MULTIVARIATE
STATISTICAL
METHODS

Third Edition

Donald F. Morrison
The Wharton School
University of Pennsylvania

CONTENTS

PREFACE TO THE THIRD EDITION

In this edition I have added a number of new topics, made current the literature survey and references, increased the number of chapter exercises and examples using actual data, and included an Appendix of seven multivariate data sets.

Among the new methods are treatments of the T^2 test for paired sets of response variables, a test for outlying observation vectors, plots and measures for assessing the normality assumption, multivariate analysis of covariance with two treatment groups, linear discrimination for two populations with unequal covariance matrices, procrustes rotation of factors, clustering rules for multivariate data, and multidimensional scaling. Other extensions are mentioned briefly in the text, or left as exercises at the end of chapters. Some topics in the previous editions which have become less important with the rise of the computer have been omitted.

My approach to multivariate inference has continued to be a pragmatic one based on the union-intersection and generalized likelihood-ratio principles. I have shown a preference for computationally feasible techniques whose required sampling distributions are known and tabulated. Limitations of space and my intention to produce a methods rather than theoretical text have precluded any development of bayesian inference. The inclusion of computer-based topics has been limited to avoid dependence on one or two statistical packages, or obsolescence as the packages or languages change. Instead, the computer aspects of the methods will be addressed in the exercise solutions manual.

The number of exercises at the ends of Chapters 4 to 9 has been doubled. The data sets in Appendix B include the classic Anderson–Fisher iris dimensions, financial ratios of healthy and insolvent firms, and samples of forest soil chemical levels. Smaller sets are given in the examples and exercises. I am very grateful to a large number of investigators for permitting the inclusion of their data.

The previous editions of the book have been the basis for a one-semester course in multivariate methods for the past twenty years at the University of Pennsylvania. The third edition was written with that schedule in mind, and in the hope that the literature references and live data sets would extend the student's horizons beyond the immediate topics.

I am indebted to Malcolm R. Heyworth, Thomas Bolland, Keith Eberhardt, and Gerald Beck for their comments on the second edition, and to Christopher Bingham, University of Minnesota; Anirban Das Gupta, Purdue University; John J. Peterson, Syracuse University; James R. Schwenke, Kansas State University; Eric P. Smith, Virginia Polytechnic Institute and State University; V. Susarla, SUNY at Binghamton; Ram C. Tiwari, University of North Carolina at Charlotte; and J. S. Verducci, Ohio State University for their reviews of the proposed third edition. Their corrections and suggestions have had a very positive effect on the book. Of course, any remaining errors are the author's sole responsibility, and I would appreciate being informed of them.

Finally, I must make a special acknowledgement to my family for their encouragement and patience during this lengthy project, and in particular, to our son Norman for his help in computer support.

Donald F. Morrison

PREFACE TO THE
FIRST EDITION

Multivariate statistical analysis is concerned with data collected on several dimensions of the same individual. Such observations are common in the social, behavioral, life, and medical sciences: the record of the prices of a commodity, the reaction times of a normal subject to several different stimulus displays, the principal bodily dimensions of an organism, or a set of blood-chemistry values from the same patient are all examples of multidimensional data. As in univariate statistics, we shall assume that a random sample of multicomponent observations has been collected from different individuals or other independent sampling units. However, the common source of each individual observation will generally lead to dependence or correlation among the dimensions, and it is this feature that distinguishes multivariate data and techniques from their univariate prototypes.

This book was written to provide investigators in the life and behavioral sciences with an elementary source for multivariate techniques which appeared to be especially useful for the design and analysis of their experimental data. The book has also been organized to serve as the text for a course in multivariate methods at the advanced undergraduate or graduate level in the sciences. The mathematical and statistical prerequisites are minimal: a semester course in elementary statistics with a survey of the fundamental sampling distributions and an exposure to the calculus for the partial differentiations and integrals required for occasional maximizations and expectations should be sufficient. The review of the essential univariate statistical concepts in the first chapter and a detailed treatment of matrix algebra in the second make the book fairly self-contained both as a reference and a text. The standard results on the multinormal distribution, the estimation of its parameters, and correlation analysis in Chapter 3 are essential background for the developments in the remaining chapters.

The selection of techniques reflects my experiential biases and preferences. Attention has been restricted to continuous observations from multivariate normal populations: no mention has been made of the newer distribution-free tests and the methods for analysis of many-way categorical data tables. It was felt that the implications of the T^2 statistic for repeated-measurements experiments justified a lengthy discussion of tests and confidence intervals for mean vectors. The multivariate general linear hypothesis and analysis of variance has been developed through the Roy union-intersection principle for the natural ease with which simultaneous confidence statements can be obtained. In my experience the Hotelling principal-component technique has proved to be exceedingly useful for data reduction, analysis of the latent structure of multivariate systems, and descriptive purposes, and its use and properties are developed at length. My approach to factor analysis has been statistical rather than psychometric, for 1 prefer to think of the initial steps, at least, of a factor analysis as a problem in statistical estimation.

For the preparation of this methods text I wish to acknowledge a considerable debt to those responsible for the theoretical development of multivariate analysis: the fundamental contributions of T. W. Anderson, Harold Hotelling, D. N. Lawley, and the late S. N. Roy are evident throughout. In particular the frequent references to S. N. Roy's monograph *Some Aspects of Multivariate Analysis* are indicative of his influence on the presentation. For the many derivations beyond the level of this book the reader has usually been referred to T. W. Anderson's standard theoretical source *An Introduction to Multivariate Statistical Analysis*.

It is a pleasure to acknowledge those who have assisted at different stages in the preparation of this book. My thanks are due to Samuel W. Greenhouse for initially encouraging me to undertake the project. I am especially indebted to Karen D. Pettigrew and John J. Bartko for their thoughtful reading of several chapters and for offering suggestions that have improved the clarity of the presentation. George Schink carefully checked the computations of the majority of the examples. However, the ultimate responsibility for the nature and accuracy of the contents must of course rest with the author. Finally, I wish to express my gratitude to the many investigators who graciously permitted the use of their original and published data for the examples and exercises.

I am indebted to A. M. Mood and the McGraw-Hill Book Company for permission to reproduce Table 1 from the first edition of *Introduction to the Theory of Statistics*. Tables 2 and 4 have been abridged from tables originally prepared by Catherine M. Thompson and Maxine Merrington, and have been reproduced with the kind permission of the editor of *Biometrika*, E. S. Pearson. I am also grateful to Professor Pearson and to H. O. Hartley for kindly permitting the reproduction of

CHAPTER

1

SOME ELEMENTARY STATISTICAL CONCEPTS

1.1 INTRODUCTION

In this chapter we shall summarize some important parts of univariate statistical theory to which we shall frequently refer in our development of multivariate methods. Certain concepts of statistical inference will be introduced, and some essential univariate distributions will be described. We shall assume that the reader has been exposed to the elements of probability and random variables and has an acquaintance with the basic univariate techniques as applied in some substantive discipline.

1.2 RANDOM VARIABLES

Every statistical analysis must be built upon a *mathematical model* linking observable reality with the mechanism generating the observations. This model should be a parsimonious description of nature: its functional form should be simple, and the number of its parameters and components should be a minimum. The model should be *parametrized* in such a way that each parameter can be interpreted easily and identified with some aspect of reality. The functional form should be sufficiently tractable to permit the sort of mathematical manipulations required for the estimation of its parameters and other inferences about its nature.

Mathematical models may be divided into three general classes: (1) purely deterministic, (2) static, or deterministic with simple random components, and (3) stochastic. Any observation from a deterministic model is strictly a function of its parameters and such variables as time, space, or inputs of energy or a stimulus. Newtonian physics states that the distance traveled by a falling object is directly related to the squared time of fall, and if atmospheric turbulence, observer error, and other transient effects can be ignored, the displacement can be calculated exactly for a given time and gravitational constant. In the second kind of model each observation is a function of a strictly deterministic component and a random term ascribable to measurement error or sampling variation in either the observed response or the input variables. The random components are assumed to be independent of one another for different observations. The models we shall encounter in the sequel will be mainly of this class, with the further restriction that the random component will merely be added to the deterministic part. Stochastic models are constructed from fundamental random events or components to explain dynamic or evolutionary phenomena: they range in complexity from the case of a sequence of Bernoulli trials as the model for a coin-tossing experiment to the birth-and-death process describing the size of a biological population. Most stochastic models allow for a "memory" effect, so that each observed response is dependent to some degree upon its predecessors in time or neighbors in space. We shall touch only tangentially on this kind of model.

Now let us define more precisely what is meant by the notions of random variation or the random components in the second and third kinds of models. We shall begin by defining a *discrete random variable*, or one which can assume only a countable number of values. Suppose that some experiment can result in exactly one of k outcomes $E_1, \ldots, E_k$. These outcomes are mutually exclusive, in the sense that the occurrence of one event precludes that of any other. To every event we assign some number p_i between zero and one called the *probability* $P(E_i)$ of that event. p_i is the probability that in a single trial of the experiment the outcome E_i will occur. Within the framework of our experiment we assign a probability of zero to impossible events and a probability of unity to any event which must happen with certainty. Then, by the mutual exclusiveness of the events, in a single trial

$$P(E_i \cap E_j) = 0$$

$$P(E_i \cup E_j) = p_i + p_j$$

where the *intersection* symbol $\cap$ denotes the event "E_i and E_j," and the *union* symbol $\cup$ indicates the event "E_i and/or E_j." By the additive property of the probabilities of mutually exclusive outcomes the total

probability of the set of events is

$$P(E_1 \cup \cdots \cup E_k) = p_1 + \cdots + p_k$$
$$= 1$$

Now assign the numerical value x_i to the ith outcome, where for convenience the outcomes have been placed in ascending order according to their x_i values. The discrete random variable X is defined as that quantity which takes on the value x_i with probability p_i at each trial of the experiment. As an example, if the experiment consists of the toss of a coin, the score of one might be assigned to the outcome heads, while zero might be the tails score. Then $x_1 = 0$, $x_2 = 1$, and $p_1 = 1 - p$, $p_2 = p$, say. This random variable would be described by its *probability function* $f(x_i)$ specifying the probabilities with which X assumes the values 0 and 1:

x_i	$f(x_i)$
0	$1 - p$
1	p

We note that the total probability is unity and that we have implicitly assigned a probability of zero to such irrelevant events as the coin's landing on edge or rolling out of sight. We have chosen *not* to assign a numerical value to the single parameter p; this reflects the intrinsic qualities of the coin as well as the manner in which it is tossed. It is only for convenience or for lack of knowledge of the coin's properties that p is ever taken as $\frac{1}{2}$.

The random variables we shall encounter in the sequel will take on values over some continuous region rather than a set of countable events and will be called *continuous random variables* or *continuous variates*. Both terms will be used synonymously. The continuous random variable X defined on the domain of real numbers is characterized by its *distribution function*

$$(1) \qquad F(x) = P(X \le x) \qquad -\infty < x < \infty$$

giving the probability that X is less than or equal to some value x of its domain. Since X is continuous, $P(X = x) = 0$. If $F(x)$ is an absolutely continuous function, the continuous analog of the discrete probability function is the *density function*

$$(2) \qquad f(x) = \frac{dF(x)}{dx}$$

Conversely, by the absolute-continuity property,

$$(3) \qquad F(x) = \int_{-\infty}^{x} f(u) \, du$$

and from this integral definition follows the equivalent term *cumulative distribution function* for $F(x)$. Note that these definitions are perfectly general: if the random variable is defined only on some interval of the real line, outside that interval $f(x)$ is defined to be zero, and to the left and right of the interval $F(x)$ is zero and one, respectively. When weighted in proportion to their density function $f(x)$, the values on the interval are said to constitute the *population* or *universe* of the random variable X.

The properties of a random variable are commonly visualized in terms of its density function, and it is to that representation that such names as *rectangular* or *exponential* refer. Figure 1.1 illustrates the densities of three familiar variates. The distribution functions of the rectangular and exponential variates follow by straightforward integrations; the normal distribution function can be evaluated only by numerical integration.

The functions of Fig. 1.1 involve parameters that determine their positions and shapes. $\frac{1}{2}(a + b)$ of the rectangular density and μ of the normal function are *location* parameters, for their values specify the positions of the densities on the real axis. The range $b - a$ of the rectangular variate, the single exponential parameter β, and σ of the normal density are *scale* parameters, for changes in their values are equivalent to changes in the units of the variates. Larger values of these parameters imply a greater spread of the density function, and hence more variation in the random variable. In general, if the density $f(x;\alpha,\beta)$ can be written as

$$f\left(\frac{x - \alpha}{\beta}\right)$$

it follows that α is a location parameter and β is a scale parameter. We note that all density functions of that form contain the factor $1/\beta$ associated with the differential element dx.

Random variables and their densities can be characterized in another way. Let us think of the density $f(x)$ of the variate X as the function measuring the density of a continuous rod occupying the position of the x axis. The kth moment of the rod about the origin of its axis is

$$(4) \qquad \mu'_k = \int_{-\infty}^{\infty} x^k f(x)\, dx$$

The first moment is the *mean, expectation, or expected value*

$$(5) \qquad E(X) = \int_{-\infty}^{\infty} x f(x)\, dx$$

of the random variable and corresponds to the physical notion of the

$$f(x) = \begin{cases} 0 & x < a \\ \dfrac{1}{b-a} & a \le x \le b \\ 0 & b < x \end{cases}$$

(a) Rectangular

$$f(x) = \begin{cases} \dfrac{1}{\beta} \exp\left(\dfrac{-x}{\beta}\right) & 0 \le x \\ 0 & x < 0 \end{cases}$$

(b) Exponential

$$f(x) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left[-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2\right]$$

(c) Normal
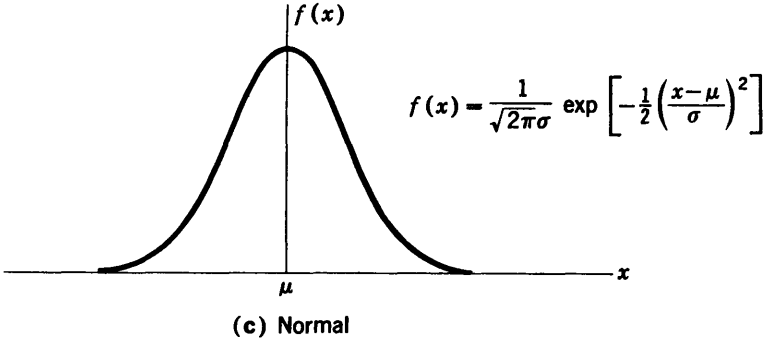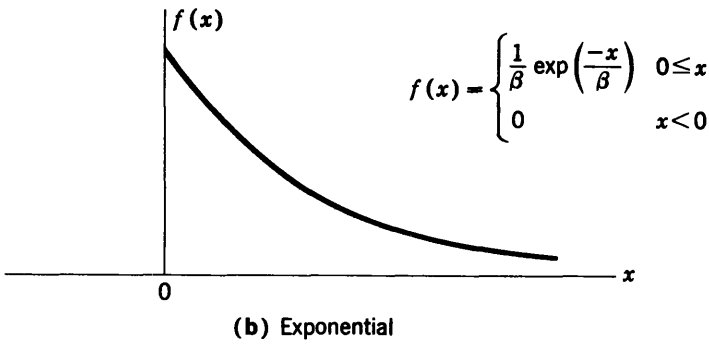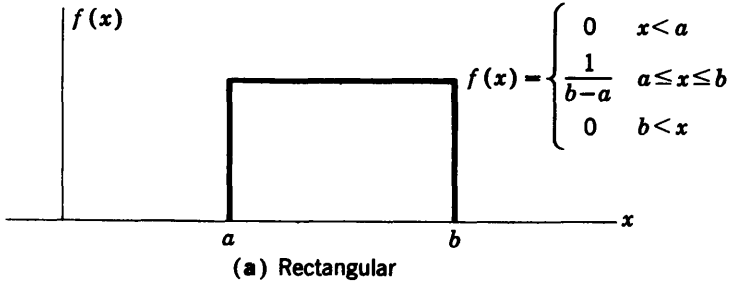
FIGURE 1.1
Density functions.

horizontal center of gravity of the rod. The symbol E denotes the operation of computing the expected value, and is called the *expectation operator*. If c and k are nonrandom quantities, these useful properties of expectations hold:

(6a) $$\mathrm{E}(c) = c$$

(6b) $$\mathrm{E}(cX) = c\mathrm{E}(X)$$

(6c) $$\mathrm{E}(k + cX) = k + c\mathrm{E}(X)$$

As an example, consider the rectangular density of Fig. 1.1. Then

$$E(X) = \frac{1}{b-a} \int_a^b x \, dx$$

$$= \frac{1}{b-a} \frac{1}{2} x^2 \Big|_a^b$$

$$= \tfrac{1}{2}(b+a)$$

As we might have reasoned from intuition, the mean value is the midpoint of the limits of the density, and if we wished, we might *reparametrize* the density function in terms of the mean as location parameter and the range $w = b - a$ as the scale parameter. The new density is

$$h(x) = \begin{cases} 0 & -\infty < x < E(X) - \tfrac{1}{2}w \\[2mm] \dfrac{1}{w} & E(X) - \tfrac{1}{2}w \leq x \leq E(X) + \tfrac{1}{2}w \\[2mm] 0 & E(X) + \tfrac{1}{2}w < x < \infty \end{cases}$$

Its functional form is unchanged, but its two parameters have different interpretations.

The *variance* of a random variable is the expected value of the squared deviations about its mean, or its *second central moment.* We shall denote the variance of X as

$$\text{var}\,(X)$$

or occasionally where space is limited as

$$\sigma_x^2$$

By definition

(7) $$\text{var}\,(X) = \int_{-\infty}^{\infty} [x - E(X)]^2 f(x) \, dx$$

$$= \int_{-\infty}^{\infty} x^2 f(x) \, dx - [E(X)]^2$$

$$= E(X^2) - [E(X)]^2$$

and the symbol var applied to any random variable will denote the operation of computing its variance. If c is a constant, the variance has these properties:

(8a) $$\text{var}\,(c) = 0$$

(8b) $$\text{var}\,(cX) = c^2 \, \text{var}\,(X)$$

(8c) $$\text{var}\,(X + c) = \text{var}\,(X)$$

The first merely states that a nonrandom variable has zero variance. The squared-units nature of the variance is reflected in the second property, for a change of scale of X by c units changes the variance by c^2. The third result follows immediately from the definition (7) and states that the variance is unaffected by changes in the origin of the X axis. It can be shown that the variances of the rectangular, exponential, and normal densities of Fig. 1.1 are $\frac{1}{12}(b - a)^2$, β^2, and σ^2, respectively.

Frequently it is desirable to have a measure of dispersion that is in the original units of the variate. The *standard deviation* of X is the positive square root of the variance

$$\sigma_x = +\sqrt{\text{var}(X)}$$

We note that the natural parameters of the normal density of Fig. 1.1c are the mean and standard deviation.

Independent variates. Earlier in the chapter we referred loosely to "independent" random variables. Now we shall give a precise definition of independence. As we shall see in Chap. 3, it is possible to extend the notions of distribution and density functions to several variates, and if we write the joint distribution function of $X_1, \ldots, X_p$ as

$$(9) \qquad F(x_1, \ldots, x_p) = \int_{-\infty}^{x_p} \cdots \int_{-\infty}^{x_1} f(u_1, \ldots, u_p)\, du_1 \cdots du_p$$

where $f(u_1, \ldots, u_p)$ is the joint density, the variates are said to be independent *if and only if*

$$(10) \qquad F(x_1, \ldots, x_p) = F_1(x_1) \cdots F_p(x_p)$$

where $F_i(x_i)$ is the distribution function of the single variate X_i. Alternatively, independence holds if and only if the factorization

$$(11) \qquad f(x_1, \ldots, x_p) = f_1(x_1) \cdots f_p(x_p)$$

of the joint density into the product of the individual densities $f_i(x_i)$ holds.

The product moment

$$(12) \quad \text{E}(X_1^{k_1} \cdots X_p^{k_p}) = \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} x_1^{k_1} \cdots x_p^{k_p} f(x_1, \ldots, x_p)\, dx_1 \cdots dx_p$$

of the variates $X_1, \ldots, X_p$ factors into the product

$$\text{E}(X_1^{k_1}) \cdots \text{E}(X_p^{k_p})$$

of the individual k_ith moments if the variates are independent. It follows from this result that the variance of a sum of *independent* random variables is merely the sum of the individual variances:

$$(13) \qquad \text{var}(X_1 + \cdots + X_p) = \text{var}(X_1) + \cdots + \text{var}(X_p)$$

Sources on probability and random variables. Certain of the large number of basic texts on probability and random variables seem particularly relevant to the purposes of this introductory chapter. A very elementary treatment of probability as applied in biology has been written by Mosimann (1968), while another lucid introductory text is that of Goldberg (1960). Parzen's book (1960) is an excellent survey at a more intermediate level, while the two volumes of Feller (1968, 1971) are the standard source for a comprehensive study of discrete and continuous probability.

1.3 NORMAL RANDOM VARIABLES

In this section we shall describe some properties of a single normal random variable in preparation for the subsequent results and techniques that will be based upon the multivariate normal distribution. Recall that the normal density function is

(1) $$f(x) = \frac{1}{\sqrt{2\pi}\,\sigma} \exp\left[-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2\right] \quad -\infty < x < \infty$$

and that its distribution function is given by the integral

(2) $$F(x) = \frac{1}{\sqrt{2\pi}\,\sigma} \int_{-\infty}^{x} \exp\left[-\frac{1}{2}\left(\frac{v-\mu}{\sigma}\right)^2\right] dv$$

$$= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{(x-\mu)/\sigma} \exp\left(-u^2/2\right) du$$

$$= \Phi\left(\frac{x-\mu}{\sigma}\right)$$

where $\Phi(z)$ denotes the *standard* or *unit* normal distribution function with zero mean and variance one. We shall denote the distribution of a normal variate by the Wilks symbol $N(\mu, \sigma^2)$; standardization of the variate will of course be indicated by $N(0,1)$.

Values of $\Phi(z)$ are contained in Table 1 of the Appendix. Conversely, the upper 100α percentage point of the unit normal distribution is defined as that value z_α such that

(3) $$\alpha = P(Z > z_\alpha)$$

$$= 1 - \Phi(z_\alpha)$$

These connections between percentage points and their probabilities are illustrated in Fig. 1.2 for the normal density and distribution functions.

Now let us offer one justification for the reliance of much of statistical methodology upon the assumption of a normal population. This is the *central-limit theorem*, which states that variates which are sums of
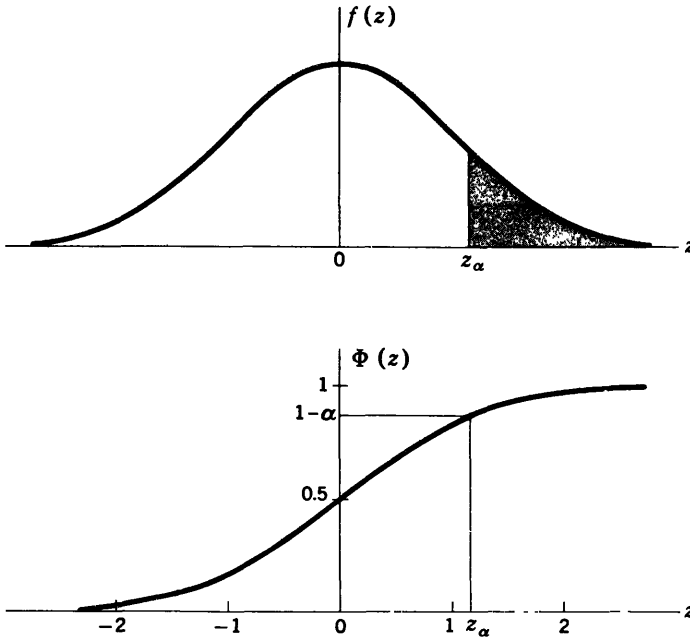
FIGURE 1.2

many independent and identically distributed effects tend to be normally distributed as the number of effects becomes large. More formally,

If the random variables $X_1, \ldots, X_N$ are independently distributed according to some common distribution function with mean $E(X_i) = \mu$ and finite variance $\text{var}(X_i) = \sigma^2$, then as the number of variates N increases without bound, the variate

$$Z = \frac{\sum\limits_{i=1}^{N} X_i - N_\mu}{\sqrt{N\sigma^2}}$$

converges in distribution to a normal variate with mean zero and variance one.

A proof of this version of the central-limit theorem can be found in most texts on probability and mathematical statistics. Feller (1968) has treated other more general theorems which do not assume identical distributions of the X_i. One immediate consequence of the theorem is that the function $\sqrt{N}(\bar{X} - \mu)$ of the sample mean

$$\bar{X} = \frac{1}{N}(X_1 + \cdots + X_N)$$

of a sequence of independent random variables whose common distribu-

tion has mean μ and variance σ^2 tends to be distributed as a $N(0,\sigma^2)$ variate as N becomes large.

We shall invoke one important property of the normal distribution continually in the sequel. If $X_1, \ldots, X_n$ are independent variates with distributions $N(\mu_1,\sigma_1^2), \ldots, N(\mu_n,\sigma_n^2)$, the linear compound

$$(4) \qquad Y = a_1 X_1 + \cdots + a_n X_n$$

is also normally distributed with mean $\sum_{i=1}^{n} a_i \mu_i$ and variance $\sum_{i=1}^{n} a_i^2 \sigma_i^2$. We shall see in Chap. 3 that this result can be extended to a linear compound of dependent normal variates.

The chi-squared distribution. Many distributions can be derived from different transformations upon a set of normal variates. One of the most important is that of the *chi-squared* variate. If the variates $X_1, \ldots, X_n$ are independently and normally distributed with mean zero and unit variance, then

$$(5) \qquad \chi^2 = X_1^2 + \cdots + X_n^2$$

has the density function

$$(6) \qquad f(\chi^2) = \frac{2^{-n/2}}{\Gamma(n/2)} (\chi^2)^{(n-2)/2} \exp\left(-\chi^2/2\right) \qquad 0 \le \chi^2 < \infty$$

and is said to be a *chi-squared variate with n degrees of freedom*. Since we started with standard normal variates, the density contains no scale or location parameters but only the single parameter n. More generally, if the X_i are independently distributed as $N(\mu_i,\sigma_i^2)$ variates, the quantity

$$\sum_{i=1}^{n} \frac{(X_i - \mu_i)^2}{\sigma_i^2}$$

has the chi-squared distribution with n degrees of freedom, for each squared term in the sum has been standardized by its mean and variance.

Table 2 of the Appendix contains percentage points of the chi-squared distribution. We shall write the 100α percentage point of the chi-squared distribution with n degrees of freedom as

$$(7) \qquad \chi^2_{\alpha,n}$$

where of course $\alpha = P(\chi^2 > \chi^2_{\alpha;n})$.

The t distribution. The t random variable with n degrees of freedom is defined as the quotient

$$(8) \qquad t = \frac{z}{\sqrt{\chi^2/n}}$$

of a standard normal variate z and the square root of an independent chi-squared variate divided by its n degrees of freedom. t is a dimensionless quantity, and its density function.

$$(9) \qquad f(t) = \frac{\Gamma[(n+1)/2]}{\sqrt{\pi n} \, \Gamma(n/2)} \frac{1}{(1 + t^2/n)^{(n+1)/2}} \quad -\infty < t < \infty$$

depends upon the single degrees of freedom parameter n. Percentage points of the distribution of t are given in Table 3 of the Appendix. We shall customarily write the upper 100α percentage point as $t_{\alpha;n}$ or

$$(10) \qquad \alpha = P(t > t_{\alpha;n})$$

The F distribution. The ratio

$$(11) \qquad F = \frac{\chi_1^2/m}{\chi_2^2/n}$$

of independent chi-squared variates divided by their respective degrees of freedom has the F, or *variance-ratio*, distribution with density function

$$(12) \quad f(F) = \frac{\Gamma((m+n)/2)}{\Gamma(m/2)\Gamma(n/2)} \left(\frac{m}{n}\right)^{m/2} F^{(m-2)/2} \left(1 + \frac{m}{n} F\right)^{-(m+n)/2} \quad 0 \le F < \infty$$

We shall denote the 100α upper percentage point of the F distribution with m, n degrees of freedom by $F_{\alpha;m,n}$:

$$(13) \qquad \alpha = P(F > F_{\alpha;m,n})$$

It follows from the definition (11) of the F variate that the lower percentage points can be obtained from the reciprocals of the upper values with reversed degrees of freedom:

$$(14) \qquad F_{1-\alpha;m,n} = \frac{1}{F_{\alpha;n,m}}$$

Table 4 of the Appendix gives upper percentage points of the F distribution.

Derivations and mathematical properties of these standard distributions can be found in many current sources, e.g., Hogg and Craig (1959), Stuart and Ord (1987), or Mood *et al.* (1974). Extensive tables of the distributions and their percentage points have been compiled by Pearson and Hartley (1966), together with illustrations of their use.

1.4 RANDOM SAMPLES AND ESTIMATION

Heretofore we have discussed random variables only in terms of the abstract populations specified by their distribution or density functions.

Occasionally these functions are known for some random phenomenon, and it is possible to describe the process directly from its mathematical model. More usually it is the case that neither the mathematical form of the distribution nor its parameters are known, and it is necessary to go beyond the realm of probability theory to the domain of *statistical inference* to obtain estimates of $F(x)$ or its parameters from finite *samples* of values of the random variable. In this section we shall consider one heuristic approach which leads to estimates with some desirable properties.

Let us begin by supposing that the values or "realizations" of the continuous random variable X can be observed and recorded. This is not such an obvious requirement, for many phenomena of interest in the physical or life sciences cannot be observed below threshold levels established by the organism or the measuring equipment, and above other levels the equipment may be saturated or paralyzed by the frequency or intensity of the responses. It is also clear that even if the values of X formed a continuum, the limitations of any recording or measuring device would yield discrete observations. Nevertheless, we shall treat such data as blood pressure in millimeters of mercury, percentage of a certain content of a projective test, and reaction time in milliseconds as observations from continuous populations. We shall assume that the mathematical form of the density function $f(x; \theta_1, \ldots, \theta_k)$ of X is known from substantive considerations, prior experience, or other good fortune, although the values of the parameters θ_i are unknown.

Next let us define the *parameter space* of a density. Suppose that the density depends upon the single real parameter θ, as in the case of the descending exponential or the normal distribution with mean μ and known unit variance. Then the parameter space of θ is *that portion of the real line which contains all admissible values of θ*. For the descending exponential the parameter space would be the positive half of the real line, for negative parameters would destroy the density property, and a parameter of zero would lead to the trivial "sure-number" distribution. For the normal distribution with known variance the space would be the entire real line. Similarly, the parameter space for the k-parameter density would be some region of k-dimensional euclidean space. For example, that of the normal distribution is the upper half of the (μ, σ^2) plane shown in Fig. 1.3.

Finally we must define the *sampling* or *experimental units* on which the values of X will be observed. The available units must constitute a homogeneous collection with respect to all characteristics which might affect the values of the variate. If the random variable is the blood level of free fatty acid (FFA) in normal adolescent American females, the available sampling units should not include female subjects with

σ^2

0   μ
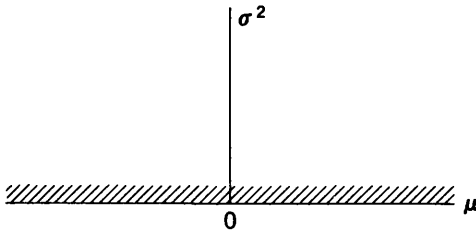
FIGURE 1.3
Parameter space for the normal distribution.

metabolic diseases, adolescent males, or prepubertal children of either sex. The sampling units must be independent of one another and must not possess common qualities which might lead to dependent values of X. Clearly, a sequence of 10 daily FFA determinations in a single subject would not yield the same information about the biological population represented by that person as 10 single determinations of FFA obtained from as many unrelated and independent individuals. We assure such independence by drawing the sampling units *randomly* from the available collection of units. The investigator who gathers data from the nearest convenient source of subjects, be it students in Psychology 1 or a group of paid volunteers, must risk whatever biases these nonrandom and unrepresentative samples may contain.

Now suppose that N units have been selected at random. Their observed values of X will be denoted by $x_1, \ldots, x_N$. We shall customarily distinguish such observations from the running value x of X by the presence of subscripts. Our initial problem will be to estimate the parameters θ_i by some suitable function of the observations. Such estimates will be denoted by the parameter with a hat, or $\hat{\theta}_i$. We shall call these quantities *point estimates*, for they are unequivocal single values of θ, as opposed to the *interval estimates* of the next section. But how should the function of the observations be chosen? Should we merely relate the parameters to the first few moments of the distribution and then equate the sample moments to those of the population? Would estimates using only extreme or middle values of the observations serve as well as those which depended upon all the data? Intuition might lead us to many other estimators, or classes of functions of the observations, and we should like to have some critiera for choosing among them. For example, we might ask whether the estimator possesses any of these desirable properties:

1. *Unbiasedness.* The expected value of the estimator should be its parameter, or $E(\hat{\theta}) = \theta$, for all θ.
2. *Consistency.* As the sample size increases without bound, $\hat{\theta}$ should converge in probability to θ.

3. *Minimum variance.* Frequently the estimate is chosen as that one which has smallest variance among all unbiased estimators. If a minimum-variance estimator does not exist for all sample sizes, it is possible to choose among competing estimators by the ratios of their asymptotic variances. An estimator with that smallest relative variance is said to be *efficient.*

4. *Sufficiency.* An estimator $\hat{\theta}$ is said to be *sufficient* if it contains all the information in the observations for the estimation of θ. That is, knowledge of the values $x_1, \ldots, x_N$ will provide no more information than that contained in $\hat{\theta}$. Stated mathematically, the conditional distribution of the x_i for a fixed value of $\hat{\theta}$ does not depend on the unknown parameter θ.

In a particular application each of these criteria must be weighed with regard to the cost of sample observations, the speed with which the data must be processed, and the consequences of small biases or larger variances on the investigator's view of nature or the policy maker's actions. As we shall see, it is sometimes possible to remove bias by a slight scaling or other redefinition of the estimate, while the common estimates of the various correlation measures to be discussed in Chap. 3 are computed in daily profusion with no concern for their biased nature. In small samples the loss of efficiency in some short-cut estimators may be offset by the ease with which they are computed.

Now let us consider a means for generating estimates known as the *method of maximum likelihood.* While that procedure is a heuristic one, or one appealing more to intuition than to the real end of producing estimates with "good" properties, it can be shown that its estimates often have a number of desirable qualities. We begin by defining the *likelihood* of the random sample of observations as the joint density of the variates of the sampling units evaluated at $x_1, \ldots, x_N$:

$$(1) \qquad L(\theta_1, \ldots, \theta_k) = \prod_{i=1}^{N} f(x_i; \theta_1, \ldots, \theta_k)$$

The likelihood function is a relative measure of the likelihood of the particular sample $x_1, \ldots, x_N$. The maximum-likelihood method of estimation directs that the estimates of the θ_i be chosen so as to maximize the function (1) for a given sample. If the likelihood has a relative maximum, this can be accomplished by straightforward differentiation and solution of certain equations. The vanishing of the derivatives is of course only a necessary condition for a relative maximum, and the sufficient conditions given by the second-order partial derivatives should also be verified (see, for example, Hancock, 1960, Chap. 5). Absolute maxima can frequently be determined by direct inspection of the

likelihood. However, since the values of the variables which maximize a function also maximize monotonic functions of it, and since the majority of likelihoods encountered in statistical inference contain exponential terms, it is usually more convenient to work with the natural logarithm of the likelihood

$$(2) \qquad l(\theta_1, \ldots, \theta_k) = \ln L(\theta_1, \ldots, \theta_k)$$

Then, if the likelihood has a relative maximum, the associated estimates of the θ_j can be found by solving the system of k simultaneous equations

$$(3) \qquad \frac{\partial l(\theta_1, \ldots, \theta_k)}{\partial \theta_j} = 0 \qquad j = 1, \ldots, k$$

for the estimates

$$(4) \qquad \hat{\theta}_1, \ldots, \hat{\theta}_k$$

If the equations possess multiple roots, it will be necessary to choose the solution leading to the greatest likelihood.

Perhaps two simple examples will help to describe the steps in finding maximum-likelihood estimators.

Example 1.1. Let us determine the maximum-likelihood estimates of a and b in the rectangular density defined in Sec. 1.2. The likelihood function of the sample $x_1, \ldots, x_N$ is

$$L(a, b) = \frac{1}{(b - a)^N}$$

Clearly a cannot exceed the smallest observation, and b cannot be less than the largest. If we denote the ordered observations by $x_{(1)} \le \cdots \le x_{(N)}$,

$$a \le x_{(1)} \le \cdots \le x_{(N)} \le b$$

The likelihood will be at its greatest value when $b - a$ is as small as possible consistent with the second set of inequalities, and the estimates minimizing that range are

$$\hat{a} = x_{(1)} \qquad \hat{b} = x_{(N)}$$

Example 1.2. The likelihood of the sample $x_1, \ldots, x_N$ of N independent normal random variables is

$$L(\mu, \sigma^2) = \frac{1}{(2\pi)^{N/2}(\sigma^2)^{N/2}} \exp\left[-\frac{1}{2\sigma^2} \sum_{i=1}^{N} (x_i - \mu)^2 \right]$$

and its logarithm is

$$l(\mu, \sigma^2) = -\frac{N}{2} \ln(2\pi) - \frac{N}{2} \ln \sigma^2 - \frac{1}{2\sigma^2} \sum_{i=1}^{N} (x_i - \mu)^2$$

The partial derivatives with respect to μ and σ^2 are

$$\frac{\partial l(\mu,\sigma^2)}{\partial \mu} = \frac{1}{\sigma^2} \sum_{i=1}^{N} (x_i - \mu)$$

$$\frac{\partial l(\mu,\sigma^2)}{\partial \sigma^2} = -\frac{N}{2\sigma^2} + \frac{1}{2\sigma^4} \sum_{i=1}^{N} (x_i - \mu)^2$$

If we equate these to zero and cancel any extraneous factors, the simultaneous equations (3) are

$$\sum_{i=1}^{N} x_i - N\mu = 0$$

$$\sum_{i=1}^{N} (x_i - \mu)^2 - N\sigma^2 = 0$$

Solve the first for the estimate of μ, and use that value in the second to obtain the solution for the estimate of σ^2:

$$\hat{\mu} = \frac{1}{N} \sum_{i=1}^{N} x_i$$

$$= \bar{x}$$

$$\hat{\sigma}^2 = \frac{1}{N} \sum_{i=1}^{N} (x_i - \bar{x})^2$$

$$= \frac{1}{N} \left[\sum_{i=1}^{N} x_i^2 - \frac{1}{N} (\sum x_i)^2 \right]$$

These estimates are intuitively plausible, for the population mean is merely estimated by the sample mean $\bar{x}$, and the estimate of the variance is the average squared deviation from the sample mean.

Let us determine whether $\hat{\mu}$ and $\hat{\sigma}^2$ are unbiased estimates. Replace the observations by the random variables X_i and take expectations:

$$E(\hat{\mu}) = \frac{1}{N} \sum_{i=1}^{N} E(X_i)$$

$$= \frac{1}{N} \sum_{i=1}^{N} \mu$$

$$= \mu$$

The sample mean is an unbiased estimate of μ. The expectation of $\hat{\sigma}^2$

involves more lengthy computations:

$$E(\hat{\sigma}^2) = \frac{1}{N} E\left[\sum_{i=1}^{N} X_i^2 - \frac{1}{N}\left(\sum X_i\right)^2\right]$$

$$= \frac{1}{N}\left[N E(X_i^2) - \frac{1}{N} E\left(\sum_{i=1}^{N}\sum_{j=1}^{N} X_i X_j\right)\right]$$

$$= \frac{1}{N}\left[N E(X_i^2) - E(X_i^2) - \frac{1}{N}\sum_i\sum_j E(X_i X_j)\right]$$

$$= \frac{1}{N}\left\{(N - 1)E(X_i^2) - \frac{1}{N} N(N - 1)[E(X_i)]^2\right\}$$

$$= \frac{N - 1}{N}\sigma^2$$

$\hat{\sigma}^2$ is not an unbiased estimate of the variance. However, if we replace the divisor N in the original formula by $N - 1$, the bias will be eliminated and the usual sample-variance expression

$$s^2 = \frac{1}{N - 1}\left[\sum_{i=1}^{N} x_i^2 - \frac{1}{N}\left(\sum x_i\right)^2\right]$$

can be obtained.

Maximum-likelihood estimates are thus not necessarily unbiased, although it is sometimes possible to remove the bias through multiplication by an appropriate factor.

1.5 TESTS OF HYPOTHESES FOR THE PARAMETERS OF NORMAL POPULATIONS

Statistical tests of hypotheses. Statistical inference can be divided into two general areas. The first is concerned with the estimation of distribution functions, the parameters of such functions when their mathematical form is specified, or the parameters of models built around random variables. The second part addresses itself to the problem of testing the validity of hypotheses about distribution functions and their parameters or the parameters or components of mathematical models. In the preceding section we touched briefly on one approach to estimation through the maximum-likelihood principle. Now we shall summarize some essentials of hypothesis testing, and subsequently we shall see how these tests can be inverted to provide interval estimates for parameters.

Perhaps a simple example will help to motivate the testing problem in terms of regions in the parameter space. It is known from extensive experience that the grade point indices (GPI) of first-year students at a

small liberal arts college have tended to be normally distributed with mean 2.43 and variance 0.04. However, in the selection of the present first-year class several admission standards were raised, and it is hypothesized that the mean GPI of the population out of which those students were drawn will be higher and the variance in turn will be a little smaller. We may summarize these statements about the population parameters in this fashion:

Original hypothesis: $\mu = 2.43 \quad \sigma^2 = 0.04$

Alternative hypothesis: $\mu > 2.43 \quad \sigma^2 < 0.04$

We shall designate the original description of the GPI population as the *null hypothesis*; this will be conventionally denoted by H_0. The *alternative hypothesis* will be denoted by H_1. The assumption of normality is common to both hypotheses and need not be mentioned in their statements. H_0 refers to the *single* point (2.43, 0.04) in the parameter space, and therefore is called a *simple* hypothesis. The alternative designates the shaded region of Fig. 1.4, and since that set contains more than one point, H_1 is called a *composite* hypothesis. An important class of composite hypotheses is formed by those statements in which the values of one or more parameters are completely unknown. For example, if the random variable X is normally distributed with *unknown* variance, the hypotheses

$$H_0: \quad \mu = \mu_0$$

and

$$H_1: \quad \mu = \mu_1 > \mu_0$$

on the mean alone specify vertical lines in the space of Fig. 1.3 terminating at $\mu = \mu_0$ and $\mu = \mu_1$ on the horizontal axis. Statistical tests of such hypotheses would have to be constructed to be unaffected by the unknown true value of σ^2.

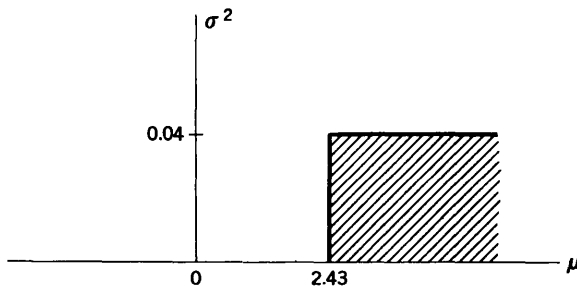It has been the purpose of much of the theory of statistical inference

FIGURE 1.4

to develop tests of the validity of these hypotheses based upon sample observations. We shall prefer to consider testing only in terms of the classical, or Neyman-Pearson, approach to two-decision rules, for the subsequent multivariate tests will be of the classical sort. The reader is referred to Lindgren (1962) and Mood *et al.* (1974) for detailed discussions and examples of test construction; considerably more advanced treatments with proofs of many of the theorems can be found in Kendall and Stuart (1979), Lehmann (1987), and Wilks (1962).

For the general case let X be a continuous random variable with the real numbers as its admissible values. The density function of X depends upon the parameters $\theta_1, \ldots, \theta_k$. The *sample space* W of all possible outcomes of N observations on X is then N-dimensional euclidean space. A particular sample of observations will be written in vector form as $[x_1, \ldots, x_N]$ and will denote a point in the sample space. Let ω_1 and ω_2 be any two disjoint (that is, having no points in common) regions of the parameter space Ω. We shall set up these hypotheses about the parameters of the distribution of X:

(1)
$$H_0: \quad [\theta_1, \ldots, \theta_k] \text{ is contained in } \omega_1$$
$$H_1: \quad [\theta_1, \ldots, \theta_k] \text{ is contained in } \omega_2$$

On the basis of the sample observations we wish to decide in some "optimal" fashion which hypothesis is tenable. Since certain sets of observations would lead us to favor H_0 over H_1 and other data would support the opposite preference, our decision rule should have this form:

(2)
$$\text{Accept } H_0 \text{ if } [x_1, \ldots, x_N] \text{ falls in } W - w$$
$$\text{Accept } H_1 \text{ if } [x_1, \ldots, x_N] \text{ falls in } w$$

where w is a specified part of the sample space called the *critical region* or *rejection region* for H_0. If the true state of nature as described by the various parameters is specified by either H_0 or H_1, the decision maker can incur two kinds of error in the application of the decision rule. An *error of the first kind,* or a *Type I error,* consists of declaring H_1 the true state when in fact H_0 is true. An *error of the second kind,* or a *Type II error,* is made upon the acceptance of H_0 as true when H_1 describes the correct state of nature. The correctness of the actions may be summarized in this two-way table:

	State of nature	
Action	H_0 **true**	H_1 **true**
Accept truth of H_0	Correct	Type II error
Accept truth of H_1	Type I error	Correct

The probabilities of the Type I and II errors provide measures of the

efficacy of the decision rule. The probability α of the Type I error is the probability that the sample observations fall in the critical region w when H_0 is true, or

$$(3) \qquad \alpha = P([x_1, \ldots, x_N] \in w \mid H_0 \text{ true})$$

where the symbol $\in$ denotes membership in the set w and the vertical bar indicates that the probability statement is conditional upon the truth of the null hypothesis. α is called the *size* of the test. The probability of the Type II error is

$$(4) \qquad \beta = P([x_1, \ldots, x_N] \in W - w \mid H_1 \text{ true})$$

The complement $1 - \beta$ of the second error probability is called the *power* of the test or decision rule. If the power is computed for a continuum of parameter values, the resulting probabilities constitute the *power function*.

   If the sample size is fixed, changes in the form of the critical region that reduce α will also increase β, and conversely, minimization of β will be at the expense of larger α. The classical approach to hypothesis testing calls for a test of fixed size α whose rejection region is chosen so as to minimize β or, equivalently, to maximize the power. If both hypotheses are simple, i.e., of the form

$$(5) \qquad H_0: \begin{array}{c} \theta_1 = \theta_{10} \\ \cdots\cdots\cdots \\ \theta_k = \theta_{k0} \end{array} \qquad H_1: \begin{array}{c} \theta_1 = \theta_{11} \\ \cdots\cdots\cdots \\ \theta_k = \theta_{k1} \end{array}$$

the *Neyman-Pearson lemma* states that the most powerful test of size α will have a critical region defined by this decision rule:

$$(6) \quad \text{Accept } H_0 \text{ if } \lambda = \frac{f(x_1; \theta_{10}, \ldots, \theta_{k0}) \cdots f(x_N; \theta_{10}, \ldots, \theta_{k0})}{f(x_1; \theta_{11}, \ldots, \theta_{k1}) \cdots f(x_N; \theta_{11}, \ldots, \theta_{k1})} > c$$

and

$$\text{Accept } H_1 \text{ if } \lambda < c$$

where c is a constant chosen such that

$$P(\lambda < c \mid H_0) = \alpha$$

The lemma defines the critical region as that set of points in the sample space for which the likelihood ratio λ is less than c. The proof of the lemma is due to Neyman and Pearson (1933); numerous applications to the derivation of standard tests may be found in the text of Mood *et al.* (1974). A more general development of two-decision rules can be obtained by assigning monetary losses or other penalties to the Type I and Type II errors.

   Note that the Neyman-Pearson lemma requires that both hypoth-

eses are simple, i.e., that the regions ω_1 and ω_2 of the parameter space are points. Tests of composite hypotheses involving several parameters can be constructed by the powerful *generalized likelihood-ratio criterion*

$$(7) \qquad \lambda = \frac{L(\hat{\omega})}{L(\hat{\Omega})}$$

where

$$(8) \qquad L(\hat{\omega}) = f(x_1; \hat{\theta}_{10}, \ldots, \hat{\theta}_{k0}) \cdots f(x_N; \hat{\theta}_{10}, \ldots, \hat{\theta}_{k0})$$

is the likelihood function maximized under the assumption that

$$H_0: \quad [\theta_1, \ldots, \theta_k] \in \omega$$

is true, and $L(\hat{\Omega})$ is the maximized likelihood for $\theta_1, \ldots, \theta_k$ permitted to take on values throughout the entire parameter space Ω. We accept H_0 if

$$\lambda > c$$

and otherwise accept the alternative

$$H_1: \quad [\theta_1, \ldots, \theta_k] \in \Omega - \omega$$

The constant c is chosen so that $P(\lambda < c \mid H_0 \text{ true}) \leq \alpha$. When, as in the case of composite hypotheses, the true size of the test is actually less than or equal to α, we shall say that the test is of *level* α. It can be shown that if H_0 is true and regularity conditions hold,

$$(9) \qquad \chi^2 = -2 \ln \lambda$$

tends as the sample size increases to be distributed according to the chi-squared distribution with degrees of freedom equal to the difference of the dimensionalities of the parameter space Ω and the null hypothesis subspace ω or, equivalently, to the number of parameters determined by H_0. The generalized likelihood-ratio criterion is also due to Neyman and Pearson (1928); examples of its use have been given by Mood *et al.* (1974), while extensive discussions of its properties have been given by Kendall and Stuart (1979) and Wilks (1962).

Tests on the mean of a normal variate with known variance. Let $x_1, \ldots, x_N$ be a sample of indep lent observations on the random variable with distribution $N(\mu, \sigma^2)$.   ie variance σ^2 is known, although μ is not. On the basis of the samp e observations we wish to test the hypothesis

$$(10) \qquad H_0: \quad \mu = \mu_0$$

that the population mean has some specified value μ_0 against the alternative

$$(11) \qquad H_1: \quad \mu = \mu_1 > \mu_0$$

that the mean is some larger value μ_1. By the Neyman-Pearson lemma the most powerful test of size α is based upon the test statistic

$$(12) \qquad z = \frac{(\bar{x} - \mu_0)\sqrt{N}}{\sigma}$$

whose critical region is

$$(13) \qquad z > z_\alpha$$

where z_α is the upper 100α percentage point of the unit normal distribution. In terms of the mean of the original observations we should reject H_0 in favor of H_1 if

$$(14) \qquad \bar{x} > \mu_0 + \frac{\sigma}{\sqrt{N}} z_\alpha$$

and otherwise accept the null hypothesis. If the alternative hypothesis had been

$$(15) \qquad H_1': \quad \mu = \mu_1 < \mu_0$$

the same test statistic would be employed, although the critical region would be

$$(16) \qquad z < -z_\alpha$$

or, equivalently,

$$(17) \qquad \bar{x} < \mu_0 - \frac{\sigma}{\sqrt{N}} z_\alpha$$

The preceding tests and alternative hypotheses H_1, H_1' are called *one-sided*, for the direction of the change from μ_0 to μ_1 is clearly indicated. When it is possible to make such predictions from subject-matter considerations or prior investigations, the power of the tests will be appreciably larger than that of the *two-sided* test with the alternative hypothesis

$$(18) \qquad H_1'': \quad \mu = \mu_1 \neq \mu_0$$

that allows for either larger or smaller alternative values of the mean. The test statistic is still (12), but the rejection region for a test of size α is

$$(19) \qquad |z| > z_{\alpha/2}$$

where $z_{\alpha/2}$ is the upper 50α percentage point of the unit normal distribution. Equivalently, we reject H_0 if *either*

$$(20) \qquad \bar{x} > \mu_0 + \frac{\sigma}{\sqrt{N}} z_{\alpha/2} \quad \text{or} \quad \bar{x} < \mu_0 - \frac{\sigma}{\sqrt{N}} z_{\alpha/2}$$

holds.

Power curves for tests against the three alternatives can be constructed from tables of the normal distribution, and since they can be found in most texts on statistical theory and methods, they will not be reproduced here. In practice one usually selects a suitable value of α and one or more tolerable β probabilities. The sample size N is then chosen to achieve the minimum β that is consistent with budgetary limitations or the size of laboratory or clinical facilities.

Finally, we note that the normal density function is a member of the exponential family cited earlier in this section, and thus tests of such composite hypotheses as

$$H_0: \quad \mu = \mu_0 \quad H_1: \quad \mu > \mu_0$$

or

$$H_0: \quad \mu < \mu_0 \quad H_1: \quad \mu > \mu_0 \qquad .$$

are uniformly most powerful.

Tests on means when the variance is unknown. In most scientific applications it is rare indeed that the population variance is known, and an important advance in statistical inference was achieved when W. S. Gosset (publishing under the pseudonym "Student") obtained the distribution of the test statistic for composite hypotheses on the mean of a normal distribution with unknown variance. The generalized likelihood-ratio criterion for testing the hypothesis (10) against the alternative (11) on the basis of N independent observations $x_1, \ldots, x_N$ with mean $\bar{x}$ and variance s^2 leads to the test statistic

$$(21) \qquad t = \frac{(\bar{x} - \mu_0)\sqrt{N}}{s}$$

If H_0 is true, t has the Student-Fisher t distribution with $N - 1$ degrees of freedom, and we reject the null hypothesis for a test of size α if

$$(22) \qquad t > t_{\alpha;N-1}$$

where $t_{\alpha;N-1}$ is the upper 100α percentage point of the t distribution defined in the preceding section. Similarly, if the alternative hypothesis had been (15), the rejection region would be defined by

$$(23) \qquad t < -t_{\alpha;N-1}$$

and for the two-sided alternative (18) the null hypothesis would be rejected if

$$(24) \qquad |t| > t_{\alpha/2,N-1}$$

The power of tests involving the t statistic can be computed from the first of the Pearson-Hartley charts of Appendix A with degrees of freedom

$v_1 = 1$ and $v_2 = N - 1$ and noncentrality parameter

$$(25) \qquad \phi = \frac{|\mu - \mu_0|}{\sigma} \left(\frac{N}{2}\right)^{1/2}$$

Then a sample size can be determined which will guarantee a power probability above a specified minimum for fixed α.

Now consider that two random samples have been independently drawn from normal populations with a common variance σ^2 but possibly different means μ_1 and μ_2. Let the observations of the samples be $x_1, \ldots, x_{N_1}, y_1, \ldots, y_{N_2}$. The generalized likelihood-ratio criterion for the test of the hypothesis

$$(26) \qquad H_0: \quad \mu_1 = \mu_2$$

of equal population means against the alternative

$$(27) \qquad H_1: \quad \mu_1 > \mu_2$$

leads to the test statistic

$$(28) \qquad t = \frac{\bar{x} - \bar{y}}{\sqrt{\dfrac{\sum\limits_{i=1}^{N_1} (x_i - \bar{x})^2 + \sum\limits_{i=1}^{N_2} (y_i - \bar{y})^2}{N_1 + N_2 - 2} \left(\dfrac{1}{N_1} + \dfrac{1}{N_2}\right)}}$$

For a test of size α we reject H_0 in favor of H_1 if

$$(29) \qquad t > t_{\alpha; N_1 + N_2 - 2}$$

The rejection regions for the other alternative hypotheses H_1': $\mu_1 < \mu_2$ and H_1'': $\mu_1 \neq \mu_2$ are of course similar to (23) and (24) of the single-sample tests.

Confidence intervals for means. The investigator who has carried out a costly or intricate experiment is rarely satisfied to hear that the observations have merely rejected some hypothesis. If the findings show that the new drug or treatment has some "significant" effect beyond that of the placebo or previous standard, the experimenter and the scientific community would prefer to know not only the best estimate of the magnitude of this effect but also some range of reasonable values of the effect parameter. Such statements of possible values are called *confidence intervals* or, in contrast with the unequivocal point estimates of Sec. 1.4, *interval estimates*.

Suppose that a random sample of N observations has been drawn from some population with continuous density $f(x; \theta)$. The $100(1 - \alpha)$ percent confidence interval for θ is that set of values

$$(30) \qquad t_1 \leq \theta \leq t_2$$

with limits computed from the percentage points of the distribution function of the estimate $\hat{\theta}$ of θ so that

(31) $$P(t_1 \le \theta \le t_2) = 1 - \alpha$$

α is usually taken as 0.05 or some smaller probability. $1 - \alpha$ is called the *confidence coefficient* of the interval. It is *essential* that the probability statement be read as "the probability that the interval with end points t_1, t_2 covers θ is $1 - \alpha$," for in our usage the parameter is hardly a random variable. We also note that an infinity of confidence intervals exists which satisfy (31); in most subsequent cases t_1 and t_2 will be chosen so that the length $t_2 - t_1$ of the interval is shortest.

Confidence intervals for the mean of a normal population or the difference of the means of two normal populations can be found from the preceding tests of hypotheses. If N independent observations with mean $\bar{x}$ have been collected on the $N(\mu, \sigma^2)$ variate with known variance, the value of μ_0 for which H_0: $\mu = \mu_0$ is just rejected in favor of

$$H_1: \quad \mu = \mu_1 > \mu_0$$

by the test of size α_1 is given by

$$\mu_0 = \bar{x} - \frac{\sigma}{\sqrt{N}} z_{\alpha_1}$$

Similarly, the smallest value of μ_0 for which the size $\alpha - \alpha_1$ test of H_0 against H_1': $\mu = \mu_1 < \mu_0$ is rejected is

$$\mu_0 = \bar{x} + \frac{\sigma}{\sqrt{N}} z_{\alpha-\alpha_1}$$

z_{α_1}, $z_{\alpha-\alpha_1}$ are of course the upper $100\alpha_1$, $100(\alpha - \alpha_1)$ percentage points of the unit normal distribution. The $100(1 - \alpha)$ percent confidence interval for μ is thus

$$\bar{x} - \frac{\sigma}{\sqrt{N}} z_{\alpha_1} \le \mu \le \bar{x} + \frac{\sigma}{\sqrt{N}} z_{\alpha-\alpha_1}$$

and its length is $(\sigma/\sqrt{N})(z_{\alpha_1} + z_{\alpha-\alpha_1})$. But it can be shown that minimum length is achieved when $z_{\alpha_1} = z_{\alpha-\alpha_1}$ or if $\alpha_1 = \frac{1}{2}\alpha$. The shortest interval with coefficient $1 - \alpha$ has the symmetric form

(32) $$\bar{x} - \frac{\sigma}{\sqrt{N}} z_{\alpha/2} \le \mu \le \bar{x} + \frac{\sigma}{\sqrt{N}} z_{\alpha/2}$$

Similarly, if σ^2 is unknown, the $100(1 - \alpha)$ percent confidence interval for μ is given by

(33) $$\bar{x} - \frac{s}{\sqrt{N}} t_{\alpha/2;N-1} \le \mu \le \bar{x} + \frac{s}{\sqrt{N}} t_{\alpha/2;N-1}$$

where s is the sample standard deviation and $t_{\alpha/2;N-1}$ is the upper 50α percentage point of the t distribution with $N-1$ degrees of freedom.

Frequently it is necessary to obtain a confidence interval for the difference of the means of two normal populations with a common, though unknown, variance. The observations from the first population might have been collected as a control for those in the second sample that had been obtained under a new treatment or experimental condition. Under the normality and common-variance assumptions the $100(1-\alpha)$ percent confidence interval for the change attributable to the experimental condition is

$$(34) \quad \bar{x} - \bar{y} - s_{\bar{x}-\bar{y}}t_{\alpha/2;N_1+N_2-2} \leq \mu_1 - \mu_2 \leq \bar{x} - \bar{y} + s_{\bar{x}-\bar{y}}t_{\alpha/2;N_1+N_2-2}$$

where $\bar{x}, \bar{y}$ are the respective means of the first and second samples of N_1 and N_2 observations and

$$(35) \qquad s_{\bar{x}-\bar{y}} = \sqrt{\frac{\sum (x_i - \bar{x})^2 + \sum (y_i - \bar{y})^2}{N_1 + N_2 - 2} \left(\frac{1}{N_1} + \frac{1}{N_2}\right)}$$

is the usual within-sample estimate of the standard deviation of the mean difference.

Tests and confidence intervals for the variance. The multivariate tests and confidence statements of the later chapters will generally be constructed for means and other location parameters. However, for the sake of completeness we shall touch upon some hypotheses and interval estimates for the variance of a normal population. If the observations $x_1, \ldots, x_N$ constitute a random sample from $N(\mu, \sigma^2)$, the quantity

$$(36) \qquad \frac{(N-1)s^2}{\sigma^2} = \frac{\sum\limits_{i=1}^{N} (x_i - \bar{x})^2}{\sigma^2}$$

is distributed as a chi-squared variate with $N-1$ degrees of freedom. The generalized likelihood-ratio criterion for the test of the hypothesis

$$(37) \qquad\qquad H_0: \quad \sigma^2 = \sigma_0^2$$

against the alternative

$$(38) \qquad\qquad H_1: \quad \sigma^2 > \sigma_0^2$$

specifies that the rejection region for a test of size α is

$$(39) \qquad\qquad \frac{(N-1)s^2}{\sigma_0^2} > \chi^2_{\alpha;N-1}$$

where $\chi^2_{\alpha;N-1}$ is the upper 100α percentage point of the chi-squared distribution with $N-1$ degrees of freedom. Similarly, the rejection

regions for testing the null hypothesis against the alternatives H'_1: $\sigma^2 < \sigma_0^2$ and H''_1: $\sigma^2 \neq \sigma_0^2$ would be

(40)
$$\frac{(N-1)s^2}{\sigma_0^2} < \chi^2_{1-\alpha, N-1}$$

and

(41)
$$\frac{(N-1)s^2}{\sigma_0^2} < \chi^2_{1-\alpha_1; N-1} \quad \text{or} \quad \frac{(N-1)s^2}{\sigma_0^2} > \chi^2_{\alpha_2; N-1}$$

respectively, where in the latter case $\alpha_1 + \alpha_2 = \alpha$. In the strict sense α_1 and α_2 should be chosen so that the latter test is *unbiased*, i.e., its power function is never less than its size α, but in most applications with moderate to large sample sizes an equal split will suffice. Confidence intervals for σ^2 can be obtained directly from the rejection region (41), and will be left as an exercise for the reader.

If independent samples of N_1 and N_2 observations have been randomly drawn from the populations $N(\mu_1, \sigma_1^2)$ and $N(\mu_2, \sigma_2^2)$, the hypothesis

(42)
$$H_0: \quad \sigma_1^2 = \sigma_2^2$$

can be tested against the alternative

(43)
$$H_1: \quad \sigma_1^2 > \sigma_2^2$$

by the statistic

(44)
$$F = \frac{s_1^2}{s_2^2}$$

If the null hypothesis is true, the statistic has the F distribution with degrees of freedom $N_1 - 1$, $N_2 - 1$, and the rejection region for a test of size α is

(45)
$$F > F_{\alpha; N_1-1, N_2-1}$$

Conversely, H_0 could be tested against the other one-sided alternative H'_1: $\sigma_1^2 < \sigma_2^2$ by the statistic

(46)
$$F = \frac{s_2^2}{s_1^2}$$

whose critical region is

(47)
$$F > F_{\alpha; N_2-1, N_1-1}$$

Finally, for the two-sided alternative H''_1: $\sigma_1^2 \neq \sigma_2^2$ the statistic (44) would

be used with the critical region defined by

(48) $$ F > F_{\alpha_1; N_1-1, N_2-1} \quad \text{or} \quad F < \frac{1}{F_{\alpha_2; N_2-1, N_1-1}} $$

where the partitioning $\alpha_1 = \alpha_2 = \frac{1}{2}\alpha$ will generally suffice.

Some further reading. The source and seed of much of modern statistical methodology can be found in Fisher's classics (1969, 1972). Snedecor and Cochran's text (1989) has a tutorial quality in its style and organization, and it treats basic methods in depth from the investigator's viewpoint. Dixon and Massey (1969) cover a wide variety of techniques. Hodges and Lehmann (1964) have integrated concepts of probability and statistical theory with many practical examples of estimation and testing. Illustrations of the normal-theory methods of this section can be found in the innumerable basic texts currently available, e.g., Freund (1971).

1.6 TESTING THE EQUALITY OF SEVERAL MEANS: THE ANALYSIS OF VARIANCE

Suppose that a certain biochemical compound is known to be taken up by the brain, although some evidence is available that the amount per gram of brain tissue appears to differ among the five strains of mice commonly used in one laboratory. It will be assumed that the relative amounts assayed from the brains of sacrificed mice are normally distributed with the same variance σ^2 for each strain. Let μ_j be the population mean for the jth strain. It is possible to construct a test of

(1) $$ H_0: \quad \mu_1 = \cdots = \mu_5 $$

against the alternative that some means are different by the generalized likelihood-ratio criterion, and furthermore, if H_0 is rejected, methods can be obtained for making simultaneous tests on the mean differences with a fixed Type I error probability for all comparisons.

In the general case of k strains, treatments, diagnostic categories, or experimental conditions we begin by postulating that the ith observation on the jth *treatment* (our generic term for whatever feature distinguishes the k groups) can be expressed by the mathematical model

(2) $$ x_{ij} = \mu + \tau_j + e_{ij} \quad i = 1, \ldots, N, \quad j = 1, \ldots, k $$

where μ = location parameter common to all observations
 τ_j = effect peculiar to jth treatment
 e_{ij} = normally distributed random variable with mean zero and variance σ^2

The variate terms e_{ij} are distributed independently of one another. The

model is said to be linear or additive, for application of the jth treatment increases μ by the increment τ_j, and the random disturbance also merely adds or subtracts some amount from the parameters. We note that in the simpler usage of the motivating example $\mu_j \equiv \mu + \tau_j$. The hypothesis of equal treatment effects can be written as

$$(3) \qquad\qquad H_0\colon \quad \tau_1 = \cdots = \tau_k$$

and we shall take as the alternative to H_0 the general model (2) for the observations.

    This is the simplest example of the *general linear model* underlying statistical experimental design. The theory of estimation and hypothesis testing in univariate linear models has been discussed in many texts; those by Scheffé (1959), Graybill (1961), and Searle (1971) are especially suitable for the theoretical background of this section and as . an introduction to the treatment of multivariate models in Chap. 5.

    The model is said to have *fixed* effects, for the μ_j are parameters, and any inferences from the observations can be made only with respect to the particular k treatments in the study. If the treatments constituted a random sample from a larger population (available laboratory technicians, experiments replicated at different times, or clinicians scoring projective tests), the treatment effects would be random variables, and a somewhat different approach would have to be employed in the analysis. This fundamental distinction between the fixed (model I) and random (model II) analysis-of-variance models was first made by Eisenhart (1947) and has been developed extensively by many other workers in experimental design. In the sequel we shall use multivariate techniques for the exact analysis of the *mixed model* for a fixed number of treatments applied repeatedly to each member of a random sample of experimental units.

    The observations can be arranged as in the following table:

Treatment		
1	$\cdots$	**k**
x_{11}	$\cdots$	x_{1k}
$\cdots\cdots$	$\cdots\cdots$	$\cdots\cdots$
$x_{N_1 1}$	$\cdots$	$x_{N_k k}$

Denote the total of the observations for the jth treatment by

$$(4) \qquad\qquad T_j = \sum_{i=1}^{N_j} x_{ij}$$

and the mean of that treatment by $\bar{x}_j = T_j/N_j$. The sum of all observations

will be denoted by

(5) $$G = T_1 + \cdots + T_k$$

the total number of experimental units by

(6) $$N = N_1 + \cdots + N_k$$

and the grand mean by $\bar{x} = G/N$. It is possible to write the total sum of squares

$$S = \sum_{j=1}^{k} \sum_{i=1}^{N_i} (x_{ij} - \bar{x})^2$$

$$= \sum_{j=1}^{k} \sum_{i=1}^{N_i} x_{ij}^2 - \frac{G^2}{N}$$

as the sum of two independent components

(8) $$\text{SST} = \sum_{j=1}^{k} N_j \left(\frac{T_j}{N_j} - \bar{x} \right)^2$$

$$= \sum_{j=1}^{k} \frac{T_j^2}{N_j} - \frac{G^2}{N}$$

and

(9) $$\text{SSE} = \sum_{j=1}^{k} \sum_{i=1}^{N_j} (x_{ij} - \bar{x}_j)^2$$

$$= \sum_{j=1}^{k} \sum_{i=1}^{N_j} x_{ij}^2 - \sum_{j=1}^{k} \frac{T_j^2}{N_j}$$

These components can be summarized in the *analysis-of-variance table* shown in Table 1.1. The statistic for the generalized likelihood-ratio test of H_0 is

(10) $$F = \frac{N - k}{k - 1} \frac{\text{SST}}{\text{SSE}}$$

TABLE 1.1
Analysis of variance

Source	Sum of squares	Degrees of freedom	Mean square
Treatments	SST	$k - 1$	$\dfrac{\text{SST}}{k - 1}$
Within treatments (error)	SSE	$N - k$	$\dfrac{\text{SSE}}{N - k}$
Total	S	$N - 1$	

and since when H_0 is true, SST/σ^2, SSE/σ^2 are independent chi-squared variates with $k - 1$ and $N - k$ degrees of freedom, respectively, the test statistic has the F distribution with $k - 1$ and $N - k$ degrees of freedom. We reject H_0 with a test of level α if

(11) $$F > F_{\alpha;k-1,N-k}$$

The power function for this analysis-of-variance test can be computed from the Pearson-Hartley noncentral F-distribution charts of the Appendix. The degrees-of-freedom parameters are $v_1 = k - 1$ and $v_2 = N - k$, and the noncentrality parameter measuring the departure of the population means of the treatments from the null hypothesis (3) is

(12) $$\phi = \frac{\sqrt{\sum_{j-1}^{k} N_j\left(\tau_j - \frac{\sum N_j\tau_j}{N}\right)^2}}{\sigma\sqrt{k}}$$

or, in the case of equal treatment samples usually encountered in experimental design problems,

(13) $$\phi = \frac{\sqrt{N_j \sum_{j-1}^{k} \tau_j^2}}{\sigma\sqrt{k}}$$

In the latter expression the correction term has vanished from the usual restraint $\tau_1 + \cdots + \tau_k = 0$ imposed on the treatment effects. Illustrations of the use of ϕ and the power charts for selecting sample sizes for the one-way design can be found in Scheffé's text (1959, chap. 3).

Multiple comparisons of treatments. An analysis of variance culminating in rejection of the hypothesis of equal treatment effects still has not indicated those effects which may be equal or those which are probably different. This is the problem of *multiple comparisons*, or simultaneous inferences about the members of some family of hypotheses. The tests are constructed so that the Type 1 error probability for the entire family will be at most α. For an excellent treatment of the theory and methods of multiple comparisons we refer the reader to Miller's monograph (1981). Two methods will be needed frequently in the later chapters, and we shall introduce them now in the context of the one-way analysis of variance.

The first technique is due to Scheffé (1953, 1959). Define a *contrast* of the parameters τ_j of the one-way model as any linear function

(14) $$\sum_{j=1}^{k} c_j\tau_j$$

whose coefficients have the property

$$(15) \qquad \sum_{j=1}^{k} c_j = 0$$

Thus $\tau_1 - \tau_2$ and $3\tau_1 - (\tau_2 + \tau_3 + \tau_4)$ are contrasts, while $\tau_2 - (\tau_3 + \tau_4)$ is not. In the particular case of the one-way analysis-of-variance model Scheffé has shown that the simultaneous confidence intervals with joint coefficient $1 - \alpha$ for all contrasts of the τ_j have the form

$$(16) \quad \sum c_j \bar{x}_j - s\sqrt{(k-1)F_{\alpha;k-1,N-k}\sum \frac{c_j^2}{N_j}} \leq \sum c_j \tau_j$$

$$\leq \sum c_j \bar{x}_j + s\sqrt{(k-1)F_{\alpha;k-1,N-k}\sum \frac{c_j^2}{N_j}}$$

where all summations are over the k treatments. $\sum c_j \bar{x}_j$ is the sample estimate of the contrast $\sum c_j \tau_j$, and

$$(17) \qquad s = \sqrt{\frac{SSE}{N-k}}$$

Note that $s^2 \sum c_j^2/N_j$ is the estimate of the variance of the estimated contrast. We accept the null hypothesis

$$(18) \qquad H_0: \sum_{j=1}^{k} c_j \tau_j = 0$$

at the α level if the simultaneous confidence interval for that contrast includes the value zero. If, on the other hand,

$$\sum c_j \bar{x}_j > s\sqrt{(k-1)F_{\alpha;k-1,N-k}\sum \frac{c_j^2}{N_j}}$$

or

$$\sum c_j \bar{x}_j < -s\sqrt{(k-1)F_{\alpha;k-1,N-k}\sum \frac{c_j^2}{N_j}}$$

we reject H_0 in favor of the respective one-sided alternatives H_1: $\sum c_j \tau_j > 0$ or H_1': $\sum c_j \tau_j < 0$. The joint level of *all* such tests is α.

The second multiple-comparison technique is called the Bonferroni method, for it is based on an inequality bearing that name. For this procedure we begin by restricting our attention to a family of m confidence-interval statements $H_1, \ldots, H_m$ about the parameters of the linear model. The probability that H_i is a true statement (that is, H_i covers the value of the ith parametric function) is $P(H_i)$, and the probability that all statements are simultaneously correct is $P(H_1 \cap \cdots \cap H_m)$, where the intersection notation $H_i \cap H_j$ denotes the event "both H_i

and H_j are correct." This probability is the simultaneous confidence coefficient for the entire family of intervals, and we should like it to be at least equal to some specified value $1 - \alpha$, where α will be called the *error rate for the family of statements*. The calculation of the joint probability is often difficult for practical statistical problems, and its value may depend on unknown "nuisance parameters" measuring the intercorrelations of the H_i statements. Instead we usually must be content with a lower bound

$$(19) \qquad P(H_1 \cap \cdots \cap H_m) \geq 1 - \sum_{i=1}^{m} P(\bar{H}_i)$$

where $P(\bar{H}_i) = 1 - P(H_i)$ is the probability that the ith individual statement is not true. The bound is a simple example of the Bonferroni inequalities (Miller, 1981, pp. 7–8; Feller, 1968, Chap. 4; David, 1956). For a set of m simultaneous confidence intervals we usually assign each statement an error rate of α/m, so that the coefficient for the family is at least $1 - \alpha$.

The Bonferroni confidence intervals on m given contrasts

$$(20) \qquad \Psi_i = \sum_{j=1}^{k} c_{ij}\tau_j \qquad i = 1, \ldots, m$$

of the one-way linear model parameters are

$$(21) \quad \sum_{j=1}^{k} c_{ij}\bar{x}_j - t_{\alpha/(2m);N-ks}\sqrt{\sum_{j=1}^{k} \frac{c_{ij}^2}{N_j}} \leq \Psi_i \leq \sum_{j=1}^{k} c_{ij}\bar{x}_j + t_{\alpha/(2m);N-ks}\sqrt{\sum_{j=1}^{k} \frac{c_{ij}^2}{N_j}}$$

The decision rule for testing H_0: $\Psi_i = 0$ is equivalent to that for the Scheffé method: if (21) does not enclose the value zero, H_0 is rejected. For all paired comparisons of the treatments, $m = \frac{1}{2}k(k - 1)$, while for successive comparisons (assuming some *a priori* ordering), $m = k - 1$. If m is small the Bonferroni intervals may be shorter on the average than those of the Scheffé technique, even though the true family confidence coefficient is greater than the nominal value $1 - \alpha$. For very large m the Bonferroni intervals will be impractically long.

A third method of multiple comparisons ascribed to Tukey (1953) is also in common use for simple experimental designs, but since it has no multivariate generalization or essential application in the later chapters we shall not discuss it here. The reader is referred to Miller (1981) or any thorough text on the analysis of variance.

Example 1.3. In a preliminary evaluation of the three tranquilizing drugs time limitations and the possibility of residual effects decreed that each subject could receive only one drug. Eighteen psychiatric patients with similar diagnoses were rated with respect to anxiety on a seven-point scale.

Six were randomly assigned to each of the three drugs, and after several days each patient was rated blindly on the same scale. These changes in anxiety ratings were observed:

	Drug		
	A	**B**	**C**
	4	0	1
	5	2	0
	3	1	0
	3	2	1
	4	2	2
	2	2	2
Mean	3.5	1.5	1.0

The pertinent sums are

$$T_1 = 21 \qquad T_2 = 9 \qquad T_3 = 6 \qquad G = 36 \qquad \sum_{j=1}^{3}\sum_{i=1}^{6} x_{ij}^2 = 106$$

The sum of squares due to drugs is

$$\text{SST} = \tfrac{1}{6}(21^2 + 9^2 + 6^2) - \frac{36^2}{18}$$

$$= 21$$

and the total sum of squares is $S = 106 - 72 = 34$. The within-drugs, or error, sum of squares follows by subtraction. These values are summarized in the analysis-of-variance table:

Source	Sum of squares	Degrees of freedom	Mean square	F
Drugs	21	2	10.5	12.1
Within drugs	13	15	0.867	
Total	34	17		

Since $F_{0.01,2,15} = 6.36$, we conclude that the hypothesis of equal drug effects is not tenable at the 1 percent level. Furthermore consultation of the F-distribution tables reveals that the observed F also exceeds the critical value for $\alpha = 0.001$.

Now we shall use the Scheffé multiple-comparison procedure to determine which drugs are different. A simultaneous confidence coefficient of 0.99 will be chosen, and thus

$$\sqrt{(k-1)F_{0.01,2,15}} = 3.567$$

First compare drugs B and C by computing the confidence interval for $\tau_2 - \tau_3$. Here $c_1 = 0$, $c_2 = 1$, $c_3 = -1$, and the estimated population

standard deviation of $\bar{x}_2 - \bar{x}_3$ is

$$\sqrt{0.867(\tfrac{1}{6} + \tfrac{1}{6})} = 0.5376$$

The confidence interval is

$$-1.42 \le \tau_2 - \tau_3 \le 2.42$$

and since this extends well across the zero value, we conclude that the hypothesis of equal drug B and C effects cannot be rejected at the 0.01 level.

Similarly, the 99 percent simultaneous confidence interval for the A and B effect difference is

$$0.08 \le \tau_1 - \tau_2 \le 3.92$$

and it is possible to accept the alternative hypothesis

$$H_1: \quad \tau_1 > \tau_2$$

at the 0.01 level. It might also be of interest to determine whether drug A is different from the average effect of drugs B and C. Here $c_1 = 1$, $c_2 = -\tfrac{1}{2}$, $c_3 = -\tfrac{1}{2}$, and the estimated standard deviation of the estimate of that contrast is

$$\sqrt{0.867(\tfrac{1}{6} + \tfrac{1}{24} + \tfrac{1}{24})} = 0.4653$$

The estimate of the contrast is of course 2.25, and the confidence interval is

$$0.59 \le \tau_1 - \tfrac{1}{2}(\tau_2 + \tau_3) \le 3.91$$

Drug A appears to be distinct from the essentially equivalent remaining drugs.

The Bonferroni simultaneous confidence intervals for the pair-wise contrasts with confidence coefficient at least 0.99 are

$$0.13 \le \tau_1 - \tau_2 \le 3.87$$

$$-1.37 \le \tau_2 - \tau_3 \le 2.37$$

$$0.63 \le \tau_1 - \tau_3 \le 4.37$$

CHAPTER

2

MATRIX ALGEBRA

2.1 INTRODUCTION

In Chap. 3 we shall see that a multidimensional random variable is merely an ordered collection

$$[X_1, \ldots, X_p]$$

of single variates. By "ordered" we mean that the variate describing the ith facet of each sampling unit drawn from the population always appears in the ith position of the sequence. The number of variates p in the array is always specified and will remain unchanged throughout the problem or analysis at hand. For example, suppose that the components of the variate are the weights of female rats in a particular strain at birth and at 10, 20, and 30 days of age. Then the weights could be described by the random variable $[X_1, X_2, X_3, X_4]$ with some distribution in four-dimensional space. If those weights were recorded in a sample of N rats, the observations might be summarized in the array

$$\begin{bmatrix} x_{11} & \cdots & x_{14} \\ \cdots \cdots \cdots \cdots \\ x_{N1} & \cdots & x_{N4} \end{bmatrix}$$

whose rows correspond to different rats. Such linear and rectangular arrangements of numbers are known respectively as *vectors* and *matrices*, and rules for their manipulation constitute that part of linear systems

known as *matrix algebra*. That algebra is the virtual language of multivariate analysis, particularly in its most common and important part based upon the multidimensional normal distribution. Indeed, it is almost inconceivable that the techniques could have been developed without the convenience, facility, and elegance of matrices.

In this chapter we shall summarize a number of properties, operations, and theorems of matrix algebra needed in the sequel. Further results and proofs of certain of the theorems can be found in the references cited at the end of the chapter.

2.2 SOME DEFINITIONS

Let us assume that we have at our disposal some elements which behave according to certain sets of axioms, for example, the real or complex numbers. We define a *matrix*

$$(1) \qquad \mathbf{A} = \begin{bmatrix} a_{11} & \cdots & a_{1c} \\ \cdots\cdots\cdots\cdots \\ a_{r1} & \cdots & a_{rc} \end{bmatrix}$$

as a rectangular ordered array of the elements. The general term of the matrix will be written as a_{ij}, where the first subscript will always refer to the *i*th row, and the second to the *j*th column. The dimensions of a matrix are important, and a matrix with r rows and c columns will be referred to as $r \times c$.

In opposition to a matrix we shall call the usual numbers and variables of everyday unidimensional transactions *scalars*. A scalar is of course a 1×1 matrix. In the initial sections of this chapter we shall think of matrices as composed of real scalar elements. Later we shall treat matrices whose elements are themselves matrices of smaller dimensions.

A *vector* is a matrix with a single row or column. We shall customarily write the *n*-component *column vector*

$$(2) \qquad \mathbf{x} = \begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix}$$

in lowercase boldface type. Similarly, a *row vector*

$$(3) \qquad \mathbf{x}' = [x_1, \ldots, x_n]$$

consists of a single row of n elements. Either vector specifies the coordinates of a point in n-dimensional euclidean space, and the connection with the physical or analytical notion of a vector is immediately apparent if we think of that point as the terminus of a line segment starting from the origin of the coordinate axes.

The prime attached to a row vector means that $\mathbf{x}'$ is the *transpose* of the column vector $\mathbf{x}$. In general, if $\mathbf{A}$ is any $r \times c$ matrix, the transpose of $\mathbf{A}$ is the $c \times r$ matrix $\mathbf{A}'$ formed by interchanging the roles of rows and columns:

$$(4) \qquad \mathbf{A}' = \begin{bmatrix} a_{11} & \cdots & a_{1c} \\ \cdots\cdots\cdots\cdots \\ a_{r1} & \cdots & a_{rc} \end{bmatrix}' = \begin{bmatrix} a_{11} & \cdots & a_{r1} \\ \cdots\cdots\cdots\cdots \\ a_{1c} & \cdots & a_{rc} \end{bmatrix}$$

If a matrix is square and equal to its transpose, it is said to be *symmetric*. Then $a_{ij} = a_{ji}$ for all pairs of i and j. For example,

$$\mathbf{A} = \begin{bmatrix} 3 & 0 & -1 \\ 0 & 1 & 2 \\ -1 & 2 & -4 \end{bmatrix}$$

is symmetric, while

$$\mathbf{B} = \begin{bmatrix} 2 & 3 \\ 1 & 2 \end{bmatrix}$$

is not. For brevity we shall frequently omit the duplicated lower elements. The elements a_{ii} of a square matrix occupy what are called the *main diagonal positions*. The sum of these diagonal elements is called the *trace* of $\mathbf{A}$, and will be denoted by

$$\operatorname{tr} \mathbf{A} = \sum_{i=1}^{n} a_{ii}$$

Certain matrices are particularly important. The *identity* matrix

$$(6) \qquad \mathbf{I} = \begin{bmatrix} 1 & \cdots & 0 \\ \cdots\cdots\cdots \\ 0 & \cdots & 1 \end{bmatrix}$$

is a square matrix with one in each main diagonal position and zeros elsewhere. The $p \times p$ *diagonal matrix*

$$(7) \qquad \mathbf{D}(a_i) = \begin{bmatrix} a_1 & \cdots & 0 \\ \cdots\cdots\cdots \\ 0 & \cdots & a_p \end{bmatrix}$$

has the elements $a_1, \ldots, a_p$ in its main diagonal positions and zeros in all other locations. Some of the a_i may be zero. In the sequel $\operatorname{diag}(\mathbf{A}) = \mathbf{D}(a_{ii})$ will denote the diagonal matrix formed from the square matrix $\mathbf{A}$.

A $p \times p$ *triangular* matrix has the pattern

(8)
$$
\begin{bmatrix}
t_{11} & t_{12} & \cdots & t_{1p} \\
0 & t_{22} & \cdots & t_{2p} \\
\cdots\cdots\cdots\cdots\cdots \\
0 & 0 & \cdots & t_{pp}
\end{bmatrix}
$$

The $r \times c$ *null matrix*

(9)
$$
\mathbf{0} =
\begin{bmatrix}
0 & \cdots & 0 \\
\cdots\cdots\cdots\cdots \\
0 & \cdots & 0
\end{bmatrix}
$$

has zero in each of its positions. Occasionally we shall also need the vector

(10)
$$
\mathbf{j}' = [1, \ldots, 1]
$$

and the matrix

(11)
$$
\mathbf{E} =
\begin{bmatrix}
1 & \cdots & 1 \\
\cdots\cdots\cdots\cdots \\
1 & \cdots & 1
\end{bmatrix}
$$

with unity in every position.

2.3 ELEMENTARY OPERATIONS WITH MATRICES AND VECTORS

The operations of addition, subtraction, and multiplication of ordinary scalar arithmetic can be carried over to matrices if certain rules are followed. The matrix analog of division is a bit more complicated and will be deferred to a later section.

Equality. Two $r \times c$ matrices $\mathbf{A}$ and $\mathbf{B}$ are said to be equal if and only if

(1)
$$
a_{ij} = b_{ij}
$$

for all pairs of i and j.

Addition. The sum of two matrices of like dimensions is the matrix of the sums of the corresponding elements. If

$$
\mathbf{A} =
\begin{bmatrix}
a_{11} & \cdots & a_{1c} \\
\cdots\cdots\cdots\cdots \\
a_{r1} & \cdots & a_{rc}
\end{bmatrix}
\qquad
\mathbf{B} =
\begin{bmatrix}
b_{11} & \cdots & b_{1c} \\
\cdots\cdots\cdots\cdots \\
b_{r1} & \cdots & b_{rc}
\end{bmatrix}
$$

then

$$(2) \qquad \mathbf{A} + \mathbf{B} = \begin{bmatrix} a_{11} + b_{11} & \cdots & a_{1c} + b_{1c} \\ \cdots\cdots\cdots\cdots\cdots\cdots\cdots \\ a_{r1} + b_{r1} & \cdots & a_{rc} + b_{rc} \end{bmatrix}$$

One matrix is subtracted from another of like dimensions by forming the matrix of differences of the individual elements. Thus,

$$\mathbf{A} + \mathbf{B} = \mathbf{B} + \mathbf{A}$$

$$(3) \qquad \mathbf{A} + (\mathbf{B} + \mathbf{C}) = (\mathbf{A} + \mathbf{B}) + \mathbf{C}$$

$$\mathbf{A} - (\mathbf{B} - \mathbf{C}) = \mathbf{A} - \mathbf{B} + \mathbf{C}$$

If the dimensions of the matrices do not conform, their sums or differences are undefined.

Multiplication by a scalar. The matrix $\mathbf{A}$ is multiplied by the scalar c by multiplying each element of $\mathbf{A}$ by c:

$$(4) \qquad c\mathbf{A} = \begin{bmatrix} ca_{11} & \cdots & ca_{1k} \\ \cdots\cdots\cdots\cdots\cdots \\ ca_{r1} & \cdots & ca_{rk} \end{bmatrix}$$

Matrix multiplication. For the matrix product $\mathbf{AB}$ to be defined it is necessary that the number of *columns* of $\mathbf{A}$ be equal to the number of *rows* of $\mathbf{B}$. The dimensions of such matrices are said to be *conformable*. If $\mathbf{A}$ is of dimensions $p \times r$ and $\mathbf{B}$ is $r \times q$, then the ijth element of the product $\mathbf{C} = \mathbf{AB}$ is computed as

$$(5) \qquad c_{ij} = \sum_{k=1}^{r} a_{ik}b_{kj}$$

This is the sum of the products of corresponding elements in the ith row of $\mathbf{A}$ and jth column of $\mathbf{B}$. The dimensions of $\mathbf{AB}$ are of course $p \times q$. For example, if

$$\mathbf{A} = \begin{bmatrix} 1 & 2 & 3 \\ -1 & 0 & 1 \end{bmatrix} \qquad \mathbf{B} = \begin{bmatrix} 6 & 5 & 4 \\ -1 & 1 & -1 \\ 0 & 2 & 0 \end{bmatrix}$$

then

$$\mathbf{AB} = \begin{bmatrix} 1(6) + 2(-1) + 3(0) & 1(5) + 2(1) + 3(2) & 1(4) + 2(-1) + 3(0) \\ -1(6) + 0(-1) + 1(0) & -1(5) + 0(1) + 1(2) & -1(4) + 0(-1) + 1(0) \end{bmatrix}$$

$$= \begin{bmatrix} 4 & 13 & 2 \\ -6 & -3 & -4 \end{bmatrix}$$

The product **BA** is undefined, for the two rows of **A** do not conform with the three columns of **B**.

The distributive and associative laws hold for matrix multiplication:

(6)
$$\mathbf{A}(\mathbf{B} + \mathbf{C}) = \mathbf{AB} + \mathbf{AC}$$
$$\mathbf{A}(\mathbf{BC}) = \mathbf{AB}(\mathbf{C})$$

However, the commutative law does *not* hold for matrix multiplication, and in general it is not true that **AB** = **BA**. For this reason the order of multiplication is crucial, and we shall speak of the product **AB** as formed from *premultiplication* of **B** by **A** or by *postmultiplication* of **A** by **B**. For example, let

$$\mathbf{A} = \begin{bmatrix} 1 & 2 \\ 2 & 3 \end{bmatrix} \qquad \mathbf{B} = \begin{bmatrix} 3 & -1 \\ -1 & 1 \end{bmatrix} \qquad .$$

Then

$$\mathbf{AB} = \begin{bmatrix} 1 & 1 \\ 3 & 1 \end{bmatrix} \qquad \mathbf{BA} = \begin{bmatrix} 1 & 3 \\ 1 & 1 \end{bmatrix}$$

Neither are the products equal, nor is the symmetry of the original matrices preserved in the multiplication.

Multiplication of any matrix by a conformable identity matrix leaves the matrix unchanged. Premultiplication by the diagonal matrix with elements $d_1, \ldots, d_r$ has the effect of multiplying each element in the ith row by d_i:

(7)
$$\mathbf{D}(d_i)\mathbf{A} = \begin{bmatrix} d_1 a_{11} & \cdots & d_1 a_{1c} \\ \cdots\cdots\cdots\cdots \\ d_r a_{r1} & \cdots & d_r a_{rc} \end{bmatrix}$$

Postmultiplication by a similar $c \times c$ diagonal matrix multiplies each element in the jth column by d_j.

A matrix can be regarded as specifying a linear transformation of the vectors in one space to those of another. If **x** has m components and **y** has n components, it is possible to express a transformation from the m-dimensional coordinate system of the elements of **x** to the n-dimensional space of those of **y** in matrix form as

(8)
$$\begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix} = \begin{bmatrix} a_{11} & \cdots & a_{1m} \\ \cdots\cdots\cdots\cdots \\ a_{n1} & \cdots & a_{nm} \end{bmatrix} \begin{bmatrix} x_1 \\ \vdots \\ x_m \end{bmatrix}$$
$$= \mathbf{Ax}$$

Transformation to a third set of variables specified by the p-component

column vector $\mathbf{z}$ could be represented as

$$(9) \qquad\qquad \mathbf{z} = \mathbf{By}$$

$$= \mathbf{BAx}$$

and thus the product of two or more matrices can be thought of as the matrix of the resultant of a succession of linear transformations.

> **Example 2.1.** It is often necessary in the social sciences to convert several disparate scores collected on individuals to a scale with a common origin and unit. If x_{ij} is the score of the ith individual on the jth measure and $\bar{x}_j$ and s_j are the sample mean and standard deviation of that measure, one common transformation is the *z score*
>
> $$z_{ij} = \frac{x_{ij} - \bar{x}_j}{s_j}$$
>
> The transformed observations can be computed conveniently by some simple matrix operations. Write the original scores as the $N \times p$ *data matrix*
>
> $$\mathbf{X} = \begin{bmatrix} x_{11} & \cdots & x_{1p} \\ \cdots & \cdots & \cdots \\ x_{N1} & \cdots & x_{Np} \end{bmatrix}$$
>
> and form the diagonal matrix
>
> $$\mathbf{D} = \begin{bmatrix} \dfrac{1}{s_1} & \cdots & 0 \\ \cdots & \cdots & \cdots \\ 0 & \cdots & \dfrac{1}{s_p} \end{bmatrix}$$
>
> from the sample standard deviations. If we introduce the $N \times N$ matrix
>
> $$\mathbf{E} = \begin{bmatrix} 1 & \cdots & 1 \\ \cdots & \cdots & \cdots \\ 1 & \cdots & 1 \end{bmatrix}$$
>
> with one in every position, the $N \times p$ matrix $\mathbf{Z}$ of standard scores can be computed as
>
> $$\mathbf{Z} = \left(\mathbf{I} - \frac{1}{N}\mathbf{E}\right)\mathbf{XD}$$
>
> Postmultiplication of $\mathbf{E}$ by $\mathbf{X}$ has the effect of summing each column of the data matrix.

Vector inner products. The inner product of two vectors with the same number of elements is defined to be the sum of the products of the

corresponding elements:

$$(10) \qquad \mathbf{x'y} = [x_1, \ldots, x_p] \begin{bmatrix} y_1 \\ \vdots \\ y_p \end{bmatrix}$$

$$= \sum_{i-1}^{p} x_i y_i$$

Since the inner product is a scalar, $\mathbf{x'y} = \mathbf{y'x}$. The inner product of $\mathbf{x}$ with itself is the sum of squares of the elements of $\mathbf{x}$.

Inner products have important geometrical interpretations. The inner product of $\mathbf{x}$ with itself is called the *squared length* of $\mathbf{x}$, for it is the square of the distance from the origin of the p-dimensional coordinate system to the point specified by the elements of $\mathbf{x}$. More generally, the distance between the points with coordinates given by $\mathbf{x}$ and $\mathbf{y}$ is

$$(11) \qquad d = \left[\sum_{i=1}^{p} (x_i - y_i)^2 \right]^{1/2}$$

The cosine of the angle θ between the vectors $\mathbf{x}$ and $\mathbf{y}$ is

$$(12) \qquad \cos \theta = \frac{\mathbf{x'y}}{(\mathbf{x'x})^{1/2}(\mathbf{y'y})^{1/2}}$$

Such division of the vectors by their respective lengths is called *normalization*, and it is easy to see that as the normalized vectors become coincident, their inner product tends to unity. Similarly, vectors at right angles to each other have an inner product of zero.

Example 2.2. In three-dimensional space the vectors

$$\mathbf{x'} = [1, 0, 0]$$
$$\mathbf{y'} = [0, 1, 0]$$
$$\mathbf{z'} = [0, 0, 1]$$

can be construed as specifying the three coordinate axes. The vector

$$\mathbf{e'} = [1, 1, 1]$$

makes an angle with the same cosine $\sqrt{3}/3$ with $\mathbf{x'}$, $\mathbf{y'}$, and $\mathbf{z'}$ and characterizes the *equiangular* line in three-space. The numbers $\sqrt{3}/3$ are called the *direction cosines* of the line. Similarly, the vectors

$$\mathbf{u'} = [1, 1, 0]$$
$$\mathbf{v'} = [1, -1, 0]$$

make an angle of 90° in the *xy* plane of the space. $\mathbf{u'}$ and $\mathbf{v'}$ each have an angle of 45° with $\mathbf{x'}$, and their angles with $\mathbf{y'}$ are 45 and −45°, respectively.

Transpose of a matrix product. If the matrix **A** is conformable for postmultiplication by another matrix **B**, it is easily verified that the transpose of their product is equal to the product of their transposes taken in the opposite order:

(13) $$(\mathbf{AB})' = \mathbf{B}'\mathbf{A}'$$

More generally, if $\mathbf{A}_1, \ldots, \mathbf{A}_k$ are conformable,

(14) $$(\mathbf{A}_1 \cdots \mathbf{A}_k)' = \mathbf{A}'_k \cdots \mathbf{A}'_1$$

We shall need these properties frequently in the later chapters.

2.4   THE DETERMINANT OF A SQUARE MATRIX

Associated with every square matrix is a unique scalar number called its *determinant*. The formal definition of the determinant of the $n \times n$ matrix **A** is the sum

(1) $$\sum_P \cdots \sum (-1)^{\alpha} a_{1j_1} a_{2j_2} \cdots a_{nj_n}$$

of all products consisting of one element from each row and column and multiplied by -1 if the number of inversions of the particular permutation $j_1 j_2 \cdots j_n$ from the standard order $1, 2, \ldots, n$ is odd. The sum is taken over the set P of all $n!$ permutations of the column subscripts. The number of inversions α in a particular permutation is the total number of times in which an element is followed by numbers which would ordinarily precede it in the standard order $1, 2, \ldots, n$.

The determinant of **A** will be written as $|\mathbf{A}|$. The determinants of the three smallest square matrices follow from the formal definition as

$$|a_{11}| = a_{11}$$

(2) $$\begin{vmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{vmatrix} = a_{11}a_{22} - a_{12}a_{21}$$

$$\begin{vmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{vmatrix} = \begin{matrix} a_{11}a_{22}a_{33} + a_{12}a_{23}a_{31} + a_{13}a_{21}a_{32} \\ -a_{13}a_{22}a_{31} - a_{11}a_{23}a_{32} - a_{12}a_{21}a_{33} \end{matrix}$$

It is more convenient to compute the determinants of larger matrices by different methods. Define the *minor* of the element a_{ij} of **A** as the determinant of the matrix formed by deleting the ith row and jth column of **A**. The *cofactor* of a_{ij} is the minor multiplied by $(-1)^{i+j}$ and will be written as A_{ij}. It can be shown that the determinant of the square matrix **A** can be expressed in terms of the cofactors of the elements of any given

row or column as

(3) $$\mathbf{|A|} = a_{i1}A_{i1} + \cdots + a_{in}A_{in} \qquad i = 1, \ldots, n$$
$$= a_{1j}A_{1j} + \cdots + a_{nj}A_{nj} \qquad j = 1, \ldots, n$$

For the simplest application of this rule we note that the matrix of cofactors for the general 2×2 matrix is

(4) $$\begin{bmatrix} a_{22} & -a_{21} \\ -a_{12} & a_{11} \end{bmatrix}$$

and the value of the determinant follows immediately.

Example 2.3. Let us evaluate the determinant of the matrix

$$\begin{bmatrix} 3 & 0 & 0 & 0 \\ 1 & 2 & 0 & 1 \\ -1 & -3 & 2 & -1 \\ 5 & 4 & 3 & 2 \end{bmatrix}$$

Note immediately that the first row contains a single nonzero element, so that it will be necessary to compute the cofactor only of the (1,1) element. If we expand that cofactor in terms of the cofactors of its first row, the original determinant is equal to

$$3\left(2\begin{vmatrix} 2 & -1 \\ 3 & 2 \end{vmatrix} - 0\begin{vmatrix} -3 & -1 \\ 4 & 2 \end{vmatrix} + 1\begin{vmatrix} -3 & 2 \\ 4 & 3 \end{vmatrix}\right) = -9$$

The method of cofactors is efficient only for small matrices or for patterned matrices with an abundance of zero elements. We shall consider a more practical technique in Sec. 2.6.

Certain properties of determinants will prove to be useful in the later chapters:

1. The determinant of a diagonal matrix is merely the product of the diagonal elements. Similarly, the determinant of a triangular matrix is the product of its diagonal elements.

2. If the elements of a single row or column of the $n \times n$ matrix $\mathbf{A}$ are multiplied by the scalar c, the determinant of the new matrix is equal to $c |\mathbf{A}|$. If every element is multiplied by c, then $|c\mathbf{A}| = c^n |\mathbf{A}|$.

3. If two columns (or rows) of a square matrix are interchanged, the sign of the determinant is reversed.

4. It follows directly from Property 3 that if two columns or two rows of a matrix are equal, the determinant must be zero. Thus, proportional rows or columns of a matrix indicate a determinant of zero.

5. The determinant of a matrix is unchanged by adding a multiple of some column to another column. A similar result holds for rows.

6. If all elements of a row or column of a square matrix are zero, the determinant is zero.

7. If **A** and **B** are each $n \times n$ matrices, the determinant of **AB** is equal to the product of the individual determinants.

8. The sum of the products of the elements of a given row of a square matrix with the corresponding cofactors of a *different* row is equal to zero. A similar result holds for columns.

2.5 THE INVERSE MATRIX

We are now ready to define the matrix analog of scalar division. The *inverse* of the square matrix **A** is that unique matrix $\mathbf{A}^{-1}$ with elements such that

(1) $$\mathbf{A}\mathbf{A}^{-1} = \mathbf{A}^{-1}\mathbf{A} = \mathbf{I}$$

It is possible that $\mathbf{A}^{-1}$ does not exist, just as it is not possible to perform scalar division by zero. Then **A** is said to be *singular*. Matrices whose inverses exist are called *nonsingular*.

The elements of $\mathbf{A}^{-1}$ can be computed from two results of the previous section. Form the matrix of cofactors

(2) $$\mathbf{C} = \begin{bmatrix} A_{11} & \cdots & A_{1n} \\ \cdots & \cdots & \cdots \\ A_{n1} & \cdots & A_{nn} \end{bmatrix}$$

called the *adjoint* of **A**. Then the inner product of the ith row of **C** and the hth row of **A** is equal to $|\mathbf{A}|$ if $i = h$ and to zero if $i \neq h$. If we take the transpose of **C** and divide each element by $|\mathbf{A}|$, we have the desired inverse

(3) $$\mathbf{A}^{-1} = \begin{bmatrix} \dfrac{1}{|\mathbf{A}|}A_{11} & \cdots & \dfrac{1}{|\mathbf{A}|}A_{n1} \\ \cdots & \cdots & \cdots \\ \dfrac{1}{|\mathbf{A}|}A_{1n} & \cdots & \dfrac{1}{|\mathbf{A}|}A_{nn} \end{bmatrix}$$

It should be apparent from this definition that the inverse exists if and only if $|\mathbf{A}|$ is not zero. Computation of $\mathbf{A}^{-1}$ by cofactors is very inefficient in most practical applications, and we shall consider other methods in Sec. 2.6.

We shall frequently use these properties of inverses:

1. The inverse of a symmetric matrix is also symmetric.
2. The inverse of the transpose of **A** is the transpose of $\mathbf{A}^{-1}$.

3. The inverse of the product of several square matrices is equal to the product of the inverses in reverse order:

(4)
$$(\mathbf{ABC})^{-1} = \mathbf{C}^{-1}\mathbf{B}^{-1}\mathbf{A}^{-1}$$

4. If c is a nonzero scalar, $(c\mathbf{A})^{-1} = 1/c\mathbf{A}^{-1}$.
5. The inverse of a diagonal matrix is a diagonal matrix consisting of the reciprocals of the original elements.

Example 2.4. The inverse of

$$\mathbf{A} = \begin{bmatrix} 2 & 0 & 0 & 0 \\ 0 & 4 & 0 & 0 \\ 0 & 0 & 3 & 2 \\ 0 & 0 & 1 & 2 \end{bmatrix}$$

is

$$\mathbf{A}^{-1} = \begin{bmatrix} \frac{1}{2} & 0 & 0 & 0 \\ 0 & \frac{1}{4} & 0 & 0 \\ 0 & 0 & \frac{1}{2} & -\frac{1}{2} \\ 0 & 0 & -\frac{1}{4} & \frac{3}{4} \end{bmatrix}$$

2.6   THE RANK OF A MATRIX

Two p-component vectors are said to be *linearly dependent* if the elements of one vector are proportional to those of the second. Thus, the row vectors

$$\mathbf{x}' = [1, 0, -1] \qquad \mathbf{y}' = [4, 0, -4]$$

are linearly dependent, while

$$\mathbf{u}' = [2, -1, 0, 7] \qquad \mathbf{v}' = [6, 2, 0, 0]$$

are linearly independent. A set of k vectors of equal dimensions is called linearly independent if it is impossible to write any vector of the set as some linear combination of the remaining vectors. That is, the vectors $\mathbf{x}_1, \ldots, \mathbf{x}_k$ form a linearly independent set if there do not exist scalars $c_1, \ldots, c_k$ such that for some vector $\mathbf{x}_i$ in the set

$$c_i\mathbf{x}_i = c_1\mathbf{x}_1 + \cdots + c_{i-1}\mathbf{x}_{i-1} + c_{i+1}\mathbf{x}_{i+1} + \cdots + c_k\mathbf{x}_k$$

The vectors

$$\mathbf{x}' = [1, -1, 2] \qquad \mathbf{y}' = [2, 0, -1] \qquad \mathbf{z}' = [0, -2, 5]$$

constitute a linearly dependent set, for $\mathbf{z}' = 2\mathbf{x}' - \mathbf{y}'$, while the unit vectors

$$\mathbf{t}' = [1, 0, 0] \qquad \mathbf{u}' = [0, 1, 0] \qquad \mathbf{v}' = [0, 0, 1]$$

are independent.

Example 2.5. Suppose that a cognitive test consists of six subscales. The first three measure certain verbal facilities, and their scores are summed to give what is called the *verbal score*. The last three reflect some motor and spatial skills, and their total is called the *performance score*. Finally, the sum of the six tests is used as a general measure of cognitive ability. The test has been administered to a large number of subjects, and it is proposed that the nine scores be used in an attempt to relate intelligence to other measures obtained on the individuals. However, if each sample of observations on a score is regarded as an *N*-component vector, it is immediately apparent that only six of the nine vectors are linearly independent, and no new information has been gained from the three derived scores. We shall see in the later chapters that the inclusion of these linear compounds may preclude certain kinds of statistical analyses.

Now let us formalize the degree of linear independence in a set of vectors as the *rank* of the matrix formed from the vectors. Assume for the moment that the number of vectors k does not exceed the dimensionality p of the vectors. Then the rank of

$$(1) \qquad \mathbf{X} = \begin{bmatrix} \mathbf{x}_1' \\ \vdots \\ \mathbf{x}_k' \end{bmatrix}$$

is the number of linearly independent row vectors in the matrix. Rank may vary from zero for any null matrix to k for a matrix of *full rank*. If, on the other hand, the number of rows in $\mathbf{X}$ exceeded the number of columns, the rank of $\mathbf{X}$ would be the number of linearly independent columns. In either case, it can be shown that the rank of the matrix is a unique number, regardless of whether it is computed from rows or columns. It follows from Property 4 of Sec. 2.4 that

the matrix $\mathbf{A}$ *is of rank r if it contains at least one nonzero r $\times$ r minor, and no nonzero minor of dimensionality greater than r.*

Example 2.6. The matrix

$$\begin{bmatrix} 1 & 2 & 3 & 4 \\ 3 & 6 & 9 & 12 \\ 4 & 3 & 2 & 1 \\ -1 & 3 & 7 & 11 \\ 8 & 6 & 4 & 2 \end{bmatrix}$$

has rank two, for it can be shown that the second row is equal to three times the first row, row four is equal to the difference of rows two and three, and row five is twice the third row. The only linearly independent rows are the first and third, and these are said to form a *basis* for the five row vectors.

Rank has these important properties:

1. The rank of $\mathbf{A}'$ is equal to that of $\mathbf{A}$. This follows from the equivalence of the row and column definitions of rank.
2. The rank of $\mathbf{A}'\mathbf{A}$ is equal to that of $\mathbf{A}$. Similarly, the rank of $\mathbf{A}\mathbf{A}'$ is equal to the rank of $\mathbf{A}$.
3. The rank of $\mathbf{A}$ is unchanged by pre- or postmultiplication of $\mathbf{A}$ by a nonsingular matrix.

Elementary row and column operations. The rank of a matrix is unchanged by these *elementary row and column operations*:

1. Interchange of any two rows (columns).
2. Multiplication of each element of a row (column) by a scalar constant.
3. Addition of a row (column) whose elements have been multiplied by a scalar constant to another row (column).

These transformations can be represented by nonsingular matrices. Row operations are performed by premultiplication of the given matrix by the elementary operation matrix, while column operations follow from postmultiplication. By Property 3 of the preceding paragraph such nonsingular transformations leave the rank invariant. By choosing the proper sequence of row or column operations we can reduce a matrix to a form consisting only of linearly independent rows or columns, and thereby determine its rank.

Example 2.7. The matrices

$$\mathbf{E}_1 = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} \qquad \mathbf{E}_2 = \begin{bmatrix} c & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \qquad \mathbf{E}_3 = \begin{bmatrix} 1 & 0 & 0 \\ d & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

can be used to make elementary transformations on the first two rows of

$$\mathbf{A} = \begin{bmatrix} 5 & 1 \\ -2 & 3 \\ 3 & 2 \end{bmatrix}$$

giving

$$\mathbf{E}_1\mathbf{A} = \begin{bmatrix} -2 & 3 \\ 5 & 1 \\ 3 & 2 \end{bmatrix} \qquad \mathbf{E}_2\mathbf{A} = \begin{bmatrix} 5c & c \\ -2 & 3 \\ 3 & 2 \end{bmatrix} \qquad \mathbf{E}_3\mathbf{A} = \begin{bmatrix} 5 & 1 \\ 5d - 2 & d + 3 \\ 3 & 2 \end{bmatrix}$$

Example 2.8. Let us use elementary row operations to compute the rank of the matrix

$$\mathbf{A} = \begin{bmatrix} 1 & 0 & 2 \\ -3 & 2 & 1 \\ -1 & 2 & 5 \\ 3 & 0 & 6 \end{bmatrix}$$

Note immediately that the last row is equal to the first row multiplied by 3. Row three is equal to row two plus twice row one. The appropriate row operations reduce **A** successively to

$$
\begin{bmatrix} 1 & 0 & 2 \\ -3 & 2 & 1 \\ -1 & 2 & 5 \\ 0 & 0 & 0 \end{bmatrix} \quad \text{and} \quad \begin{bmatrix} 1 & 0 & 2 \\ -3 & 2 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}
$$

Since the remaining rows are linearly independent, we conclude that **A** is of rank two.

Both row and column operations can be applied simultaneously to any $m \times n$ matrix to reduce it to its *canonical form*

$$
\text{(2)} \qquad \mathbf{F} = \begin{bmatrix} 1 & \cdots & 0 & \cdots & 0 \\ \cdots\cdots\cdots\cdots\cdots\cdots \\ 0 & \cdots & 1 & \cdots & 0 \\ \cdots\cdots\cdots\cdots\cdots\cdots \\ 0 & \cdots & 0 & \cdots & 0 \end{bmatrix}
$$

of one in the first r diagonal positions and zero everywhere else. This means that for every matrix **A** there exist elementary row and column transformation matrices $\mathbf{R}_1, \ldots, \mathbf{R}_p, \mathbf{C}_1, \ldots, \mathbf{C}_q$ such that

$$
\text{(3)} \qquad \mathbf{R}_p \cdots \mathbf{R}_1 \mathbf{A} \mathbf{C}_1 \cdots \mathbf{C}_q = \mathbf{PAQ}
$$
$$
= \mathbf{F}
$$

is the canonical form of **A**. *But* if **A** is square and of full rank n, then row operations alone produce

$$
\text{(4)} \qquad \mathbf{R}_p \cdots \mathbf{R}_1 \mathbf{A} = \mathbf{I}
$$

and

$$
\text{(5)} \qquad \mathbf{A}^{-1} = \mathbf{R}_p \cdots \mathbf{R}_1 \mathbf{I}
$$

Hence, the *same* sequence of elementary row operations that reduces **A** to the identity matrix transforms the $n \times n$ identity matrix to the inverse of **A**. This property of elementary transformations provides us with a powerful tool for inverting matrices: we merely write down the $n \times 2n$ matrix

$$
\text{(6)} \qquad\qquad\qquad [\mathbf{A} \quad \mathbf{I}]
$$

and apply elementary operations to each row with the aim of transforming the first n columns to the identity matrix. When this has been accomplished, $\mathbf{A}^{-1}$ will appear in the last n columns. For symmeric matrices this method had been formalized as the abbreviated Gauss-Doolittle technique (Dwyer, 1951).

Example 2.9. The successive transformations in the inversion of

$$A = \begin{bmatrix} 1 & 1 & 2 \\ 2 & 3 & 3 \\ 3 & -1 & 8 \end{bmatrix}$$

are shown below:

$$\begin{bmatrix} 1 & 1 & 2 & 1 & 0 & 0 \\ 2 & 3 & 3 & 0 & 1 & 0 \\ 3 & -1 & 8 & 0 & 0 & 1 \end{bmatrix}$$

$$\begin{bmatrix} 1 & 1 & 2 & 1 & 0 & 0 \\ 0 & 1 & -1 & -2 & 1 & 0 \\ 0 & -4 & 2 & -3 & 0 & 1 \end{bmatrix}$$

$$\begin{bmatrix} 1 & 0 & 3 & 3 & -1 & 0 \\ 0 & 1 & -1 & -2 & 1 & 0 \\ 0 & 0 & -2 & -11 & 4 & 1 \end{bmatrix}$$

$$\begin{bmatrix} 1 & 0 & 0 & -13.5 & 5 & 1.5 \\ 0 & 1 & 0 & 3.5 & -1 & -0.5 \\ 0 & 0 & 1 & 5.5 & -2 & -0.5 \end{bmatrix}$$

and

$$A^{-1} = \begin{bmatrix} -13.5 & 5 & 1.5 \\ 3.5 & -1 & -0.5 \\ 5.5 & -2 & -0.5 \end{bmatrix}$$

The determinant of a matrix can also be computed by elementary row or column operations, for by Property 5 of Sec. 2.4 those transformations do not alter its value. The process, called *pivotal condensation*, consists of reducing the matrix to triangular form, from which the determinant is computed as the product of the diagonal elements. If row operations are used, the matrix is written with the largest element of the first column in the (1,1) position. That element is used as the pivot for reducing the remaining elements of the column to zero. This rearrangment and reduction is continued until the triangular form is attained. Choice of the greatest element is in the interests of numerical accuracy.

Example 2.10. Let us evaluate the determinant of the matrix

$$A = \begin{bmatrix} 10 & 5 & -2 & 0 \\ 6 & 3 & 2 & 1 \\ 4 & 5 & 12 & 3 \\ 5 & 1 & 3 & 8 \end{bmatrix}$$

We begin by subtracting appropriate multiples of the first row from the remaining rows:

$$\begin{bmatrix} 10 & 5 & -2 & 0 \\ 0 & 0 & 3.2 & 1 \\ 0 & 3 & 12.8 & 3 \\ 0 & -1.5 & 4 & 8 \end{bmatrix}$$

Since the (2,2) element is zero, we interchange the second and third rows of the matrix, and compensate for the resulting change of sign in the determinant by multiplying each element of the new second row by -1:

$$\begin{bmatrix} 10 & 5 & -2 & 0 \\ 0 & -3 & -12.8 & -3 \\ 0 & 0 & 3.2 & 1 \\ 0 & -1.5 & 4 & 8 \end{bmatrix}$$

A single row operation in the second column transforms this to

$$\begin{bmatrix} 10 & 5 & -2 & 0 \\ 0 & -3 & -12.8 & -3 \\ 0 & 0 & 3.2 & 1 \\ 0 & 0 & 10.4 & 9.5 \end{bmatrix}$$

Finally we have

$$\begin{bmatrix} 10 & 5 & -2 & 0 \\ 0 & -3 & -12.8 & -3 \\ 0 & 0 & 3.2 & 1 \\ 0 & 0 & 0 & 6.25 \end{bmatrix}$$

and the determinant is

$$|\mathbf{A}| = (10)(-3)(3.2)(6.25)$$
$$= -600$$

Generalized inverse matrices. Several generalizations of the inverse matrix have been proposed for rectangular matrices of any rank. One generalized inverse that is useful for solving systems of linear equations is defined as the matrix $\mathbf{G}$ satisfying

(7) $$\mathbf{AGA} = \mathbf{A}$$

$\mathbf{A}$ is $p \times q$ and of rank r, while $\mathbf{G}$ is necessarily $q \times p$ and of the same rank as $\mathbf{A}$. Other kinds of generalized inverses exist, e.g., those due to Penrose (1955) which satisfy the additional conditions

(8) $$\mathbf{GAG} = \mathbf{G} \quad (\mathbf{GA})' = \mathbf{GA} \quad (\mathbf{AG})' = \mathbf{AG}$$

Their properties have been discussed at length by Graybill (1983), Searle

(1966, 1971), and Searle and Hausman (1970); more advanced treatments have been written by Albert (1972), Boullion and Odell (1971), and Rao and Mitra (1971). However, the restricted form defined by (7) will suffice for our purposes.

Our matrix **G** can be computed from the canonical reduction (3) of **A**. We write

$$(9) \qquad \mathbf{PAQ} = \begin{bmatrix} \mathbf{D} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix}$$

where **D** is an $r \times r$ diagonal matrix (not necessarily the identity) and the null matrices have appropriate dimensions. **P** and **Q** are the respective products defined in (3) of the row and column elementary matrices. We introduce the $q \times p$ matrix

$$(10) \qquad \mathbf{F}^{-1} = \begin{bmatrix} \mathbf{D}^{-1} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix}$$

Then $\mathbf{G} = \mathbf{QF}^-\mathbf{P}$ is a generalized inverse of the matrix **A**, as one may verify by replacing **A** in (7) by its representation $\mathbf{P}^{-1}\mathbf{FQ}^{-1}$. **G** is not a unique matrix, unless of course **A** is square and nonsingular.

> **Example 2.11.** Let us find a generalized inverse of the matrix **A** in Example 2.8. The row operator matrices which reduce the third and fourth rows to null vectors are
>
> $$\mathbf{R}_1 = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ -3 & 0 & 0 & 1 \end{bmatrix} \qquad \mathbf{R}_2 = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ -2 & -1 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$
>
> Then
>
> $$\mathbf{P} = \mathbf{R}_2\mathbf{R}_1 = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ -2 & -1 & 1 & 0 \\ -3 & 0 & 0 & 1 \end{bmatrix}$$
>
> The column transformations which reduce **PA** to a diagonal canonical form are
>
> $$\mathbf{C}_1 = \begin{bmatrix} 1 & 0 & 0 \\ \frac{3}{2} & 1 & -\frac{1}{2} \\ 0 & 0 & 1 \end{bmatrix} \qquad \mathbf{C}_2 = \begin{bmatrix} 1 & 0 & -2 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$
>
> and
>
> $$\mathbf{Q} = \mathbf{C}_1\mathbf{C}_2 = \begin{bmatrix} 1 & 0 & -2 \\ \frac{3}{2} & 1 & -\frac{7}{2} \\ 0 & 0 & 1 \end{bmatrix}$$

Then

$$\mathbf{F} = \mathbf{PAQ} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \qquad \mathbf{F} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

and

$$\mathbf{G} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ \frac{3}{2} & \frac{1}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

is one generalized inverse of $\mathbf{A}$.

2.7 SIMULTANEOUS LINEAR EQUATIONS

The set of equations in the unknowns $x_1, \ldots, x_n$

$$a_{11}x_1 + \cdots + a_{1n}x_n = c_1$$

(1)
$$\cdots \cdots \cdots \cdots \cdots$$

$$a_{m1}x_1 + \cdots + a_{mn}x_n = c_m$$

is called *a system of m-simultaneous linear equations in n unknowns* and can be compactly written in matrix form as

(2) $$\mathbf{Ax} = \mathbf{c}$$

where $\mathbf{A}$ is the $m \times n$ matrix of the coefficients, $\mathbf{x}' = [x_1, \ldots, x_n]$, and $\mathbf{c}' = [c_1, \ldots, c_m]$. The general system $\mathbf{Ax} = \mathbf{c}$ of m equations in n unknowns possesses a solution if and only if the $m \times (n + 1)$ *augmented matrix*

$$[\mathbf{A} \quad \mathbf{c}]$$

is of the same rank r as $\mathbf{A}$. Otherwise the system is said to be inconsistent. It is essential to distinguish between homogeneous systems, for which $\mathbf{c} = \mathbf{0}$, and nonhomogeneous systems. We shall consider three types of equations that are particularly relevant for our purposes.

Nonhomogeneous system: A square and nonsingular. Since $\mathbf{A}^{-1}$ exists, the unique solution to the system is

(3) $$\mathbf{x} = \mathbf{A}^{-1}\mathbf{c}$$

This follows from premultiplying both sides of equation (1) by $\mathbf{A}^{-1}$.

Example 2.12. The inverse matrix of the system

$$x_1 + x_2 - x_3 = 1$$
$$-x_1 + x_2 + x_3 = -1$$
$$x_1 - x_2 + x_3 = 1$$

is

$$\begin{bmatrix} \frac{1}{2} & 0 & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} & 0 \\ 0 & \frac{1}{2} & \frac{1}{2} \end{bmatrix}$$

The solution is

$$x_1 = \tfrac{1}{2}(1) + 0(-1) + \tfrac{1}{2}(1)$$
$$= 1$$
$$x_2 = \tfrac{1}{2}(1) + \tfrac{1}{2}(-1) + 0(1)$$
$$= 0$$
$$x_3 = 0(1) + \tfrac{1}{2}(-1) + \tfrac{1}{2}(1)$$
$$= 0$$

Nonhomogeneous system: A $m \times n$ and of rank r. If the condition on the ranks of the coefficient and augmented matrices is satisfied, a solution may be found by selecting any r linearly independent equations and solving for r of the n unknowns in terms of the constants c_i and the remaining $n - r$ variables.

Example 2.13. The equations

$$x_1 + x_2 = 2$$
$$x_1 + x_2 = 1$$

can be interpreted geometrically as defining parallel lines in the $x_1 x_2$ plane. Since they do not intersect, the system cannot have a solution. The rank of the coefficient matrix

$$\begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}$$

is one, while that of the augmented matrix

$$\begin{bmatrix} 1 & 1 & 2 \\ 1 & 1 & 1 \end{bmatrix}$$

is two.

Example 2.14. The system

$$2x_1 + 3x_2 - x_3 = 1$$
$$x_2 + x_3 = 2$$

has coefficient and augmented matrices of rank two. Write the equations as

$$2x_1 + 3x_2 = 1 + x_3$$

$$x_2 = 2 - x_3$$

and solve for x_1 by substitution. The general solution is given by the vector

$$[\tfrac{1}{2}(-5 + 4x_3), 2 - x_3, x_3]$$

wherein x_3 can assume any value.

Homogeneous systems of equations. It is not possible for a homogeneous system of linear equations to be inconsistent, for the rank of $[\mathbf{A} \quad \mathbf{0}]$ is the same as that of $\mathbf{A}$. Every homogeneous system is satisfied by the trivial null solution $\mathbf{x}' = [0, \ldots, 0]$, and in fact if the rank of the coefficient matrix is equal to the number of unknowns n, this is the *only* solution. Hence a homogeneous system will have a nontrivial solution if and only if the rank r of $\mathbf{A}$ is strictly less than n, and it is always possible to find $n - r$ *linearly independent* solutions of the system such that any linear combination of these solutions is itself a solution. In statistical applications we shall frequently encounter systems with as many unknowns as equations; such systems have nontrivial solutions if and only if their coefficient determinants vanish.

Example 2.15. The system

$$3x_1 - 2x_2 = 0$$

$$5x_1 + x_2 = 0$$

defines two lines in the x_1x_2 plane that intersect at the origin. Hence the only solution is the trivial one $[0,0]$.

Example 2.16. In the system

$$x_1 - x_2 + 2x_3 = 0$$

$$x_1 + 3x_2 - 2x_3 = 0$$

$$3x_1 + x_2 + 2x_3 = 0$$

the third equation is equal to the sum of twice the first plus the second, and the rank is thus two. The single independent solution may be determined in units of x_3 by solving the system

$$x_1 - x_2 = -2x_3$$

$$x_1 + 3x_2 = 2x_3$$

The general solution for the original set is, in units of x_3,

$$x_1 = -x_3$$

$$x_2 = x_3$$

Example 2.17. The system

$$
\begin{aligned}
x_1 + x_2 - x_3 - x_4 &= 0 \\
-2x_2 + 3x_3 + x_4 &= 0 \\
x_1 - x_2 + 2x_3 &= 0 \\
3x_1 + x_2 \quad\quad - 2x_4 &= 0
\end{aligned}
$$

is also of rank two. The first and third equations can be solved conveniently in terms of x_3 and x_4 to give the solution vector

$$[\tfrac{1}{2}(-x_3 + x_4), \tfrac{1}{2}(3x_3 + x_4), x_3, x_4]$$

If we set x_3 equal to zero and x_4 equal to one, and alternatively set x_3 to unity and x_4 to zero, we shall have these *linearly independent* values of the solution vector:

$$[\tfrac{1}{2}, \tfrac{1}{2}, 0, 1]$$

$$[-\tfrac{1}{2}, \tfrac{3}{2}, 1, 0]$$

Since any linear combination of these solutions is also a solution, the most general solution to the original system is

$$
\begin{aligned}
x_1 &= \tfrac{1}{2}(a - b) \\
x_2 &= \tfrac{1}{2}(a + 3b) \\
x_3 &= b \\
x_4 &= a
\end{aligned}
$$

for arbitrary a and b.

Solution by generalized inverses. Rao (1962) has shown that the system $\mathbf{Ax} = \mathbf{c}$ of m consistent equations in n unknowns has the solution

(4) $$\mathbf{x}^* = \mathbf{Gc} + (\mathbf{GA} - \mathbf{I})\mathbf{z}$$

where $\mathbf{G}$ is a generalized inverse of $\mathbf{A}$ defined by equation (7) of Sec. 2.6, $\mathbf{I}$ is the $n \times n$ identity matrix, and $\mathbf{z}$ is any $n \times 1$ vector of arbitrary constants. We note that the term containing $\mathbf{z}$ vanishes when $\mathbf{G} = \mathbf{A}^{-1}$. The algebraic properties, computing methods, and illustrations of such solutions have been treated by Basilevsky (1983), Graybill (1983), and Searle (1971, 1982).

Example 2.18. We shall obtain solutions to the equations of Examples 2.14 and 2.16 by the method of generalized inverses. For the first system, $\mathbf{P} = \mathbf{I}$ and

$$
\mathbf{Q} = \begin{bmatrix} 1 & -\tfrac{3}{2} & 2 \\ 0 & 1 & -1 \\ 0 & 0 & 1 \end{bmatrix} \quad
\mathbf{F} = \begin{bmatrix} 2 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix}
$$

$$
\mathbf{G} = \begin{bmatrix} \tfrac{1}{2} & -\tfrac{3}{2} \\ 0 & 1 \\ 0 & 0 \end{bmatrix} \quad
\mathbf{GA} = \begin{bmatrix} 1 & 0 & -2 \\ 0 & 1 & 1 \\ 0 & 0 & 0 \end{bmatrix}
$$

The most general solution is

$$\mathbf{x}' = [-\tfrac{1}{2}(5 + 4z_3), 2 + z_3, -z_3]$$

For Example 2.16,

$$\mathbf{P} = \begin{bmatrix} 1 & 0 & 0 \\ -1 & 1 & 0 \\ -2 & -1 & 1 \end{bmatrix} \qquad \mathbf{Q} = \begin{bmatrix} 1 & 1 & -1 \\ 0 & 1 & 1 \\ 0 & 0 & 1 \end{bmatrix} \qquad \mathbf{F}^- = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \tfrac{1}{4} & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

$$\mathbf{G} = \begin{bmatrix} \tfrac{3}{4} & \tfrac{1}{4} & 0 \\ -\tfrac{1}{4} & \tfrac{1}{4} & 0 \\ 0 & 0 & 0 \end{bmatrix} \qquad \mathbf{GA} = \begin{bmatrix} 1 & 0 & 1 \\ 0 & 1 & -1 \\ 0 & 0 & 0 \end{bmatrix}$$

If we let z_3 equal $-x_3$ the general solution is $\mathbf{x}' = [-x_3, x_3, x_3]$.

Numerical methods for linear equations. Perhaps the most common direct means of solving a system of rank r in r unknowns is the Gauss-Doolittle elimination method. As we have indicated before, this technique amounts to reduction of the system to triangular form by elementary row operations, followed by a backward solution of the new equations until all unknowns have been obtained. The usual form of the scheme supposes a symmetric coefficient matrix, but generalized procedures are also available. The reader is referred to Dwyer (1951), Faddeeva (1959), Graybill (1961), and Ralston and Rabinowitz (1978) for discussion and worked examples of the Gauss-Doolittle method.

Another efficient direct solution is the square-root method. If the original system has been reduced to a square nonhomogeneous form $\mathbf{Ax} = \mathbf{c}$ of full rank r, it can be shown that the coefficient matrix can be factored into the product of a triangular matrix $\mathbf{T}$ and its transpose:

$$\mathbf{A} = \mathbf{TT}'$$

It is first necessary to determine the elements of $\mathbf{T}$ by a sequence of quadratic recurrence relationships. Then, letting $\mathbf{y} = \mathbf{T}'\mathbf{x}$, the triangular system

$$\mathbf{Ty} = \mathbf{c}$$

can be solved backward for the elements of $\mathbf{y}$. Finally, it is necessary to solve the other triangular system

$$\mathbf{T}'\mathbf{x} = \mathbf{y}$$

for the original unknown vector $\mathbf{x}$. The expressions for the elements of $\mathbf{T}$ and efficient arrangements of computing worksheets have been given by Dwyer (1951) and Faddeeva (1959).

Often it is necessary to find explicitly the inverse of the coefficient matrix rather than the solution to its equations. This is especially true in regression analysis, for the sampling variances and covariances of the

least-squares estimates of the regression parameters are determined from the elements of the inverse. Inversion of the matrix may be formulated as the solution of r systems of equations with a common coefficient matrix $\mathbf{A}$ but with constant vectors $\mathbf{c}$, the successive columns of the $r \times r$ identity matrix. Solution of the systems can be carried out compactly by the abbreviated Gauss-Doolittle method. Details and examples of this procedure can be found in the texts of Dwyer and Graybill. Alternatively, with the computer language APL (STSC, 1986) inverse matrices can be calculated on a microcomputer with a single primitive function operation. Most of the matrices in the sequel were inverted in that way.

   The preceding methods based upon elementary row operations are all *exact*, in the sense that a finite number of arithmetical operations will lead to a solution with an accuracy dependent only upon the precision maintained at each step in the computations and of course upon the exact or approximate nature of the coefficients in the original matrix. *Iterative* methods start with an approximation or plausible guess at the solution and repeatedly correct these trial values until they converge with a specified degree of accuracy to the actual solution. Perhaps the most familiar iterative technique for solving systems of linear equations is the Gauss-Seidel method (Faddeeva, 1959; Hotelling, 1943; Ralston and Rabinowitz, 1978). Convergence of this algorithm is highly dependent upon the magnitude of the elements in the coefficient matrix. Necessary and sufficient conditions for convergence have been considered by Faddeeva, together with other iterative methods possessing accelerated or more general convergence properties.

2.8   ORTHOGONAL VECTORS AND MATRICES

In Sec. 2.3 we introduced the expression

$$(1) \qquad \cos \theta = \frac{\mathbf{x}'\mathbf{y}}{(\mathbf{x}'\mathbf{x})^{1/2}(\mathbf{y}'\mathbf{y})^{1/2}}$$

for the cosine of the angle between the vectors $\mathbf{x}$ and $\mathbf{y}$ and saw that if their inner product vanished, the vectors must lie at right angles to one another. Such vectors are called *orthogonal*, or *orthonormal* if their lengths have been normalized to unity. An *orthogonal matrix* $\mathbf{T}$ is a square matrix whose rows are a set of orthonormal vectors. Hence

$$(2) \qquad \mathbf{T}\mathbf{T}' = \mathbf{T}'\mathbf{T}$$
$$= \mathbf{I}$$

and the inverse of $\mathbf{T}$ is merely its transpose $\mathbf{T}'$. A simple 2×2 orthogonal

matrix is

$$\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

This is the transformation matrix of a reflection of the points in the xy plane about the 45° line. A more general orthogonal matrix of that dimension is

(3)
$$\mathbf{T} = \begin{bmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{bmatrix}$$

and is interpretable as the transformation matrix for a rotation of the xy coordinate axes through an angle θ. That is, if x and y were the coordinates of a point under the old axes, the point would have coordinates

(4)
$$u = x\cos\theta + y\sin\theta$$
$$v = -x\sin\theta + y\cos\theta$$

after a rigid rotation of the axes through an angle of θ degrees. Larger orthogonal matrices can be constructed by the Gram-Schmidt orthogonalization process (Hohn, 1964, Chap. 7) by starting with one normalized row and building up the matrix according to the requirement of mutual row orthogonality. For example, the Helmert matrix

$$\mathbf{T} = \begin{bmatrix} \dfrac{1}{\sqrt{3}} & \dfrac{1}{\sqrt{3}} & \dfrac{1}{\sqrt{3}} \\ \dfrac{1}{\sqrt{2}} & -\dfrac{1}{\sqrt{2}} & 0 \\ \dfrac{1}{\sqrt{6}} & \dfrac{1}{\sqrt{6}} & -\dfrac{2}{\sqrt{6}} \end{bmatrix}$$

is one particular 3 × 3 orthogonal matrix.

The $n \times n$ orthogonal matrix $\mathbf{T}$ is interpretable as the matrix of the linear transformation equivalent to a *rigid rotation* or a rotation followed by a *reflection* of the n coordinate axes about their origin. Distances in the space are unchanged by this rotation, for if we make the transformation

$$\mathbf{y} = \mathbf{Tx}$$

then

$$\mathbf{x'x} = \mathbf{y'T'Ty}$$
$$= \mathbf{y'Iy}$$

and the sums of squares are invariant.

Orthogonal matrices have these useful properties:

1. The columns of an orthogonal matrix are orthogonal.
2. The determinant of an orthogonal matrix is always either 1 or -1. Since $|\mathbf{TT'}| = |\mathbf{I}| = 1$ and $|\mathbf{T}| = |\mathbf{T'}|$, $|\mathbf{T}| = \pm 1$.
3. The product of orthogonal matrices of the same dimension is itself orthogonal. That is, a succession of rigid rotations and reflections of the coordinate axes is expressible as a single rigid rotation and appropriate reflections.

2.9 QUADRATIC FORMS

A *quadratic form* in the variable $x_1, \ldots, x_n$ is an expression of the type

$$(1) \quad f(x_1, \ldots, x_n) = a_{11}x_1^2 + a_{22}x_2^2 + \cdots + a_{nn}x_n^2$$

$$+ 2a_{12}x_1x_2 + \cdots + 2a_{1n}x_1x_n + \cdots + 2a_{n-1,n}x_{n-1}x_n$$

$$= \sum_{i=1}^{n} \sum_{j=1}^{n} a_{ij}x_i x_j$$

where $a_{ij} = a_{ji}$. Some of the a_{ij} may be zero. We note immediately that the quadratic form can be written in the matrix notation as

$$\mathbf{x'Ax}$$

where $\mathbf{x'} = [x_1, \ldots, x_n]$ and $\mathbf{A}$ is the $n \times n$ symmetric matrix of the coefficients. The simplest quadratic form is merely $f(x) = a_{11}x^2$, the equation of a parabola in the single variable x. Quadratic forms in which the x_i are random variables play an important role in both univariate and multivariate statistical theory. For example, the sum of squared deviations about the sample mean

$$(2) \qquad \sum_{i=1}^{N} (x_i - \bar{x})^2 = \sum_{i=1}^{N} x_i^2 - \frac{1}{N}\left(\sum x_i\right)^2$$

can be written as a quadratic form in the observations x_i with matrix

$$(3) \qquad \mathbf{A} = \begin{bmatrix} \dfrac{N-1}{N} & \dfrac{-1}{N} & \cdots & \dfrac{-1}{N} \\[2mm] \dfrac{-1}{N} & \dfrac{N-1}{N} & \cdots & \dfrac{-1}{N} \\[2mm] \cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots \\[2mm] \dfrac{-1}{N} & \dfrac{-1}{N} & \cdots & \dfrac{N-1}{N} \end{bmatrix}$$

A symmetric matrix $\mathbf{A}$ and its associated quadratic form are called *positive definite* if $\mathbf{x}'\mathbf{Ax} > 0$ for all nonnull $\mathbf{x}$. If $\mathbf{x}'\mathbf{Ax} \geq 0$, the form and its matrix are called *positive semidefinite*. Similar definitions apply for *negative definite* and *semidefinite* quadratic forms. An *indefinite* form can assume either positive, zero, or negative values. We shall need the special properties of positive definite and semidefinite matrices and quadratic forms frequently in the sequel.

Positive definite quadratic forms have matrices of *full rank*. It is possible by repeatedly completing squares to reduce such a form in n variables to the form

$$(4) \qquad\qquad d_1 y_1^2 + \cdots + d_n y_n^2$$

containing only squares of the new variables y_t and with coefficients $d_i > 0$. Similarly, a positive semidefinite quadratic form can be reduced to

$$(5) \qquad\qquad d_1 y_1^2 + \cdots + d_r y_r^2$$

where all coefficients are positive, and $r \leq n$ is the rank of the form matrix. However, these properties are not convenient means of determining the nature of the form, and we shall now state a necessary and sufficient condition for positive definiteness or semidefiniteness. From the matrix form the sequence of *leading principal minor determinants*

$$(6) \qquad p_0 = 1 \qquad p_1 = a_{11} \qquad p_2 = \begin{vmatrix} a_{11} & a_{12} \\ a_{12} & a_{22} \end{vmatrix} \quad \cdots$$

$$p_t = \begin{vmatrix} a_{11} & \cdots & a_{1t} \\ \cdots\cdots\cdots\cdots \\ a_{1t} & \cdots & a_{tt} \end{vmatrix} \quad \cdots \quad p_n = |\mathbf{A}|$$

If $\mathbf{A}$ is of rank r it is said to be *regular* if $p_r \neq 0$ and no two consecutive p_i in the sequence $p_0, p_1, \ldots, p_r$ are zero. It is always possible to put any symmetric matrix into regular form by interchanging rows and, simultaneously, the corresponding columns. Then, if $\mathbf{A}$ is a regularly arranged matrix,

1. A necessary and sufficient condition for positive definiteness is that $p_t > 0$ for $i = 1, \ldots, n$.
2. A necessary and sufficient condition for positive semidefiniteness is that $p_1 > 0, \ldots, p_r > 0$ and the remaining $n - r$ p_t equal zero, where r may equal n.

Example 2.19. The matrix

$$\begin{bmatrix} 4 & 6 & 0 \\ 6 & 9 & 0 \\ 0 & 0 & 2 \end{bmatrix}$$

has the leading-principal-minor-determinant sequence $p_0 = 1$, $p_1 = 4$, $p_2 = 0$, $p_3 = 0$, and so it is not regularly arranged. We can reorder the rows and columns to give the new matrix

$$\begin{bmatrix} 2 & 0 & 0 \\ 0 & 4 & 6 \\ 0 & 6 & 9 \end{bmatrix}$$

with the sequence $p_0 = 1$, $p_1 = 2$, $p_2 = 8$, $p_3 = 0$. The matrix and its quadratic form are positive semidefinite of rank two.

Example 2.20. The matrix (3) of the sample sum of squares is a particular case of the patterned matrix with a common diagonal element a and equal off-diagonal elements b. The determinant of such an $i \times i$ matrix is

$$(a - b)^{i-1}[a + (i - 1)b]$$

so that the leading principal minor determinants of (3) are

$$p_i = \frac{1}{N}[N - 1 - (i - 1)]$$

The first $N - 1$ of these are positive, while the Nth is always zero. The sum of squared deviations is then a positive semidefinite quadratic form of rank $N - 1$.

2.10 THE CHARACTERISTIC ROOTS AND VECTORS OF A MATRIX

The *characteristic roots* of the $p \times p$ matrix $\mathbf{A}$ are the solutions to the *determinantal equation*

(1) $$|\mathbf{A} - \lambda\mathbf{I}| = 0$$

The determinant is a pth-degree polynomial in λ, and thus $\mathbf{A}$ has just p characteristic roots. The Laplace expansion of the *characteristic determinant* enables us to write the *characteristic polynomial* as

(2) $$|\mathbf{A} - \lambda\mathbf{I}| = (-\lambda)^p + S_1(-\lambda)^{p-1} + S_2(-\lambda)^{p-2} + \cdots - S_{p-1}\lambda + |\mathbf{A}|$$

where S_i is the sum of all $i \times i$ principal minor determinants. S_1 is merely the sum of the diagonal elements of $\mathbf{A}$, or tr $\mathbf{A}$. It follows immediately from the theory of polynomial equations that:

1. The *product* of the characteristic roots of $\mathbf{A}$ is equal to $|\mathbf{A}|$.

2. The *sum* of the characteristic roots of $\mathbf{A}$ is equal to the *trace* of $\mathbf{A}$.

Example 2.21. The matrix

$$\mathbf{A} = \begin{bmatrix} 2 & 1 & 1 \\ 1 & 2 & 1 \\ 1 & 1 & 2 \end{bmatrix}$$

has trace 6 and three 2×2 principal minor determinants equal to

$$\begin{vmatrix} 2 & 1 \\ 1 & 2 \end{vmatrix} = 3$$

while $|\mathbf{A}| = 4$. The characteristic equation of $\mathbf{A}$ is

$$\lambda^3 - 6\lambda^2 + 9\lambda - 4 = 0$$

and its roots are $1, 1$, and 4.

In the sequel we shall frequently need these properties of characteristic roots:

1. The characteristic roots of a symmetric matrix with real elements are all real.
2. The characteristic roots of a positive definite matrix are all positive.
3. If an $n \times n$ symmetric matrix is positive semidefinite of rank r, it contains exactly r positive characteristic roots and $n - r$ zero roots.
4. The nonzero characteristic roots of the product $\mathbf{AB}$ are equal to the nonzero roots of $\mathbf{BA}$. Hence the traces of $\mathbf{AB}$ and $\mathbf{BA}$ are equal.
5. The characteristic roots of a diagonal matrix are the diagonal elements themselves.

Associated with every characteristic root λ_t of the square matrix $\mathbf{A}$ is a *characteristic vector* $\mathbf{x}_i$ whose elements satisfy the homogeneous system of equations

$$(3) \qquad\qquad [\mathbf{A} - \lambda_i \mathbf{I}]\mathbf{x}_t = \mathbf{0}$$

By the definition of the characteristic root the determinant of the system vanishes, and a nontrivial solution $\mathbf{x}_t$ always exists. We note immediately that the elements of the vector are determined only up to a scale factor. Many of the characteristic vectors we shall encounter in the sequel will be computed from symmetric matrices. The characteristic roots and vectors of such matrices have these important properties:

1. If λ_t and λ_j are distinct characteristic roots of the symmetric matrix $\mathbf{A}$, their associated vectors $\mathbf{x}_t$ and $\mathbf{x}_j$ are orthogonal. This is readily apparent if we premultiply the definitions of the vectors

$$\mathbf{A}\mathbf{x}_t = \lambda_i \mathbf{x}_t \qquad \mathbf{A}\mathbf{x}_j = \lambda_j \mathbf{x}_j$$

by $\mathbf{x}_j'$ and $\mathbf{x}_i'$, respectively. But this implies that

$$\lambda_t \mathbf{x}_j' \mathbf{x}_t = \lambda_j \mathbf{x}_i' \mathbf{x}_j$$

and since $\lambda_i \neq \lambda_j$, we conclude that the vectors are orthogonal.

2. For every real symmetric matrix **A** there exists an orthogonal matrix **P** such that

(4) $$\mathbf{P'AP} = \mathbf{D}$$

where **D** is the diagonal matrix of the characteristic roots of **A**. The normalized characteristic vectors of **A** can be taken as the columns of **P**. Even if the characteristic roots are not distinct, it is still possible to select the elements of their vectors to give a mutually orthogonal set of characteristic vectors.

These properties of symmetric matrices have an important implication for quadratic forms. If we apply the orthogonal transformation

(5) $$\mathbf{x} = \mathbf{Py}$$

to the p variables in the quadratic form $\mathbf{x'Ax}$, the form becomes

(6) $$\mathbf{x'Ax} = \mathbf{y'P'APy}$$
$$= \mathbf{y'Dy}$$
$$= \lambda_1 y_1^2 + \cdots + \lambda_r y_r^2$$

where the λ_i are the characteristic roots of the coefficient matrix, and r is the rank of the form. Any real quadratic form can be reduced to a weighted sum of squares by computing the characteristic roots and vectors of its matrix.

Example 2.22. The characteristic vector of the largest root of Example 2.21 must satisfy the equations

$$-2x_{11} + x_{12} + x_{13} = 0$$
$$x_{11} - 2x_{12} + x_{13} = 0$$
$$x_{11} + x_{12} - 2x_{13} = 0$$

If we arbitrarily set x_{13} equal to one and solve the first two non-homogeneous equations, the characteristic vector is

$$\mathbf{x'} = [1, 1, 1]$$

and of course any nonnull vector $[a, a, a]$ is a characteristic vector for $\lambda_3 = 4$. The vector associated with the double root $\lambda_1 = \lambda_2 = 1$ must satisfy the system with the single linearly independent equation

$$x_{21} + x_{22} + x_{23} = 0$$

The most general solution to this is the vector

$$[a, b, -a - b]$$

and by properly selecting a and b we can generate two linearly independent

characteristic vectors for the double root. Note that *any* choice of a and b will give vectors orthogonal to the first vector $[1, 1, 1]$. We may elect to choose a and b in the second and third vectors to continue this orthogonality. For example,

$$\mathbf{x}_1' = [0, 1, -1]$$
$$\mathbf{x}_2' = [-2, 1, 1]$$

Example 2.23. Square matrices with the property

$$\mathbf{AA} = \mathbf{A}$$

are called *idempotent* and play an exceedingly important role in the theory of the analysis of variance. The characteristic roots of an idempotent matrix are either zero or one, and a quadratic form with such a matrix can be reduced to a sum of r squared terms. It is easy to check that the matrix (3) of Sec. 2.9 is idempotent and that it is therefore possible to make the transformation

$$\sum_{i=1}^{N} (x_i - \bar{x})^2 = y_1^2 + \cdots + y_{N-1}^2$$

into a sum of squares of $N - 1$ new random variables whose statistical independence follows from the orthogonality of the transformation.

Numerical methods for calculating characteristic roots and vectors have been described by Bodewig (1956), Faddeeva (1959), Householder (1953), and Ralston and Rabinowitz (1978). The APL Plus version (STSC, 1986) of the APL computer language contains functions for extracting characteristic roots and vectors of symmetric and general square matrices. In Sec. 8.2 we shall describe an iterative scheme for computing the largest roots of small matrices with a calculator.

Bounds for characteristic roots have been obtained by a number of algebraists. Such results have been collected and summarized by Marcus and Minc (1964).

2.11 PARTITIONED MATRICES

Frequently we shall find it convenient to think of certain rows and columns of a matrix as grouped together because of common characteristics of their associated variables. Such a matrix can be written as an array

$$(1) \qquad \mathbf{A} = \begin{bmatrix} \mathbf{A}_{11} & \cdots & \mathbf{A}_{1n} \\ \cdots\cdots\cdots\cdots\cdots \\ \mathbf{A}_{m1} & \cdots & \mathbf{A}_{mn} \end{bmatrix}$$

of submatrices $\mathbf{A}_{ij}$ containing r_i rows and c_j columns, where it is obvious that all submatrices in a given row of $\mathbf{A}$ must have the same number of rows and each column must be composed of matrices with a like number

of columns. Operations with partitioned matrices are akin to those in the ungrouped case, except that the nonscalar nature of the elements must be kept in mind. The sum of the partitioned matrices $\mathbf{A}$ and $\mathbf{B}$ whose submatrices have similar dimensions is

$$
(2) \qquad \mathbf{A} + \mathbf{B} = \begin{bmatrix} \mathbf{A}_{11} + \mathbf{B}_{11} & \cdots & \mathbf{A}_{1n} + \mathbf{B}_{1n} \\ \cdots\cdots\cdots\cdots\cdots\cdots\cdots \\ \mathbf{A}_{m1} + \mathbf{B}_{m1} & \cdots & \mathbf{A}_{mn} + \mathbf{B}_{mn} \end{bmatrix}
$$

The product of the partitioned matrices $\mathbf{A}$ and $\mathbf{B}$ is

$$
(3) \qquad \mathbf{AB} = \begin{bmatrix} \sum_{j=1}^{n} \mathbf{A}_{1j}\mathbf{B}_{j1} & \cdots & \sum_{j=1}^{n} \mathbf{A}_{1j}\mathbf{B}_{jp} \\ \cdots\cdots\cdots\cdots\cdots\cdots\cdots \\ \sum_{j=1}^{n} \mathbf{A}_{mj}\mathbf{B}_{j1} & \cdots & \sum_{j=1}^{n} \mathbf{A}_{mj}\mathbf{B}_{jp} \end{bmatrix}
$$

The dimensions within each submatrix product must conform; if the submatrices of $\mathbf{A}$ have respective column numbers $c_1, \ldots, c_n$, those of $\mathbf{B}$ must have the row dimensions $c_1, \ldots, c_n$.

When the elements of partitioned matrices must be shown, as in numerical examples, it will be convenient to separate the submatrices by dashed lines or appropriate spacing.

Example 2.24. Let

$$
\mathbf{A} = \begin{bmatrix} 1 & 0 & \vdots & 3 \\ -2 & 3 & \vdots & 1 \\ \cdots\cdots\cdots\cdots \\ 1 & 1 & \vdots & 2 \end{bmatrix} \qquad \mathbf{B} = \begin{bmatrix} 1 & 1 \\ 2 & 0 \\ \cdots\cdots \\ 3 & 1 \end{bmatrix}
$$

Then

$$
\mathbf{AB} = \begin{bmatrix} 10 & 4 \\ 7 & -1 \\ \cdots\cdots \\ 9 & 3 \end{bmatrix}
$$

It is also possible to express the inverse of a nonsingular partitioned matrix in terms of its submatrices. In the particularly important case of

$$
(4) \qquad \mathbf{A} = \begin{bmatrix} \mathbf{A}_{11} & \mathbf{A}_{12} \\ \mathbf{A}_{21} & \mathbf{A}_{22} \end{bmatrix}
$$

where $\mathbf{A}_{11}$ and $\mathbf{A}_{22}$ are both square and by their principal-minor nature nonsingular, it can be verified that

$$
(5) \quad \mathbf{A}^{-1} =
$$

$$
\begin{bmatrix} (\mathbf{A}_{11} - \mathbf{A}_{12}\mathbf{A}_{22}^{-1}\mathbf{A}_{21})^{-1} & -(\mathbf{A}_{11} - \mathbf{A}_{12}\mathbf{A}_{22}^{-1}\mathbf{A}_{21})^{-1}\mathbf{A}_{12}\mathbf{A}_{22}^{-1} \\ -\mathbf{A}_{22}^{-1}\mathbf{A}_{21}(\mathbf{A}_{11} - \mathbf{A}_{12}\mathbf{A}_{22}^{-1}\mathbf{A}_{21})^{-1} & \mathbf{A}_{22}^{-1} + \mathbf{A}_{22}^{-1}\mathbf{A}_{21}(\mathbf{A}_{11} - \mathbf{A}_{12}\mathbf{A}_{22}^{-1}\mathbf{A}_{21})^{-1}\mathbf{A}_{12}\mathbf{A}_{22}^{-1} \end{bmatrix}
$$

An alternate expression can be obtained by reversing the positions of $\mathbf{A}_{11}$ and $\mathbf{A}_{22}$ in the original matrix.

Frequently it is necessary to compute the determinant of the partitioned matrix (4). If $\mathbf{A}_{11}$ is nonsingular,

(6) $$|\mathbf{A}| = |\mathbf{A}_{11}| \cdot |\mathbf{A}_{22} - \mathbf{A}_{21}\mathbf{A}_{11}^{-1}\mathbf{A}_{12}|$$

If $\mathbf{A}_{22}$ is nonsingular,

(7) $$|\mathbf{A}| = |\mathbf{A}_{22}| \cdot |\mathbf{A}_{11} - \mathbf{A}_{12}\mathbf{A}_{22}^{-1}\mathbf{A}_{21}|$$

Example 2.25. The preceding expressions for the inverses and determinants are often valuable in practical computation if the submatrices are small or conveniently patterned. If

$$\mathbf{A} = \begin{bmatrix} 1 & 0 & 1 & 1 & 1 \\ 0 & 1 & 2 & 2 & 2 \\ 3 & -1 & 4 & 0 & 0 \\ 3 & -1 & 0 & 4 & 0 \\ 3 & -1 & 0 & 0 & 4 \end{bmatrix}$$

we can compute $\mathbf{A}^{-1}$ by partitioning the matrix in terms of the first and second and third to fifth rows and columns. Then

$$\mathbf{A}_{11}^{-1} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \qquad \mathbf{A}_{22}^{-1} = \begin{bmatrix} \frac{1}{4} & 0 & 0 \\ 0 & \frac{1}{4} & 0 \\ 0 & 0 & \frac{1}{4} \end{bmatrix}$$

$$\mathbf{A}_{11} - \mathbf{A}_{12}\mathbf{A}_{22}^{-1}\mathbf{A}_{21} = \begin{bmatrix} -\frac{5}{4} & \frac{3}{4} \\ -\frac{9}{2} & \frac{5}{2} \end{bmatrix}$$

$$(\mathbf{A}_{11} - \mathbf{A}_{12}\mathbf{A}_{22}^{-1}\mathbf{A}_{21})^{-1} = \begin{bmatrix} 10 & -3 \\ 18 & -5 \end{bmatrix}$$

$$\mathbf{A}_{12}\mathbf{A}_{22}^{-1} = \begin{bmatrix} \frac{1}{4} & \frac{1}{4} & \frac{1}{4} \\ \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \end{bmatrix} \qquad \mathbf{A}_{22}^{-1}\mathbf{A}_{21} = \begin{bmatrix} \frac{3}{4} & -\frac{1}{4} \\ \frac{3}{4} & -\frac{1}{4} \\ \frac{3}{4} & -\frac{1}{4} \end{bmatrix}$$

Hence

$$\mathbf{A}^{-1} = \begin{bmatrix} 10 & -3 & -1 & -1 & -1 \\ 18 & -5 & -2 & -2 & -2 \\ -3 & 1 & \frac{1}{2} & \frac{1}{4} & \frac{1}{4} \\ -3 & 1 & \frac{1}{4} & \frac{1}{2} & \frac{1}{4} \\ -3 & 1 & \frac{1}{4} & \frac{1}{4} & \frac{1}{2} \end{bmatrix}$$

The determinant of $\mathbf{A}$ can be computed from (6) or (7) to be 16.

The two forms of the partitioned inverse (5) lead to a useful matrix

identity. If we equate the alternative expressions for the (1,1) submatrix of $\mathbf{A}^{-1}$, we have

$$(8) \quad (\mathbf{A}_{11} - \mathbf{A}_{12}\mathbf{A}_{22}^{-1}\mathbf{A}_{21})^{-1} = \mathbf{A}_{11}^{-1} + \mathbf{A}_{11}^{-1}\mathbf{A}_{12}(\mathbf{A}_{22} - \mathbf{A}_{21}\mathbf{A}_{11}^{-1}\mathbf{A}_{12})^{-1}\mathbf{A}_{21}\mathbf{A}_{11}^{-1}$$

In particular, if $\mathbf{A}$ is $p \times p$ and nonsingular, $\mathbf{b}$ is a $p \times 1$ vector, and c is a scalar, then we have Bartlett's (1951) form of the identity:

$$(9) \qquad (\mathbf{A} + c\mathbf{b}\mathbf{b}')^{-1} = \mathbf{A}^{-1} - \frac{c}{1 + c\mathbf{b}'\mathbf{A}^{-1}\mathbf{b}}\mathbf{A}^{-1}\mathbf{b}\mathbf{b}'\mathbf{A}^{-1}$$

Example 2.26. We shall use (9) to compute the inverse of the $p \times p$ matrix

$$\mathbf{K} = \begin{bmatrix} a & c & \cdots & c \\ c & a & \cdots & c \\ \cdots\cdots\cdots\cdots \\ c & c & \cdots & a \end{bmatrix}$$

Let $\mathbf{A} = (a - c)\mathbf{I}$, $\mathbf{b}' = [1, \ldots, 1]$, and write $\mathbf{E} = \mathbf{b}\mathbf{b}'$. Then

$$\mathbf{K}^{-1} = \frac{1}{a - c}\mathbf{I} - \frac{c}{(a - c)[a + c(p - 1)]}\mathbf{E}$$

or a matrix with a common diagonal element

$$\frac{a + (p - 2)c}{(a - c)[a + (p - 1)c]}$$

and off-diagonal elements each equal to

$$-\frac{c}{(a - c)[a + (p - 1)c]}$$

2.12 DIFFERENTIATION WITH VECTORS AND MATRICES

In the later chapters we shall need formulas for finding the partial derivatives of likelihoods and other scalar functions of vectors and matrices. Let $f(\mathbf{x})$ be a continuous function of the elements of the vector $\mathbf{x}' = [x_1, \ldots, x_p]$ whose first and second partial derivatives

$$\frac{\partial f(\mathbf{x})}{\partial x_i} \qquad \frac{\partial^2 f(\mathbf{x})}{\partial x_i \, \partial x_j}$$

exist for all points $\mathbf{x}$ in some region of p-dimensional euclidean space of interest to us. Define the partial derivative operator vector as

$$(1) \qquad \frac{\partial}{\partial \mathbf{x}} = \begin{bmatrix} \dfrac{\partial}{\partial x_1} \\ \vdots \\ \dfrac{\partial}{\partial x_p} \end{bmatrix}$$

Application of it to $f(\mathbf{x})$ yields the vector of partial derivatives

(2)
$$\frac{\partial f(\mathbf{x})}{\partial \mathbf{x}} = \begin{bmatrix} \dfrac{\partial f(\mathbf{x})}{\partial x_1} \\ \vdots \\ \dfrac{\partial f(\mathbf{x})}{\partial x_p} \end{bmatrix}$$

The following functions and their derivatives are especially important:

1. If $f(\mathbf{x})$ is constant for all $\mathbf{x}$,

(3)
$$\frac{\partial f(\mathbf{x})}{\partial \mathbf{x}} = \begin{bmatrix} 0 \\ \vdots \\ 0 \end{bmatrix}$$

2. $f(\mathbf{x}) = \mathbf{a}'\mathbf{x}$:

(4)
$$\frac{\partial f(\mathbf{x})}{\partial \mathbf{x}} = \begin{bmatrix} a_1 \\ \vdots \\ a_p \end{bmatrix}$$

Note that the columnar form of the derivative vector is unchanged if we write $f(\mathbf{x}) = \mathbf{x}'\mathbf{a}$.

3. To compute the vector of derivatives of the quadratic form $\mathbf{x}'\mathbf{A}\mathbf{x}$ write

$$\mathbf{x}'\mathbf{A}\mathbf{x} = \sum_{i=1}^{p} \sum_{j=1}^{p} a_{ij} x_i x_j = a_{ii} x_i^2 + 2x_i \sum_{\substack{j=1 \\ j \neq i}} a_{ij} x_j + \sum_{\substack{h \neq i \\ j \neq i}} \sum a_{hj} x_h x_j$$

and differentiate with respect to x_i. If we let $\mathbf{a}_i'$ be the ith row of the symmetric matrix $\mathbf{A}$, the partial derivative of the quadratic form with respect to x_i is

$$2\mathbf{a}_i'\mathbf{x} = 2 \sum_{j=1}^{p} a_{ij} x_j$$

and the vector of partial derivatives is

(5)
$$\frac{\partial \mathbf{x}'\mathbf{A}\mathbf{x}}{\partial \mathbf{x}} = 2\mathbf{A}\mathbf{x}$$

In particular, the vector of derivatives of the sum of squares $\mathbf{x}'\mathbf{x}$ is merely $2\mathbf{x}$.

4. In the more general quadratic function

(6)
$$h(\mathbf{x}) = (\mathbf{a} - \mathbf{C}\mathbf{x})'\mathbf{K}(\mathbf{a} - \mathbf{C}\mathbf{x})$$

let $\mathbf{K}$ be an $N \times N$ symmetric matrix, $\mathbf{C} = [\mathbf{C}_1, \ldots, \mathbf{C}_p]$ is an $N \times p$ matrix of constants, and $\mathbf{a}$ is an $N \times 1$ vector. If we let $\mathbf{u} = \mathbf{a} - \mathbf{C}\mathbf{x}$, the derivatives of $h(\mathbf{x})$ can be computed by the chain rule:

(7)
$$\frac{\partial h(\mathbf{x})}{\partial x_i} = \sum_{j \cdot 1}^{p} \frac{\partial(\mathbf{u}'\mathbf{K}\mathbf{u})}{\partial u_j} \frac{\partial u_j}{\partial x_i}$$

$$= -2\mathbf{u}'\mathbf{K}\mathbf{C}_i \qquad i = 1, \ldots, p$$

and

(8)
$$\frac{\partial h(\mathbf{x})}{\partial \mathbf{x}} = -2\mathbf{C}'\mathbf{K}(\mathbf{a} - \mathbf{C}\mathbf{x})$$

5. The matrix of second-order partial derivatives of a function of p variables is called the *hessian* matrix:

(9)
$$\mathbf{H} = \frac{\partial^2 f(\mathbf{x})}{\partial \mathbf{x}' \partial \mathbf{x}} = \begin{bmatrix} \dfrac{\partial^2 f(\mathbf{x})}{\partial x_1^2} & \cdots & \dfrac{\partial^2 f(\mathbf{x})}{\partial x_1 \partial x_p} \\ \cdots \cdots \cdots \cdots \cdots \cdots \\ \dfrac{\partial^2 f(\mathbf{x})}{\partial x_1 \partial x_p} & \cdots & \dfrac{\partial^2 f(\mathbf{x})}{\partial x_p^2} \end{bmatrix} .$$

For example, the hessian matrix of $f(\mathbf{x}) = \mathbf{x}'\mathbf{A}\mathbf{x}$ is merely $2\mathbf{A}$. The hessian is necessarily symmetric if our original conditions of continuity and existence of all first and second derivatives are satisfied by $f(\mathbf{x})$.

Determination of maxima and minima. A necessary condition for a maximum or minimum of $f(\mathbf{x})$ at $\mathbf{x} = \mathbf{x}_0$ is that

(10)
$$\frac{\partial f(\mathbf{x})}{\partial \mathbf{x}} = \mathbf{0}$$

at that point. Such a value of the function is called a *stationary* maximum or minimum, as opposed to a *global* extremum which might exist on the boundary of the admissible region of $\mathbf{x}$, or as a cusp or other form at which the derivatives were undefined. A sufficient condition for a maximum at the point $\mathbf{x}_0$ satisfying (10) is that the hessian matrix evaluated at $\mathbf{x}_0$ is negative definite. Similarly, a positive definite hessian is a sufficient condition for a stationary minimum. If the hessian is semidefinite the test fails, and higher-order terms in the Taylor expansion of $f(\mathbf{x})$ must be examined in the vicinity of the stationary point. If the hessian is an indefinite matrix $\mathbf{x}_0$, that point is neither a maximum nor a minimum.

As an application of these rules let us determine the stationary extremum of the function $h(\mathbf{x})$ given by (6). By equating (8) to the null vector we see that the stationary point must satisfy the system of linear equations

(11)
$$\mathbf{C}'\mathbf{K}\mathbf{C}\mathbf{x} = \mathbf{C}'\mathbf{K}\mathbf{a}$$

and if $\mathbf{C'KC}$ is of full rank p,

(12) $\mathbf{x} = (\mathbf{C'KC})^{-1}\mathbf{C'Ka}$

If $\mathbf{K}$ is positive definite and $\mathbf{C}$ has rank p, the hessian $2\mathbf{C'KC}$ will be positive definite and the solution (12) will minimize $h(\mathbf{x})$.

Maximization subject to constraints. Frequently it will be necessary to maximize or minimize one function $f(\mathbf{x})$ subject to a constraint $g(\mathbf{x}) = c$ on the values of $\mathbf{x}$. Although one might be able to handle this problem by eliminating one variable by the constraint, a more general and efficient method is that of *Lagrange multipliers*. The mathematical basis for that technique can be found in most modern calculus texts, e.g., Courant (1966) or Hadley (1964). Essentially, we form a new function

(13) $h(\mathbf{x}, \lambda) = f(x) - \lambda[g(\mathbf{x}) - c]$

For a constrained stationary value these conditions must be met:

(14a) $\dfrac{\partial h(\mathbf{x},\lambda)}{\partial \mathbf{x}} = \dfrac{\partial f(\mathbf{x})}{\partial \mathbf{x}} - \lambda \dfrac{\partial g(\mathbf{x})}{\partial \mathbf{x}}$

$$= \mathbf{0}$$

(14b) $\dfrac{\partial h(\mathbf{x},\lambda)}{\partial \lambda} = -g(\mathbf{x}) + c$

$$= 0$$

The second condition is of course nothing more than the original constraint. In practice one must solve the equations (14a) for $\mathbf{x}$ after eliminating λ by algebraic manipulation or from the nature of the equations.

As an example, let us find the maximum value of the quadratic function $f(\mathbf{x}) = \mathbf{x'Ax}$, where $\mathbf{A}$ is a positive definite matrix, subject to the constraint $\mathbf{x'x} = 1$. Then

$$h(\mathbf{x},\lambda) = \mathbf{x'Ax} - \lambda(\mathbf{x'x} - 1)$$

and (14a) is the system of linear equations

(15) $[\mathbf{A} - \lambda\mathbf{I}]\mathbf{x} = \mathbf{0}$

defining the characteristic vectors of $\mathbf{A}$. Premultiplication by $\mathbf{x'}$ and use of the constraint yields $\lambda = \mathbf{x'Ax}$; clearly, if that quadratic form is to be a maximum then λ must be the *greatest* characteristic root of $\mathbf{A}$, and $\mathbf{x}$ its associated vector. The constraint directs that the vector be normalized to length one. Similarly, the minimum value of $f(\mathbf{x})$ subject to the condition would be given by the characteristic vector corresponding to the smallest characteristic root.

Sufficient conditions for maxima and minima in the presence of one or more constraints have been given by Hancock (1960, pp. 114–116) and in certain more current texts, e.g., Goldberger (1964, pp. 45–48).

The derivative of the determinant of the $n \times n$ matrix $\mathbf{A}$ with respect to its element a_{ij} can be found from the expansion of $\mathbf{A}$ in the cofactors of the ith row or jth column. By the first expansion,

$$(16) \qquad \frac{\partial |\mathbf{A}|}{\partial a_{ij}} = \frac{\partial}{\partial a_{ij}} (a_{i1} A_{i1} + \cdots + a_{ij} A_{ij} + \cdots + a_{in} A_{in})$$

$$= A_{ij}$$

If $\mathbf{A}$ is symmetric,

$$(17) \qquad \frac{\partial |\mathbf{A}|}{\partial a_{ii}} = A_{ii} \qquad .$$

and it can be shown from more general formulas for derivatives of determinants, whose elements are in turn functions of other variables, that

$$(18) \qquad \frac{\partial |\mathbf{A}|}{\partial a_{ij}} = 2A_{ij}$$

In the sequel it will be necessary to differentiate quadratic forms and other scalars with respect to elements of their constituent matrices. If $\mathbf{X}$ is an $m \times n$ matrix with general element x_{ij}, its derivative with respect to that element is

$$(19) \qquad \frac{\partial \mathbf{X}}{\partial x_{ij}} = \mathbf{J}_{ij}$$

where $\mathbf{J}_{ij}$ is the $m \times n$ matrix with a one in the ijth position and zeros everywhere else. If $\mathbf{X}$ is symmetric,

$$(20) \qquad \frac{\partial \mathbf{X}}{\partial x_{ij}} = \mathbf{J}_{ij} + \mathbf{J}_{ji} \qquad i \neq j$$

The rule for differentiating a matrix product is similar to that for scalars. Suppose that the elements of the conformable matrices $\mathbf{X}$ and $\mathbf{Y}$ are functions $x_{ij}(z)$, $y_{ij}(z)$ of some variable z. Then

$$(21) \qquad \frac{\partial \mathbf{X}\mathbf{Y}}{\partial z} = \frac{\partial \mathbf{X}}{\partial z} \mathbf{Y} + \mathbf{X} \frac{\partial \mathbf{Y}}{\partial z}$$

This formula leads to a means of differentiating the inverse of the square nonsingular matrix $\mathbf{X}$. Write

$$\mathbf{I} = \mathbf{X}\mathbf{X}^{-1}$$

Then

$$\frac{\partial \mathbf{I}}{\partial x_{ij}} = \mathbf{J}_{ij}\mathbf{X}^{-1} + \mathbf{X}\frac{\partial \mathbf{X}^{-1}}{\partial x_{ij}}$$

$$= 0$$

and

(22)
$$\frac{\partial \mathbf{X}^{-1}}{\partial x_{ij}} = -\mathbf{X}^{-1}\mathbf{J}_{ij}\mathbf{X}^{-1}$$

If **X** is symmetric,

(23)
$$\frac{\partial \mathbf{X}^{-1}}{\partial x_{ij}} = \begin{cases} -\mathbf{X}^{-1}\mathbf{J}_{ii}\mathbf{X}^{-1} & i = j \\ -\mathbf{X}^{-1}(\mathbf{J}_{ij} + \mathbf{J}_{ji})\mathbf{X}^{-1} & i \neq j \end{cases}$$

Many other formulas for matrix and vector differentiation have been given in a series of papers by Dwyer and MacPhail (1948), Dwyer (1967), and Tracy and Dwyer (1969).

2.13 FURTHER READING

The texts of Basilevsky (1983), Browne (1958), Graybill (1983), Hadley (1961), Hohn (1964), Perlis (1952), Searle (1966, 1982), and Searle and Hausman (1970) serve well both as surveys of matrix algebra and as sources for the proofs of the results of this chapter. Horst (1963) has developed matrix operations at a more verbal level for workers in the social sciences. Frazer, Duncan, and Collar (1963) have discussed a wide variety of topics in the algebra and numerical-analysis methods of matrices. A more advanced treatment motivated by physical and probabilistic applications has been written by Bellman (1970). Householder (1964) has given a theoretical development of numerical techniques for the solution of systems of linear equations, matrix inversion, and extraction of characteristic roots. Roy's monograph (1957) contains in its appendices a wealth of special theorems on partitioned matrices, quadratic forms, and characteristic roots.

2.14 EXERCISES

1. Let

$$\mathbf{A} = \begin{bmatrix} 1 & 2 & -1 \\ -1 & 3 & -1 \\ 2 & 2 & 4 \end{bmatrix} \quad \mathbf{B} = \begin{bmatrix} 3 & 2 & -1 \\ 2 & 3 & 1 \\ -1 & 1 & 3 \end{bmatrix} \quad \mathbf{C} = \begin{bmatrix} 2 & 0 \\ -1 & 1 \\ 3 & 2 \end{bmatrix}$$

Perform those matrix operations that are defined:

(a) **A + B** (b) **A − 2B** (c) **A′ + B** (d) **A + C**
(e) **(A + B)′** (f) **(3A′ − 2B)′**

2. If

$$
P = \begin{bmatrix} 3 & 2 & 1 \\ 2 & 5 & -1 \\ 1 & -1 & 3 \end{bmatrix} \quad
Q = \begin{bmatrix} 1 & 2 & 2 & 1 \\ 1 & 1 & 1 & 4 \\ 1 & 2 & 2 & 1 \end{bmatrix} \quad
R = \begin{bmatrix} 1 & 2 \\ -5 & 2 \\ 3 & -1 \\ -2 & 2 \end{bmatrix}
$$

$$
x = \begin{bmatrix} 1 \\ 0 \\ -1 \end{bmatrix} \quad
y = \begin{bmatrix} 2 \\ 3 \\ 2 \end{bmatrix} \quad
z = \begin{bmatrix} -1 \\ -2 \\ -3 \\ -4 \end{bmatrix}
$$

compute those matrix products that are defined:

(a) **PQ** (b) **PQR** (c) **QR′** (d) **yx′**
(e) **x′y** (f) **x′Px** (g) **x′Py** (h) **P(x + y)**

3. If **A** is the general $n \times n$ matrix and **j** and **E** have the patterns defined in Sec. 2.2, interpret these expressions:

(a) **j′A** (b) **Aj** (c) **diag (EA)** (d) **diag (AE)**
(e) **j′j** (f) **Ej** (g) **E²**

4. Which of the following matrices are commutative under multiplication?

$$
A = \begin{bmatrix} 3 & 1 & 0 \\ 1 & 2 & 1 \\ 0 & 1 & 2 \end{bmatrix} \quad
B = \begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{bmatrix} \quad
C = \begin{bmatrix} 3 & 0 & 0 \\ 0 & 3 & 0 \\ 0 & 0 & 3 \end{bmatrix} \quad
D = \begin{bmatrix} 2 & 1 & 0 \\ 1 & 2 & 1 \\ 0 & 1 & 2 \end{bmatrix}
$$

5. Calculate the determinants of these matrices using the most convenient methods:

$$
(a) \begin{bmatrix} 4 & 2 & 0 \\ 5 & 3 & 0 \\ 6 & 9 & 2 \end{bmatrix} \quad
(b) \begin{bmatrix} 1 & 0.8 & 0.5 \\ 0.8 & 1 & 0.6 \\ 0.5 & 0.6 & 1 \end{bmatrix} \quad
(c) \begin{bmatrix} 5 & 0 & 0 \\ 0 & 3 & 0 \\ 0 & 0 & 1 \end{bmatrix}
$$

$$
(d) \begin{bmatrix} 1 & 4 & -1 \\ 3 & 12 & -3 \\ 0 & 35 & 7 \end{bmatrix} \quad
(e) \begin{bmatrix} 2 & 0 & 4 & 0 \\ 0 & 3 & 0 & 5 \\ 5 & 0 & 1 & 0 \\ 0 & 4 & 0 & 1 \end{bmatrix} \quad
(f) \begin{bmatrix} 2 & 0 & 1 & 1 & 1 \\ 0 & 2 & 3 & 3 & 3 \\ 1 & 3 & 1 & 0 & 0 \\ 1 & 3 & 0 & 1 & 0 \\ 1 & 3 & 0 & 0 & 1 \end{bmatrix}
$$

6. Compute the inverses of these matrices:

$$
(a) \begin{bmatrix} 5 & 1 & -2 \\ 2 & 6 & 3 \\ -1 & 0 & 3 \end{bmatrix} \quad
(b) \begin{bmatrix} a & b & b \\ b & a & b \\ b & b & a \end{bmatrix}
$$

$$
(c) \begin{bmatrix} 5 & 0 & 0 \\ 0 & 8 & 6 \\ 0 & 6 & 5 \end{bmatrix} \quad
(d) \begin{bmatrix} 4 & 3 & 2 & 1 \\ 0 & 3 & 2 & 1 \\ 0 & 0 & 2 & 1 \\ 0 & 0 & 0 & 1 \end{bmatrix}
$$

7. Use elementary row or column operations to calculate the ranks of these matrices:

(a) $\begin{bmatrix} 1 & 0 & 2 & 1 \\ 1 & 1 & 2 & 0 \\ 1 & -1 & 2 & 2 \\ 1 & 1 & 2 & 0 \end{bmatrix}$
   (b) $\begin{bmatrix} 1 & 2 & 3 & 4 & 5 \\ 1 & 0 & -1 & 3 & 1 \\ 2 & 1 & 1 & 0 & 1 \\ 0 & 3 & 8 & -5 & 3 \\ -1 & 2 & 6 & -2 & 3 \\ 1 & 1 & 2 & -3 & 0 \end{bmatrix}$

8. Find a generalized inverse of the matrix

$$\mathbf{A} = \begin{bmatrix} 3 & 4 & 5 \\ 4 & 5 & 6 \\ 5 & 6 & 7 \end{bmatrix}$$

and use it to solve the system of equations $\mathbf{x}'\mathbf{A}' = [0, 1, 2]$.

9. Determine the solution to the system of equations

$$2x_1 - x_2 + x_3 = 2$$
$$x_1 + 4x_2 - 2x_3 = -1$$
$$2x_1 + 2x_2 + x_3 = 0$$

10. Verify that the system of homogeneous equations

$$x_1 + x_2 + x_3 = 0$$
$$-x_1 + 2x_2 - x_3 = 0$$
$$3x_1 + 3x_3 = 0$$

has a nontrivial solution and obtain all linearly independent solutions to the system.

11. Determine the rank of the system of equations

$$2x_1 + x_2 + x_3 = 0$$
$$x_1 + 2x_2 - x_3 + 3x_4 = 0$$
$$x_1 - x_2 + 3x_3 - 4x_4 = 0$$
$$3x_2 - 4x_3 + 7x_4 = 0$$

and compute its solution by the method of generalized inverses.

12. Identity those vectors of the set

$$\mathbf{t}' = [\tfrac{1}{2}, \tfrac{1}{2}, \tfrac{1}{2}, \tfrac{1}{2}]$$
$$\mathbf{u}' = [1, 0, -1, 0]$$
$$\mathbf{v}' = \left[\frac{\sqrt{2}}{2}, 0, \frac{\sqrt{2}}{2}, 0\right]$$

that are orthogonal or orthonormal, and compute the angles of each pair of vectors.

13. Verify that the matrix

$$\begin{bmatrix} \dfrac{\sqrt{3}}{2} & \dfrac{1}{2} & 0 \\[2mm] -\dfrac{\sqrt{2}}{4} & \dfrac{\sqrt{6}}{4} & -\dfrac{\sqrt{2}}{2} \\[2mm] -\dfrac{\sqrt{2}}{4} & \dfrac{\sqrt{6}}{4} & \dfrac{\sqrt{2}}{2} \end{bmatrix}$$

is orthogonal.

14. Write the matrix of the quadratic form

$$2x_1^2 - 2x_1x_2 + x_2^2 + 4x_1x_3 - 3x_3^2$$

and determine whether it is positive definite.

15. Classify the following matrices as positive definite or positive semidefinite:

$$(a)\ \begin{bmatrix} 4 & 1 & 2 \\ 1 & 4 & -1 \\ 2 & -1 & 4 \end{bmatrix} \quad (b)\ \begin{bmatrix} 1 & 0 & -1 \\ 0 & 1 & 0 \\ -1 & 0 & 1 \end{bmatrix} \quad (c)\ \begin{bmatrix} 2 & 1 & -1 \\ 1 & 2 & 1 \\ -1 & 1 & 2 \end{bmatrix}$$

16. Given the matrix

$$\mathbf{A} = \begin{bmatrix} 2 & \sqrt{2} & 0 \\ \sqrt{2} & 2 & \sqrt{2} \\ 0 & \sqrt{2} & 2 \end{bmatrix}$$

compute its characteristic roots and vectors, and determine the orthogonal matrix reducing it to diagonal form.

17. If

$$\mathbf{A} = \begin{bmatrix} 2 & -1 \\ -1 & 3 \end{bmatrix} \quad \mathbf{B} = \begin{bmatrix} 5 & 3 \\ 3 & 6 \end{bmatrix}$$

compute the sums and products of the characteristic roots of

(a) $\mathbf{A}^{-1}\mathbf{B}$ (b) $\mathbf{AB}^{-1}$

18. From the matrix of the function

$$f(x,y,z) = 4x^2 + 4y^2 + 2z^2 + 4xy + 2xz + 2yz$$

can you determine its extremal properties at the point $x = y = z = 0$?

19. Maximize $f(\mathbf{x}) = (\mathbf{a}'\mathbf{x})^2$ subject to the constraint $\mathbf{x}'\mathbf{x} = 1$.

20. Minimize the function

$$f(x,y) = x^2 + 2axy + y^2$$

where $|a| \le 1$, under the condition $xy = 1$. What is the geometrical interpretation of this problem?

21. Using expressions (5) and (7) of Sec. 2.11, show that the determinant of the

$p \times p$ matrix $\mathbf{A}$ can be written as

$$|\mathbf{A}| = 1/(a_p^{11} \cdots a_1^{11})$$
$$= a_{pp}/(a_p^{11} \cdots a_2^{11})$$

where $a_j^{11} = (1, 1)$ element of the inverse of the $j \times j$ matrix formed from the last j rows and columns of $\mathbf{A}$

$a_{pp} = pp$th element of $\mathbf{A}$