbb{R} \) to \( \mathbb{R} \) if and only if \( x \ll y \).

Also, the same inequality holds for all continuous increasing convex functions \( g \) if and only if \( x \llw y \). It holds for continuous decreasing convex functions \( g \) if and only if \( x \llw y \).

23.18. The following are examples of strictly convex functions.

(a) For \( a > 0 \), \( g(x) = [x + (1/x)]^a \) is strictly convex on \((0, 1]\). For \( a \geq 1 \), \( g \) is strictly convex on \((0, \infty)\).

(b) \( -\log x \) is strictly convex on \((0, \infty)\).

(c) \( g(x) = 1/x \) is strictly convex on \((0, \infty)\).
In each case \( \phi(x) = \sum_{i=1}^{n} g(x_i) \) is strictly Schur-convex. If \( x_i > 0 \) and \( \sum_{i=1}^{n} x_i = 1 \), then \( n^{-1}1_n \ll x \) (by 23.2b) and \( \phi(n^{-1}1_n) \leq \phi(x) \). We can use this result to set up inequalities. For example, using (a),

\[
\sum_{i=1}^{n} \left( x_i + \frac{1}{x_i} \right)^a \geq \left( \frac{n^2 + 1}{n^{a-1}} \right)^a.
\]

**23.19.** (Product) Let \( g \) be a continuous non-negative function defined on an interval \( I \). Then \( \phi(x) = \prod_{i=1}^{n} g(x_i) \) is (strictly) Schur-convex on \( I^n \) if and only if \( \log g \) is (strictly) convex on \( I \). Since, by (23.2b), \( \bar{x} 1_n \ll x \), we can use this result to obtain various inequalities. For example, \( \log \Gamma(x) \) is strictly convex on \( \mathbb{R}_{++} = (0, \infty) \) so that \( \phi(x) = \prod_{i=1}^{n} \Gamma(x_i) \) is strictly Schur-convex on \( \mathbb{R}_{++}^n \). Hence

\[
[\Gamma(\bar{x})]^n \leq \prod_{i=1}^{n} \Gamma(x_i).
\]

For further details about Schur-convex or Schur-concave functions see Marshall and Olkin [1979: chapter 3].

**Proofs.** Section 23.2.


### 23.3 PROBABILITIES AND RANDOM VARIABLES

**23.20.** (Probabilities) For \( i = 1, 2, \ldots, n \), let \( p_i = \text{pr}(E_i) \), and let \( q_i \) be the probability that at least \( k \) of the events \( E_1, E_2, \ldots, E_n \) occurs.

(a) If \( p = (p_1, \ldots, p_n)' \) and \( q = (q_1, \ldots, q_n)' \), then \( p \ll q \).

(b) From (a) we have \( \sum_{i=1}^{n} p_i = \sum_{i=1}^{n} q_i \) and \( \prod_{i=1}^{n} p_i \geq \prod_{i=1}^{n} q_i \).

**23.21.** (Expectations) Let \( x = (x_1, x_2, \ldots, x_n)' \) be a random vector with finite expectation, and define \( a_i = E(x_i) \), \( \bar{a}_i = a_{(i)} \), and \( b_i = E(x_{(i)}) \), where \( a_{(1)} \geq a_{(2)} \geq \cdots \geq a_{(n)} \) and \( x_{(1)} \geq x_{(2)} \geq \cdots \geq x_{(n)} \). Then:

(a) \( a \ll b \).

(b) \( \bar{a} \ll b \).
23.22. (Eigenvalues) Let $Z$ be a random Hermitian $n \times n$ matrix with eigenvalues $\lambda_1(Z) \geq \lambda_2(Z) \geq \ldots \geq \lambda_n(Z)$ (which are all real). Then
\[
(\lambda_1(E[Z]), \ldots, \lambda_n(E[Z]))' \prec (E[\lambda_1(Z)], \ldots, E[\lambda_n(Z)])',
\]
where the $\lambda_i(E[Z])$ are the eigenvalues of $E[Z]$, the expectation of $Z$.

23.23. (Singular Values) Let $W$ be an $m \times n$ random complex matrix with singular values $\sigma_1(W) \geq \ldots \geq \sigma_t(W)$, where $t = \min(m, n)$. Then
\[
(\sigma_1(E[Z]), \ldots, \sigma_n(E[Z]))' \prec_w (E[\sigma_1(Z)], \ldots, E[\sigma_n(Z)])'.
\]

Proofs. Section 23.2.


CHAPTER 24

OPTIMIZATION AND MATRIX APPROXIMATION

The subject of finding unconstrained or constrained maxima and minima of functions is an extensive one. Schott [2005: section 9.7] gives a helpful summary. We consider only a few basic results in this chapter.

24.1 STATIONARY VALUES

Definition 24.1. Let \( f : \mathbb{R}^n \rightarrow \mathbb{R}^n \) be a real-valued function defined on \( S \), a subset of \( \mathbb{R}^n \). Then \( f \) has a local maximum at \( c \) if, for some \( \delta > 0 \), \( f(c) \geq f(x) \) for all \( x \) such that \( \|x - c\| < \delta \). It has a strict local maximum if \( f(c) > f(x) \) for all \( x \neq c \) such that \( \|x - c\| < \delta \). Also, \( f \) has a global (absolute) maximum at \( c \) if \( f(c) \geq f(x) \) for all \( x \in S \). The function \( f \) has a local minimum at \( c \) if \( -f \) has a local maximum at \( c \), and a global (absolute) minimum at \( c \) if \( -f \) has a global maximum at \( c \).

Let \( c \) be an interior point of \( S \) (cf. Definition 2.29 below (2.63)). Then there exists a \( \delta > 0 \) such that \( x \in S \) for all \( x \) satisfying \( \|x - c\| < \delta \). Suppose \( f \) is differentiable at \( c \). If

\[
\frac{\partial f(c)}{\partial x'} = \frac{\partial f(\mathbf{x})}{\partial x'} \bigg|_{\mathbf{x} = c} = 0,
\]

then any point \( c \) satisfying the above equation is called a stationary point. (Note that \( f(c) \) is also called a critical value of \( f \) at \( c \).) Such a point can be a local maximum, a local minimum, or a saddle point.
24.1. (Unconstrained Local Optimization) Let \( f \) be defined as in Definition 24.1 above, and suppose that \( f \) is twice differentiable at \( c \), where \( c \) is an interior point of \( S \). If \( c \) is a stationary value of \( f \) and \( \nabla^2 f(c) \) is the Hessian of \( f \) at \( c \) (cf. Section 17.11), then:

(a) \( f \) has a strict local minimum at \( c \) if \( \nabla^2 f(c) \) is positive definite.

(b) \( f \) has a strict local maximum at \( c \) if \(-\nabla^2 f(c)\) is positive definite (i.e., \( \nabla^2 f(c) \) is negative definite).

(c) \( f \) has a saddle point at \( c \) if \( \nabla^2 f(c) \) is neither positive definite nor negative definite, but is nonsingular.

(c) \( f \) may have a local minimum, a local maximum, or a saddlepoint at \( c \) if \( \nabla^2 f(c) \) is singular.

24.2. Minimizing a function is equivalent to minimizing a monotonically increasing transformation of that function. This result is particularly useful in maximum likelihood estimation, which is discussed in Section 24.3.1 below.

24.3. (Method of Lagrange Multipliers for Constrained Optimization) We now give sufficient conditions for finding a strict local maximum or minimum of a real-valued function \( f \) defined on \( S \subseteq \mathbb{R}^n \) subject to the vector of constraints \( g(x) = 0 \), where \( g = (g_1, g_2, \ldots, g_m)' \) is \( m \times 1 \) (\( m < n \)).

Let \( c \) be an interior point of \( S \), let \( F(x, \lambda) = f(x) + \lambda' g(x) \), where \( \lambda \in \mathbb{R}^m \) (called the Lagrange multiplier; some use \(-\lambda\)), and suppose that the following conditions hold:

1. \( f \) and \( g \) are twice differentiable at \( c \).
2. \( B = \partial g(x)/\partial x' = (\partial g_i(x)/\partial x_j) \) has full row rank \( m \) at \( x = c \).
3. \( x = c \) is a solution of \( g(x) = 0 \) and \( \partial F(x, \lambda)/\partial x = 0 \) (for some \( \lambda \)).

If \( \mathbf{A} \) is \( \nabla^2 f(x) - \sum_{i=1}^m \lambda_i \nabla^2 g_i(x) \) evaluated at \( x = c \), then \( f \) has a strict local maximum at \( x = c \), subject to \( g(x) = 0 \), if

\[
x' \mathbf{A} x < 0, \quad \text{for all } x \neq 0 \text{ for which } \mathbf{B} x = 0.
\]

A similar result holds for a strict local minimum with the inequality \( x' \mathbf{A} x > 0 \) replacing \( x' \mathbf{A} x < 0 \). In practice, one can often just simply solve the equations \( \partial F(x, \lambda)/\partial x = 0 \) and \( g(x) = 0 \) for \( x \) and \( \lambda \), and then use ad hoc methods to check the nature of the constrained stationary value without having to investigate \( \mathbf{A} \).

24.4. Assuming that the conditions of the previous result (24.3) hold, we now give some equivalent sufficient conditions for a strict local maximum or a strict local minimum to exist. Let \( \mathbf{A} \) be a symmetric \( n \times n \) matrix and \( \mathbf{B} \) an \( m \times n \) matrix of rank \( m \). Let \( \mathbf{A}_{rr} \) be the leading principal \( r \times r \) submatrix of \( \mathbf{A} \), and let \( \mathbf{B}_r \) be the \( m \times r \) matrix obtained by deleting the last \( n - r \) columns of \( \mathbf{B} \). For \( r = 1, 2, \ldots, n \), define the \( (m + r) \times (m + r) \) matrix \( \mathbf{\Delta}_r \) as

\[
\mathbf{\Delta}_r = \begin{pmatrix}
0 & \mathbf{B}_r \\
\mathbf{B}_r' & \mathbf{A}_{rr}
\end{pmatrix}.
\]
If $B_m$ is nonsingular (which can be achieved by rearranging the $x_i$ variables in (24.3)), then $x'Ax > 0$ holds for all $x \neq 0$ satisfying $Bx = 0$ if and only if

$$(-1)^m \det \Delta_r > 0 \quad \text{for all } r = m + 1, \ldots, n.$$ 

Also, $x'Ax < 0$ holds for all $x \neq 0$ satisfying $Bx = 0$ if and only if

$$(-1)^r \det \Delta_r > 0 \quad \text{for all } r = m + 1, \ldots, n.$$ 

Examples using the above theory are given by Schott [2005: 380–381] and Magnus and Neudecker [1999: 138].

24.5. (Global Optimization) Finding the global maximum or minimum is sometimes best achieved by using the ideas of convex sets and functions, as seen in the following results.

(a) On a convex set, the set of points at which the minimum of a convex function is attained is convex, and any local minimum is a global minimum. The same is true for a concave function, except replacing minimum by maximum.

A strictly convex function attains a minimum at no more than one point of a convex set, and a stationary (critical) point is necessarily a minimum.

(b) On a compact convex set, the maximum of a convex function occurs at an extreme point. The same is true for the minimum of a concave function.

We now focus on convex and concave functions.

Proofs. Section 24.1.


24.5. Quoted by Horn and Johnson [1985: 535].

24.2 USING CONVEX AND CONCAVE FUNCTIONS

24.6. Let $f : x \rightarrow f(x)$ be a real-valued convex function defined on $S$, a convex subset of $\mathbb{R}^n$.

(a) Corresponding to each interior point $a \in S$, an $n \times 1$ vector $t$ exists, such that

$$f(x) \geq f(a) + t'(x - a)$$

for all $x \in S$. 
(b) If $S$ is an open convex set, $f$ is differentiable, and $a \in S$, then
\[ f(x) \geq f(a) + \frac{\partial f(a)}{\partial a^T}(x - a) \]
for all $x \in S$.

24.7. (Global Minimum or Maximum) Let $f(x)$ be a real-valued convex (respectively concave) function defined for all $x \in S$, an open convex subset of $\mathbb{R}^n$. If $f$ is differentiable and $c \in S$ is a stationary point of $f$, then $f$ has a global minimum (respectively maximum) at $c$. If $f$ is strictly convex or strictly concave, then $c$ is unique.

24.8. Let $y = f(X)$. If $d^2f \geq 0$, then $f$ is convex and $f$ has a global minimum at $df = 0$. However, if $d^2f > 0$ for all $dX \neq 0$, then $f$ is strictly convex and $f$ has a strict global minimum at $df = 0$. For second-order differentials see Section 17.11.

24.9. (Constrained Global Minimum) Let $f$ be a real-valued function defined and differentiable on an open convex set $S$ in $\mathbb{R}^n$, and let $g$ be an $m \times 1$ vector function ($m < n$) defined and differentiable on $S$. Let $c$ be a point of $S$, and let $F(x) = f(x) + \lambda^T g(x)$, where $\lambda \in \mathbb{R}^m$. Assume that $x = c$ is a solution of $g(x) = 0$ and $\partial F(x)/\partial x = 0$. If $F$ is convex (respectively strictly convex) on $S$, then $f$ has an absolute minimum (respectively unique absolute minimum) at $c$ under the constraint $g(c) = 0$. Under the same conditions, if $F$ is (strictly) concave, then $f$ has a (unique) absolute maximum at $c$ under the constraint $g(c) = 0$.

24.10. Suppose we wish to minimize $y = f(X)$ subject to the constraints $G(X) = 0$, where $G$ is a matrix function of $X$. Define the Lagrangian function $\psi(X) = f(X) - \text{trace}[L^T G(X)]$, where $L$ is a matrix of Langrange multipliers. (If $G$ happens to be symmetric, then we can take $L$ to be symmetric also.) If $\psi$ is (strictly) convex, then $\psi$ has a (strict) global minimum at the point where $d\psi = 0$ under the constraint $G(X) = 0$.

Proofs. Section 24.2.


24.10. Abadir and Magnus [2005: 354].

24.3 TWO GENERAL METHODS

24.3.1 Maximum Likelihood

Definition 24.2. Suppose we have a set of random variables denoted by $x$ with continuous probability density function or discrete probability function $f(x | \theta)$ depending on $d$ unknown parameters $\theta = (\theta_1, \theta_2, \ldots, \theta_d)'$, where $\theta \in \Omega$ (often
We now express this function as a function of $\theta$, namely $l(\theta)$, called the likelihood function. (Any constants or unknown functions of $x$ are sometimes suppressed.)

A value of $\theta, \hat{\theta}$, say, that maximizes $l(\theta)$ or equivalently $L(\theta) = \log l(\theta)$ for $\theta \in \Omega$, is called a maximum likelihood estimate of $\theta$. There is no guarantee that such an estimate exists for (almost) every $y$, nor that it is unique if it exists. If $L$ is based on a set of $n$ independent observations, we denote the estimate by $\hat{\theta}_n$ to emphasize its dependence on $n$.

The vector $u(\theta) = \partial L(\theta)/\partial \theta$, or more briefly $\partial L/\partial \theta$, is usually referred to as the score vector. The equations $u(\theta) = 0$ are called the likelihood equations.

24.11. Under fairly general conditions (e.g., Cox and Hinkley [1974] and Mäkeläinen et al. [1981]), we have the following results.

(a) $E(u) = 0$.

(b) $E(uu') = \text{var}(u) = -E(\partial u/\partial \theta') = E(I) = I_\theta$, where $I = -\partial^2 L/\partial \theta \partial \theta'$ is usually called the (observed) information matrix and $I_\theta$ the expected (Fisher) information matrix.

(c) As $n \to \infty$, $u(\theta)$ is approximately distributed as the multivariate normal distribution $N_d(0, I_\theta)$.

(d) $\hat{\theta}$ is the unique solution of $u(\theta) = 0$.

(e) If $L$ is based on a set of $n$ independent observations and $\theta_0$ is the true value of $\theta$, then as $n \to \infty$,

(i) $(\hat{\theta}_n - \theta_0)$ is approximately distributed as $N_n(0, I_\theta^{-1})$, and

(ii) $-2[L(\hat{\theta}_n) - L(\theta_0)]$ is approximately distributed as $\chi^2_d$, the chi-square distribution.

With additional assumptions, the above theory extends to mutually independent non-identically distributed random variables, and even to dependent variables.

24.12. (Constrained Maximization) Recalling that $\theta \in \Omega \subseteq \mathbb{R}^d$, sometimes $\Omega$ is restricted in some way. For example, in multivariate analysis (cf. Chapter 21) a matrix of parameters may be symmetric or even positive definite, as in the case of a variance matrix, so that technically these constraints should be built into the optimization process. For example, if we wish to maximize an expression subject to a matrix restricted to being positive definite, what frequently happens is that the unrestricted maximum turns out to be positive definite with probability 1. This unrestricted maximum is then also the restricted maximum (e.g., Calvert and Seber [1978: 274–276]). Alternatively, we can express the positive definite matrix in the form $A' A$ (cf. 10.32), where $A$ is unknown. For a selection of examples and proofs see Abadir and Magnus [2005: section 13.12] and Magnus and Neudecker [1999: chapters 15 and 16].

A major problem with maximum likelihood is showing that the estimate obtained is actually a maximum. As a result, various ad hoc methods are used such as convexity arguments.
24.13. Let \( \Sigma \) and \( A \) be \( n \times n \) matrices. Consider the matrix function \( f \), where

\[
f(\Sigma) = \log(\det A) + \text{trace}(\Sigma^{-1}A).\]

If \( A \) is positive definite, then, subject to \( \Sigma \) being positive definite, \( f(\Sigma) \) is minimized uniquely at \( \Sigma = A \).

24.14. Let \( A \) be \( n \times n \), then:

(a) \( \text{trace}(AA') \) is a strictly convex function of \( A \).
(b) If \( A \) is positive definite then \( -\log(\det A) \) is a convex function.

Proofs. Section 24.3.1.

24.3.2 Least Squares

**Definition 24.3.** Let \( y \) be an \( n \times 1 \) random vector with mean \( \text{E}(y) = f(\theta) \), where \( \theta \) is a \( d \times 1 \) vector of parameters and \( \theta \in \Omega \). Then \( \hat{\theta} \) is a least squares estimate of \( \theta \) if \( \hat{\theta} \) minimizes \( [y - f(\theta)]'[y - f(\theta)] \) with respect to \( \theta \in \Omega \). In practice, \( f(\theta) \) will also depend on some data observations.

If a weight matrix function \( W(\theta) \) (generally a positive definite matrix) is included, then a minimum of \( [y - f(\theta)]'W(\theta)[y - f(\theta)] \), \( \theta_w \) say, is called a generalized or weighted least squares estimate. Various iterative methods such as Iteratively Reweighted Least Squares (IRLS) (e.g., Seber and Wild [1989: 37]) are available. In some applications \( W \) does not depend on \( \theta \).

Under certain general conditions, least squares and generalized least squares estimates are unique and have certain optimal properties. They generally have some useful asymptotic properties as well, which do not depend on normality assumptions. However, under normality assumptions, such estimates may be the same as the maximum likelihood estimates, for example in univariate (Seber and Lee [2003]) and multivariate (Seber [1984]) linear models, and nonlinear models (Seber and Wild [1989]). For a further discussion of least squares with respect to regression models see Section 20.7.

24.4 OPTIMIZING A FUNCTION OF A MATRIX

24.4.1 Trace

24.15. Let \( A \) be a real \( n \times n \) matrix with singular values \( \sigma_1(A) \geq \cdots \geq \sigma_n(A) \) and singular value decomposition \( A = P\Sigma Q' \), where \( \Sigma = \text{diag}(\sigma_1(A), \ldots, \sigma_n(A)) \) and \( P \) and \( Q \) are \( n \times n \) orthogonal matrices. Let \( T_n \) be the collection of all \( n \times n \) orthogonal matrices. Then

\[
\max_{T \in T_n} \text{trace}(AT) = \sum_{i=1}^{n} \sigma_i(A),
\]
and the maximum is attained at $T_0 = QP'$, where $T_0$ is not necessarily unique. Also $AT_0$ is non-negative definite. Furthermore, if $T_1$ is an orthogonal matrix such that $AT_1$ is non-negative definite, then $T_1$ is the maximizer.

24.16. Let $A$ be an $m \times n$ real matrix with singular value decomposition $P\Sigma_1Q'$, let $B$ be a real $n \times m$ matrix with singular value decomposition $B = RS_2'S'$, $p = \min\{m, n\}$, and let $T_p$ be the set of all $p \times p$ orthogonal matrices. Here $P$, $Q$, $R$, and $S$ are conformable orthogonal matrices. Then

$$\max_{T \in T_p, U \in T_m} \text{trace}(ATBU) = \sum_{i=1}^{p} \sigma_i(A)\sigma_i(B) \quad (= \text{trace}(\Sigma_1\Sigma_2)).$$

By substitution we see that equality occurs when $T = QR'$ and $U = SP'$. The above holds for complex matrices if we replace orthogonal matrices by unitary matrices and the trace by its real part.

24.17. Let $\mathcal{V}$ be the set of all real $m \times n$ matrices $C$. Suppose $X$ is a given $n \times r$ matrix, $V_1, V_2, \ldots, V_k$ are given $m \times n$ matrices, and $a_1, a_2, \ldots, a_k$ are given real scalars. Let $V_1 = \{C : C \in \mathcal{V}, CX = 0, \text{trace}(CV_i') = a_i \text{ for each } i\}$, and let $Q = I_n - X(X'X)^{-1}X$ represent the orthogonal projection perpendicular to $C(X)$. Then:

(a) $\min_{C \in V_1} \text{trace}(CC') = \text{trace}(C_0C_0')$,

where $C_0 = \sum_{i=1}^{k} \alpha_iV_iQ$, and $(\alpha_1, \alpha_2, \ldots, \alpha_k)$ is a solution to the following system of linear equations:

$$\sum_{i=1}^{k} \text{trace}(V_iQV_j')\alpha_i = a_j, \quad j = 1, 2, \ldots, k.$$ 

(b) Suppose now that $m = n$, $V_1$ is the set of all symmetric $m \times m$ matrices, and the $V_i$ are now all symmetric $m \times m$ matrices. Then

$$\min_{C \in V_1} \text{trace}(C^2) = \text{trace}(C_1^2),$$

where $C_1 = \sum_{i=1}^{k} \alpha_iQV_iQ$, and $(\alpha_1, \alpha_2, \ldots, \alpha_k)$ is a solution to the following system of linear equations:

$$\sum_{i=1}^{k} \text{trace}(QV_iQV_j')\alpha_i = a_j, \quad j = 1, 2, \ldots, k.$$ 

The above solutions are not necessarily unique if the matrices in the linear equations are singular. This theory can be applied to variance estimation (Rao and Rao [1998: sections 12.5–12.10]).

24.18. Let $X$ be an $n \times p$ matrix of rank $p$, $V$ be an $n \times n$ positive definite matrix, and $W$ be an $m \times p$ matrix. Then $\text{trace}(GVG')$ is minimized with respect to $G$, subject to $GX = W$, when $G = G_0$ and

$$G_0 = W(X'V^{-1}X)^{-1}X'V^{-1}. $$
If we drop the assumption that \( \text{rank} \ X = p \), then \( \text{trace}(GVG') \) is minimized with respect to \( G \), subject to \( GX = X \), when \( G = G_1 \) and

\[
G_1 = X(X'V^{-1}X)^+X'V^{-1},
\]

where \((X'V^{-1}X)^+\) is the Moore–Penrose inverse.

**24.19.** Let \( X \) be an \( n \times p \) matrix of rank \( r \) and \( V \) be a non-negative definite \( n \times n \) matrix. Then the minimum of \( \left[ \text{trace}(V^2)/n \right] \) subject to \( VX = 0 \) and \( \text{trace} \ V = 1 \) is given by \( V_0 \), where

\[
V_0 = \frac{1}{n-r}(I_n - XX^+),
\]

and \( X^+ \) is the Moore–Penrose inverse of \( X \).

**Proofs.** Section 24.4.1.


**24.18.** Abadir and Magnus [2005: 384–386].

**24.19.** Abadir and Magnus [2005: 386].

### 24.4.2 Norm

In this section we are also involved with matrix approximation as well as optimization.

**Definition 24.4.** Let \( U \) be the vector space of all \( m \times n \) real matrices, and let \( V \) be a subspace. Given \( A \in U \) and \( B \in V \), we say that \( B \) is the closest to \( A \) with respect to a given norm \( \| \cdot \| \) if \( B \) minimizes \( \| A - B \| \). Note that \( B \) may not be unique.

**24.20.** (Eckart–Young) Some of the dimension reduction techniques of Section 21.5 may be described as approximating an \( n \times d \) data matrix \( X \) by another \( n \times r \) matrix, with \( r < d \). We now consider the broader problem of approximating one matrix by another of lower rank.

Let \( A \) be an \( m \times n \) real matrix of rank \( r \) with singular value decomposition

\[
A = P\Sigma Q' = \sum_{i=1}^{r} \sigma_i p_i q_i',
\]

where \( P = (p_1, \ldots, p_m), Q = (q_1, \ldots, q_n), \) and \( \sigma_i = \sigma_i(A) \), the ordered singular values of \( A \). Let \( V \) be the set of \( m \times n \) matrices of rank \( s \) (\( s < r \)).

(a) Then

\[
\min_{B \in V} \| A - B \|_{\sigma_i} = \| A - B_0 \|_{\sigma_i},
\]
for all orthogonally invariant norms $\| \cdot \|_{oi}$, where

$$B_0 = \sum_{i=1}^{s} \sigma_i p_i' q_i' = (\mathbf{P} \Sigma_i \mathbf{Q}')$$

(b) We have from (a) the special case

$$\| \mathbf{A} - B_0 \|_F^2 = \text{trace}[(\mathbf{A} - B_0)(\mathbf{A} - B_0)']$$

$$= \sum_{i=s+1}^{r} \sigma_i^2 \text{trace}(p_i' q_i' p_i' q_i')$$

$$= \sigma_{s+1}^2 + \sigma_{s+2}^2 + \cdots + \sigma_r^2,$$

where $\| \cdot \|_F$ is the Frobenius norm.

(c) If the rows of $\mathbf{A}$ sum to zero (i.e., $\mathbf{A}' \mathbf{1}_m = 0$), then, in terms of the Frobenius norm, $\mathbf{B}$ is the rank $s$ matrix whose column differences best approximate the column differences of $\mathbf{A}$. The same result applies to row differences if $\mathbf{A} \mathbf{1}_n = 0$.

The above results are used in many places in statistics such as the biplot (Jolliffe [2002: section 5.3] and Seber [1984: section 5.3]), classical multidimensional scaling (Seber [1984: 240]), sample principal components (Jolliffe [2002: 36–38]), and procrustes analysis (Gower and Dijksterhuis [2004] and Seber [1984: 252]).

24.21. Let $\mathbf{A}$ and $\mathbf{B}$ be $m \times n$ real matrices, $p = \min\{m, n\}$, and let $\mathcal{T}_k$ be the set of $k \times k$ real orthogonal matrices. Then, if $\| \cdot \|_F$ is the Frobenius norm,

$$\| \mathbf{A} - \mathbf{UBV} \|_F^2 = \| \mathbf{A} \|_F^2 - 2 \text{trace}(\mathbf{AV}'\mathbf{B}'\mathbf{U}') + \| \mathbf{B} \|_F^2$$

and

$$\min_{\mathbf{U} \in \mathcal{T}_m, \mathbf{V} \in \mathcal{T}_n} \| \mathbf{A} - \mathbf{UBV} \|_F = \left\{ \sum_{i=1}^{p} (\sigma_i(\mathbf{A}) - \sigma_i(\mathbf{B}))^2 \right\}^{1/2}.$$ 

The minimizing values of $\mathbf{U}$ and $\mathbf{V}$ follow from (24.16) above with appropriate substitutions.

24.22. Let $\mathbf{A}$ and $\mathbf{B}$ be $m \times n$ real matrices with respective singular value decompositions $\mathbf{A} = \mathbf{P} \Sigma_i \mathbf{Q}'$ and $\mathbf{B} = \mathbf{R} \Sigma_j \mathbf{S}'$. Let $\mathcal{T}_p$ be the set of all $p \times p$ real orthogonal matrices. Then, if $\| \cdot \|_F$ is the Frobenius norm,

$$\min_{\mathbf{U} \in \mathcal{T}_m, \mathbf{T} \in \mathcal{T}_n} \| \mathbf{UA} - \mathbf{BT} \|_F = \| \mathbf{U}_0 \mathbf{A} - \mathbf{BT}_0 \|_F,$$

where $\mathbf{U}_0 = \mathbf{RP}'$ and $\mathbf{T}_0 = \mathbf{SQ}'$.

24.23. If $\mathbf{A}$ is an $n \times n$ symmetric matrix, $\mathbf{Q}_r$ is an $n \times r$ matrix with orthonormal columns, and $\mathbf{S}$ is any $r \times r$ matrix, then

$$\min_{\mathbf{S}} \| \mathbf{AQ}_r - \mathbf{Q}_r \mathbf{S} \|_F = \| (\mathbf{I}_n - \mathbf{Q}_r \mathbf{Q}_r') \mathbf{AQ}_r \|_F$$

and $\mathbf{S} = \mathbf{Q}_r' \mathbf{AQ}_r$ is the minimizer.
We now find nearest approximations for several matrices.

(a) (Symmetric Matrix) Let $A$ be an $n \times n$ real matrix, and define $B = \frac{1}{2}(A + A')$. Then $B$ is a symmetric matrix closest to $A$ with respect to any orthogonally invariant norm $\| \cdot \|_{oi}$. Thus if $C$ is any $n \times n$ real symmetric matrix, then

$$\|A - B\|_{oi} \leq \|A - C\|_{oi}.$$  

(b) (Skew-Symmetric Matrix) Referring to (a), if we now have $B = \frac{1}{2}(A - A')$, then $B$ is a skew-symmetric matrix closest to $A$ with respect to any orthogonally invariant norm.

(c) (Orthogonal Matrix) Let $A$ be a real $n \times n$ matrix with singular value decomposition $PSQ'$, and let $T_n$ be the set of $n \times n$ real orthogonal matrices. Then, if $\| \cdot \|_F$ is the Frobenius norm,

$$\min_{T \in T_n} \|A - T\|_F = \|A - T_0\|_F,$$

with $T_0 = PQ'$.

(d) (Non-negative Definite Matrix) Let $A$ be a real $n \times n$ matrix, $B = \frac{1}{2}(A + A')$, and $B = QH$ be a polar decomposition with $Q$ orthogonal and $H$ non-negative definite. If $\mathcal{N}$ is the set of all non-negative definite matrices, then

$$\min_{C \in \mathcal{N}} \|A - C\|_F = \|A - C_0\|_F,$$

where $C_0 = \frac{1}{2}(B + H)$ is non-negative definite and unique. Rao and Rao [1998: Sections 11.6 and 11.7] give a number of approximations like the above based on the $M, N$-invariant generalized matrix norm.

Suppose $X = (x_1, \ldots, x_n)$ is an $m \times n$ matrix, $B = (b_1, \ldots, b_k)$ is an $m \times k$ matrix of rank $k$ ($k \leq m$), $Z = (z_1, \ldots, z_m)$ is $k \times n$ matrix, and $a \in \mathbb{R}^m$. If $\| \cdot \|_{ui}$ is any unitarily invariant norm, then $\|X - a_{11}' - BZ\|_{ui}$ is minimized with respect to $a$, $B$, and $Z$ when

$$b = n^{-1}X1_n (= \bar{x}, \text{ say}), \quad B = (u_1, \ldots, u_k), \quad \text{and} \quad Z' = (\sigma_1 v_1, \ldots, \sigma_k v_k),$$

where $\sigma_i$, $u_i$, and $v_i$ are defined by the singular value decomposition

$$X - \bar{x}1_n' = U\Sigma V' = \sigma_1 u_1 v_1' + \cdots + \sigma_r u_r v_r'.$$

In particular,

$$\min_{a, B, Z} \|X - a_{11}' - BZ\|_F = \sigma_{k+1}^2 + \cdots + \sigma_r^2.$$

This problem is related to that of finding a hyperplane that is "nearest" to a set of points (Rao and Rao [1998: 399-400]).

Proofs. Section 24.4.2.


24.4.3 Quadratics

24.26. Suppose \( q(x) = x'Ax + b'x + c \), where \( A \) is a real symmetric matrix. Then:

(a) \( q(x) = (x + \frac{1}{2}A^{-1}b)'A(x + \frac{1}{2}A^{-1}b) + (c - \frac{1}{4}b'A^{-1}b) \).

(b) \( q(x) \) has a maximum if and only if \( b \in C(A) \) and \( -A \) is non-negative definite. If such is the case, a maximizer of \( q(x) \) is of the form

\[
x_{\text{max}} = -\frac{1}{2}A^{-1}b + (I - A^{-1}A)x_0,
\]

where \( x_0 \) is arbitrary.

(c) \( q(x) \) has a minimum if and only if \( b \in C(A) \) and \( A \) is non-negative definite. If such is the case, a minimizer of \( q(x) \) is of the same form

\[
x_{\text{min}} = -\frac{1}{2}A^{-1}b + (I - A^{-1}A)x_0,
\]

where \( x_0 \) is arbitrary.

24.27. Suppose \( x, a \in \mathbb{R}^m \), \( c \in \mathbb{R}^k \), and \( B \) is \( m \times k \) of rank \( k \). If \( \Sigma \) is a positive definite \( m \times m \) matrix, then

\[
\min_c (x - a - Bc)'\Sigma^{-1}(x - a - Bc) = (x - a)'(\Sigma^{-1} - \Sigma^{-1}PB)(x - a),
\]

occurs at

\[
c = (B'\Sigma B)^{-1}B'\Sigma^{-1}(x - a),
\]

where

\[
P_B = B(B'\Sigma^{-1}B)^{-1}B'\Sigma^{-1}.
\]

If we now have \( x_i, c_i, \) and \( w_i > 0 \) for \( i = 1, 2, \ldots, n \), then

\[
\min_{a, B, c_1, \ldots, c_n} \sum_{i=1}^{n} w_i(x_i - a - Bc_i)'\Sigma^{-1}(x_i - a - Bc_i)
\]

\[
= \sum_{i=1}^{n} w_i(x_i - \bar{x})'\Sigma^{-1}(x_i - \bar{x}) - \text{trace}(\Sigma^{-1}P_{B_0}S),
\]

where \( S = \sum_{i=1}^{n} w_i(x_i - \bar{x})'\Sigma^{-1}(x_i - \bar{x}) \), \( B_0 = \Sigma^{1/2}Q_* \), and \( Q_* \) is the matrix of the first \( k \) eigenvectors of \( \Sigma^{-1/2}S\Sigma^{-1/2} \).
24.28. Let $A$ be a real symmetric matrix.

(a) If $r(x) = x'Ax/x'x$, then by differentiation the stationary values of $r(x)$ occur when $x$ is an eigenvector of $A$ and are equal to the eigenvalues of $A$. Note that we can set $x'x = 1$ without any change in the result. We then have that $r(x)$ is maximized with respect to $x$ when $x$ is a unit-norm eigenvector of $A$ corresponding to its largest eigenvalue. The minimum relates to the minimum eigenvalue (see 6.58a). If we also have $C'x = 0$, where $C$ is $n \times p$ ($p \leq n$), then Golub and Van Loan [1996: 621] give a method for finding the stationary values of $r(x)$ subject to this constraint.

(b) Suppose, in addition to $C'x = 0$, we also have $x'Bx = 1$, where $B$ is positive definite.

(i) The stationary values of $x'Ax$ subject to these constraints are attained at the eigenvectors of $B^{-1}(I_n - P)A$, where $P$ is the projection matrix

$$P = C(C'B^{-1}C)^{-1}C'B^{-1},$$

that is, $x$ satisfies $(I_n - P)Ax = \lambda Bx$. Setting $B = I_n$ gives a solution to the second part of (a).

(ii) If $A = aa'$, then $x'Ax$ has a maximum value when $x \propto B^{-1}(I_n - P)a$. This result occurs in problems of genetic selection. Rao and Rao [1998: 507] give references to two extensions of the above.

24.29. Let $A$, $B$, and $C$ be $n \times n$ matrices with $A$ and $B$ positive definite and $C$ symmetric. The stationary values of

$$\frac{x'Cx}{(x'Ax)^{1/2}(x'Bx)^{1/2}}$$

are $\lambda_i^2 \nu_i$ ($i = 1, 2, \ldots$), where $\lambda_i$ and $\nu_i$ are solutions of the equations

$$2Cx = \lambda(A + \nu B)x,$$

$$\nu = x'Ax/(x'Bx).$$

This result occurs in the study of canonical variates (Rao and Rao [1987]).

24.30. Let $A$ be a positive definite $n \times n$ matrix, let $B$ be an $n \times k$ matrix, and let $c$ be a given $1 \times 1$ vector.

(a) If $S^-$ is any weak inverse of $B'A^{-1}B$, then for $n \times 1 \ x$,

$$\min_{B'x = c} x'Ax = c'S^-c,$$

where the minimum attained at $x = A^{-1}BS^-$.

(b) If rank $B = k$, then from (a) we have

$$\min_{B'x = c} x'x = c'(B'B)^{-1}c,$$

where the minimum is attained at $x = B(B'B)^{-1}c$. 
(c) Suppose \( x' = (x'_1, x'_2) \) and \( (B'_1, B'_2) \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = c \). If

\[
\begin{pmatrix} B'_1 & B'_2 \\ B_2 & 0 \end{pmatrix}^{-1} = \begin{pmatrix} C_1 & C_2 \\ C_3 & C_4 \end{pmatrix},
\]

then

\[
\min_{B'x = c} x'_1 x_1 = c'C_1 c,
\]

where the minimum is attained at \( x_1 = B_1 C_1' c \).

(d) Suppose \( A \) is now non-negative definite and \( c \in \mathcal{C}(B') \). Let

\[
\begin{pmatrix} A & B \\ B' & 0 \end{pmatrix}^{-1} = \begin{pmatrix} C_1 & C_2 \\ C_3 & -C_4 \end{pmatrix},
\]

then

\[
\min_{B'x = c} x' Ax = c'C_4 c.
\]

24.31. Let \( 0 < p_0 < 1 \) be given, and let \( p = (p_1, p_2, \ldots, p_m)' \), where \( 0 < p_0 \leq p_i \leq 1 \) for \( i = 1, 2, \ldots, m \). Let \( \mathcal{R} \) be the region

\[
\mathcal{R} = \{p: 0 < p_0 \leq p_i \leq 1, i = 1, \ldots, m, p_0 < 1\},
\]

and define

\[
f(p) = \frac{1 + p_0 + 1^m_p}{(1 + p_0^2 + p^p p)^{1/2}}.
\]

Then

\[
\max_{p \in \mathcal{R}} f(p) = \left( m + \frac{(1 + p_0)^2}{1 + p_0^2} \right)^{1/2},
\]

and it occurs in the interior of \( \mathcal{R} \) at the point given by

\[
p_i = \frac{1 + p_0^2}{1 + p_0}, \quad i = 1, 2, \ldots, m.
\]

The minimum occurs at one or more of the extreme points of \( \mathcal{R} \). For a proof and further details see Thibaudeau and Styan [1985]. They point out that their above result applies to a measure of imbalance for experimental designs introduced by Chakabarti [1963].

Proofs. Section 24.4.3.


24.28b(i). Rao and Rao [1998: 507]. Note that \( x'(I_n - P)Ax = \lambda \).

24.28b(ii). When \( A = aa' \), \( a \) is an eigenvector of \( A \). We then set \( \lambda = a'B^{-1}(I_n - P)a \) in (i) and substitute for \( x \).


24.5 OPTIMAL DESIGNS

In fitting the linear model $y = X\beta + \epsilon$, where $X$ is $n \times p$ of rank $p$ (cf. Section 20.7), we may wish to find the best design for minimizing some function of $\text{var}(\hat{\beta}) = \sigma^2(X'X)^{-1}$, where $\hat{\beta} = (X'X)^{-1}X'y$, the least squares estimate of $\beta$. Depending on which function is chosen, there are three main criteria, namely:

1. **A-optimality**: minimize $\text{trace}[(X'X)^{-1}]$.

2. **E-optimality**: minimize the largest eigenvalue (i.e., the spectral radius $\rho[(X'X)^{-1}]$) of $(X'X)^{-1}$.

3. **D-optimality**: minimize $\text{det}[(X'X)^{-1}]$ or maximize $\text{det}(X'X)$.

For general references to optimal designs see Atkinson and Donev [1992], Druilhet [2004], and Melas [2006].

24.32. (D-Optimality) This is probably the most commonly used criterion for two reasons. Firstly, when $\epsilon$ in the above linear model is multivariate normal $N_n(0, \sigma^2 I_n)$, the D-optimal design gives the smallest volume of the confidence ellipsoid for $\beta$. Secondly, the computations are the simplest. To find the optimal $X$ with a given number $n$ rows from a set of $N$ potential rows, one begins with an initial choice of $n$ rows, for example at random, and then determines the effect on the determinant by exchanging a deleted row with a different row from the set of potential rows using a result like (15.13b). For further references and details see Gentle [1998: 190].


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