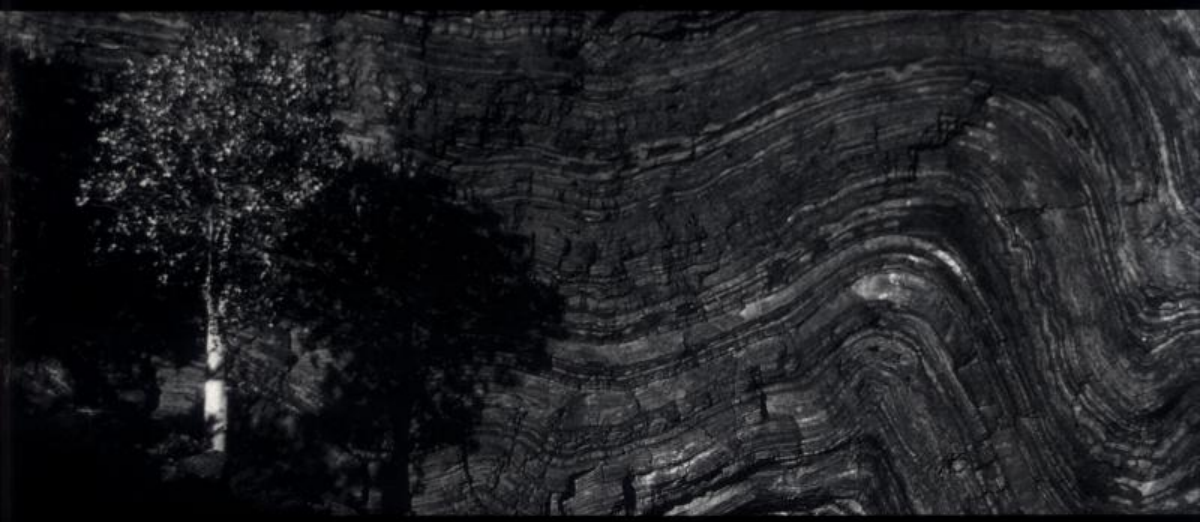
STATISTICS AND DATA ANALYSIS IN GEOLOGY

THIRD EDITION



JOHN C. DAVIS

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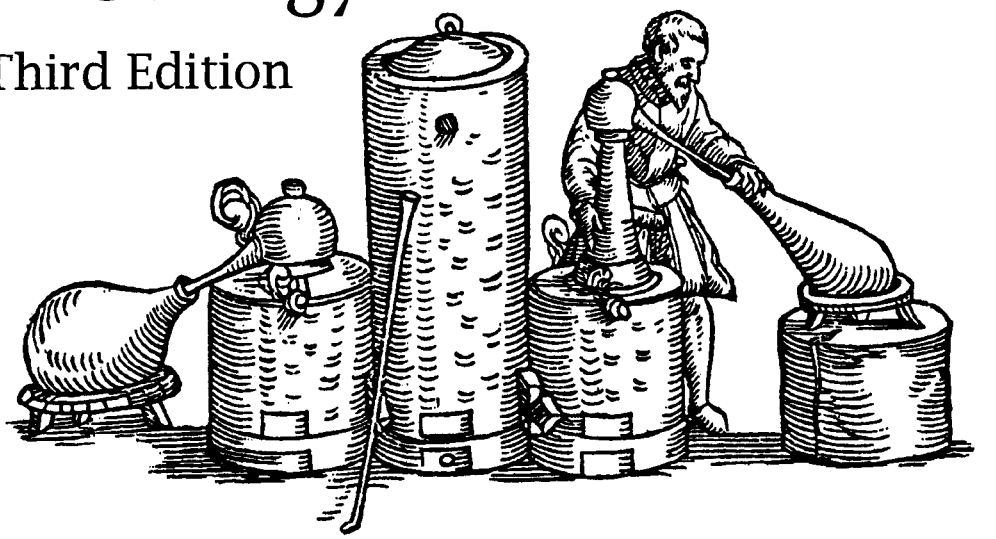

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Preface

My original motivation for writing this book, back in 1973, was very simple. Teaching the techniques of data analysis to engineers and natural scientists, both university students and industry practitioners, would be easier, I reasoned, if I had a suitable textbook. It was. By 1986 when I revised *Statistics and Data Analysis in Geology* for its second edition, technology had progressed to the point that personal computers were almost commonplace and every young geologist was expected to have at least some familiarity with computing and analysis of data. This was a time of transition when personal computers offered the freedom of access and ease of use missing in the centralized mainframe environment, but these PC's lacked the power and speed necessary for many geological applications. In the intervening years since the appearance of the second edition, computing technology has evolved with almost unbelievable speed. I now have on my desktop a small crystalline cube, a "supercomputer" capable of outperforming devices that existed a decade ago at only a few sites in the world.

Although computing tools have advanced rapidly, our skills as educators have not kept pace. Almost all undergraduate students in the natural sciences and engineering, including the Earth sciences, are required to take classes in mathematics, statistics, data analysis, and computing. Graduate students, as a matter of course, are expected to have proficiency in these areas. Unfortunately, Earth science students voice an almost universal complaint: material taught in such courses is not relevant to their studies. In part this criticism reflects a certain mental rigidity present in some young minds that refuse to make an effort to stretch their imaginations. But it also reflects, in part, the absence of anything quantitative in many geology courses.

It is not surprising when students protest, "Why should I study this dull and boring topic when the material is never used in my field?" In an attempt to contribute to the solution of this educational impasse, I've made a major change in this edition of my book. The text now includes numerous geological data sets that illustrate how specific computational procedures can be applied to problems in the Earth sciences. In addition, each chapter ends with a set of exercises of greater or lesser complexity that the student can address using methods discussed in the text. It should be noted that there is no "teacher's manual" containing correct answers. Like most real-world situations, there may be more than one solution to a problem. An answer may depend upon how a question is framed. Acknowledging that no students, not even graduate assistants, like to do drudge work such as data entry, I've provided all of the data for examples and exercises as digital files on the World Wide Web. Thus, while there may be many excuses for failing to work an exercise, entering data incorrectly should not be one of them!

We have already noted that computing technology has changed enormously during the 28 years this book has been in print. Computers are no longer made that can read floppy disks and double-sided diskettes are being phased out by optical disks. We can be sure that computer technology will continue to evolve at a dizzying pace; to provide some degree of security from obsolescence, the data files are available on the World Wide Web at two sites, one maintained by John Wiley & Sons and the other by the Kansas Geological Survey. The WWW addresses are

http://www.wiley.com/college/davis

and

http://www.kgs.ku.edu/Mathgeo/Books/Stat/index.html

In addition to the downloadable files from the 3rd edition of *Statistics and Data Analysis in Geology*, you may also find additional data sets and exercises at this site as they are made available from time to time.

The basic arrangement of topics covered in the book is retained from earlier editions, progressing from background information to the analysis of geological sequences, then maps, and finally to multivariate observations. The discussion of elementary probability theory in Chapter 2 has been revised in recognition of the unfortunate fact that fundamentals of probability often are passed over in introductory courses in favor of a cookbook recitation of elementary statistical tests. These tests are also included here, but because probability forms the basis for almost all data analysis procedures and a thorough grounding in the concepts of probability is essential to understanding statistics, this introductory section has been expanded. The discussion of nonparametric methods introduced in the 2nd edition has been expanded because geologic data, particularly data collected in the field, seldom satisfy the distribution assumptions of classical parametric statistics. The effects of closure, which results in unwarranted relationships between variables when they are forced to sum to a constant value, are examined in detail. Geological measurements such as geochemical, petrographic, and petrophysical analyses, grain-size distributions—in fact, any set of values expressed as percentages—constitute compositional data and are subject to closure effects. The statistical transformations proposed by John Aitchison to overcome these problems are discussed at length.

In the 2nd edition, I revised the discussion of eigenvalues and eigenvectors because these topics had proved to be difficult for students. They are still difficult, so their treatment in the chapter on matrix algebra has been rewritten and a new section on singular value decomposition and the relationship between R- and Q-mode factor methods has been added to the final chapter on multivariate analysis.

The central role of geostatistics and regionalized variable theory in the study of the spatial behavior of geological and other properties is now firmly established. With the help of Ricardo Olea, I have completely revised the discussion of the many varieties of kriging and provide a series of simple demonstrations to illustrate how geostatistical methodologies work. I also have revised the section on contour mapping to reflect modern practices.

A discussion of fractals has been added, not because fractals have demonstrated any particular utility in geological investigations, but because they seem to hold a promise for the future. On a more prosaic topic, the section on regression has been expanded to include several variants that have special significance in the Earth sciences. To make room for these and other discussions, some subjects that proved to be of limited utility in geologic research have been deleted. Moving most tables to the WWW sites has made additional room in the text.

Because this is not a reference book, references are not emphasized. Citations are made to more specialized or advanced texts that I have found to contain especially lucid discussions of the points in question rather than to the most definitive or original sources. Those who wish to pursue a topic in depth will find ample references to the literature in the books I have included; those that simply want an elaboration on some point will probably find the books in Suggested Readings adequate for their needs.

I am fortunate to have enjoyed the help and encouragement of many people in the creation and evolution of this book throughout its several editions. The

list of those who provided technical reviews and critical comments over the years reads like a "Who's Who" of mathematical geology and includes, in alphabetical order, Frits Agterberg, Dave Best, Paul Brockington, Jim Campbell, Ted Chang, Felix Chayes, Frank Ethridge, Je-an Fang, Colin Ferguson, John Griffiths, Jan Harff, Günther Hausberger, Ute Herzfeld, George Koch, Michael McCullagh, Gerry Middleton, Vera Pawlowsky, Floyd Preston, Nick Rock, Robert Sampson, Paul Switzer, Keith Turner, Leopold Weber, and Zhou Di. In addition, there have been dozens of others who have called or written to clarify a specific point or to bring an error to my attention, or to suggest ways in which the text could be improved. To all of these people, named and unnamed, I owe my deepest appreciation.

My esteem for my two mentors, Dan Merriam and John Harbaugh, was expressed in my dedication to the second edition of this book. My debt to these dear friends and colleagues remains as large as ever. However, those to whom I owe the greatest debt of gratitude for help with this 3rd edition are my associates and coworkers at the Kansas Geological Survey, particularly Ricardo Olea, John Doveton, and David Collins, who have provided examples, data, and exercises, and who have patiently reviewed specific topics with me in order to clarify my thoughts and to help me correct my misconceptions and errors. Ricardo has been my guide through the sometimes controversial field of geostatistics, and John has generously shared the store of instructional material and student exercises that he has patiently assembled through years of teaching petrophysics.

Most especially, I must acknowledge the assistance of Geoff Bohling, who volunteered to shoulder the burden of reading every word in the manuscript, working each example and exercise, and checking all of the computations and tables. Geoff created many of the statistical tables in the Appendix from the basic equations of distributions, and all of the calculations in the text have benefited from his careful checking and verification. Of course, any errors that remain are the responsibility of the author alone, but I would be remiss if I did not acknowledge that the number of such remaining errors would be far greater if it were not for Geoff's careful scrutiny.

I would also like to note that I have benefited from the nurturing environment of the Kansas Geological Survey (KGS) at The University of Kansas. KU has provided an intellectual greenhouse in which mathematical geology has flourished for over 30 years. I especially wish to acknowledge the support and encouragement of two previous directors of the Kansas Geological Survey, Bill Hambleton and Lee Gerhard, who recognized the importance of geology's quantitative aspects. Bill had the foresight to realize that the massive, expensive mainframe dinosaurs of computing in the 1960's would evolve into the compact, indispensable personal tools of every working geologist, and his vision kept the KGS at the forefront of computer applications. Mathematical geology advances, as does all of science, by the cumulative efforts of individuals throughout the world who share a common interest and who have learned that methodologies created in one part of the globe will find important applications elsewhere. Aware of this synergistic process, Lee encouraged visits and exchanges with the world's leaders in mathematical geology and its related disciplines, creating a heady ferment of intellectual activity that remains unique. It was with their support and encouragement that I have been able to write the three editions of this book.

My final expression of gratitude is the deepest and is owed to my editor, layout designer, proofreader, typesetter, reviewer, critic, companion, and source of

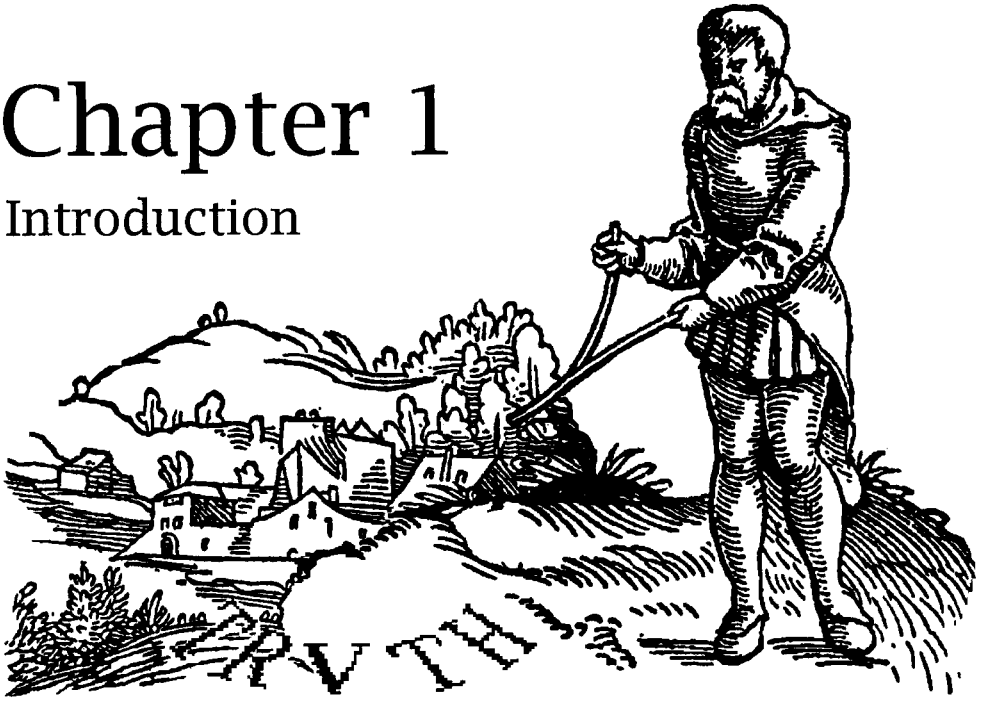
inspiration—Jo Anne DeGraffenreid, without whose tireless efforts this edition would never have been completed. She carefully polished my words, refined my grammar, and detected obscure passages, insisting that I rewrite them until they were understandable. She checked the illustrations and equations for consistency in style and format, designed the layout, selected the book type, and in a Herculean effort, set the entire manuscript in camera-ready form using the TEX typesetting language. Most importantly, she encouraged me throughout the process of seemingly never-ending revision, and took me home and poured for me a generous libation when I despaired of ever laying this albatross to rest. To her I dedicate this book.

John C. Davis
Lawrence, KS

CONTENTS

Chapter 1

Introduction



Mathematical methods have been employed by a few geologists since the earliest days of the profession. For example, mining geologists and engineers have used samples to calculate tonnages and estimate ore tenor for centuries. As Fisher pointed out (1953, p. 3), Lyell's subdivision of the Tertiary on the basis of the relative abundance of modern marine organisms is a statistical procedure. Sedimentary petrologists have regarded grain-size and shape measurements as important sources of sedimentological information since the beginning of the last century. The hybrid Earth sciences of geochemistry, geophysics, and geohydrology require a firm background in mathematics, although their procedures are primarily derived from the non-geological parent. Similarly, mineralogists and crystallographers utilize mathematical techniques derived from physical and analytical chemistry.

Although these topics are of undeniable importance to specialized disciplines, they are not the subject of this book. Since the spread of computers throughout universities and corporations in the late 1950's, geologists have been increasingly attracted to mathematical methods of data analysis. These methods have been borrowed from all scientific and engineering disciplines and applied to every facet of Earth science; it is these more general techniques that are our concern. Geology itself is responsible for some of the advances, most notably in the area of mapping and spatial analysis. However, our science has benefited more than it has contributed to the exchange of quantitative techniques.

The petroleum industry has been among the largest nongovernment users of computers in the United States, and is also the largest employer of geologists. It is not unexpected that a tremendous interest in geomathematical techniques has developed in petroleum companies, nor that this interest has spread back into the

academic world, resulting in an increasing emphasis on computer languages and mathematical skills in the training of geologists. Unfortunately, there is no broad heritage of mathematical analysis in geology—adequate educational programs have been established only in scattered institutions, through the efforts of a handful of people.

Many older geologists have been caught short in the computer revolution. Educated in a tradition that emphasized the qualitative and descriptive at the expense of the quantitative and analytical, these Earth scientists are inadequately prepared in mathematics and distrustful of statistics. Even so, members of the profession quickly grasped the potential importance of procedures that computers now make so readily available. Many institutions, both commercial and public, provide extensive libraries of computer programs that will implement geomathematical applications. Software and data are widely distributed over the World Wide Web through organizations such as the International Association for Mathematical Geology (http://www.iamg.org/). The temptation is strong, perhaps irresistible, to utilize these computer programs, even though the user may not clearly understand the underlying principles on which the programs are based.

The development and explosive proliferation of personal computers has accelerated this trend. In the quarter-century since the first appearance of this book, computers have progressed from mainframes of ponderous dimensions (but minuscule capacity) to small cubes that perch on the corner of a desk and contain the power of a supercomputer. Any geologist can buy an inexpensive computer for personal use that will perform more computations faster than the largest mainframe computers that served entire corporations and universities only a few short years ago. For many geologists, a personal computer has replaced a small army of secretaries, draftsmen, and bookkeepers. However, these ubiquitous plastic boxes with their colorful screens seem to promise much more than just word-processing and spreadsheet calculations—if only geologists knew how to put them to use in their professional work.

This book is designed to help alleviate the difficulties of geologists who feel that they can gain from a quantitative approach to their research, but are inadequately prepared by training or experience. Ideally, of course, these people should receive formal instruction in probability, statistics, numerical analysis, and programming; then they should study under a qualified geomathematician. Such an ideal is unrealistic for all but a few fortunate individuals. Most must make their way as best they can, reading, questioning, and educating themselves by trial and error. The path followed by the unschooled is not an orderly progression through topics laid out in curriculum-wise fashion. The novice proceeds backwards, attracted first to those methods that seem to offer the greatest help in the research, exploration, or operational problems being addressed. Later the self-taught amateur fills in gaps in his or her background and attempts to master the precepts of the techniques that have been applied. This unsatisfactory and even dangerous method of education, comparable perhaps to a physician learning by on-the-job training, is one many people seem destined to follow. The aim of this book is to introduce organization into the self-educational process, and guide the impatient neophyte rapidly through the necessary initial steps to a glittering algorithmic Grail. Along the way, readers will be exposed to those less glamorous topics that constitute the foundations upon which geomathematical procedures are built.

This book is also designed to aid another type of geologist-in-training—the student who has taken or is taking courses in statistics and programming. Such curriculum requirements are now nearly ubiquitous in universities throughout the world. Unfortunately, these topics are frequently taught by persons who have little knowledge of geology or any appreciation for the types of problems faced by Earth scientists. The relevance of these courses to the geologist's primary field is often obscure. A feeling of skepticism may be compounded by the absence of mathematical applications in geology courses. Many faculty members in the Earth sciences received their formal education prior to the current emphasis on geomathematical methodology, and consequently are untrained in the quantitative subjects their students are required to master. These teachers may find it difficult to demonstrate the relevance of mathematical topics. In this book, the student will find not only generalized developments of computational techniques, but also numerous examples of their applications in geology and a library of problem sets for the exercises that are included. Of course, it is my hope that both the student and the instructor will find something of interest in this book that will help promote the widening common ground we refer to as geomathematics.

The Book and the Course it Follows

Readers are entitled to know at the onset where a book will lead and how the author has arranged the journey. Because the author has made certain assumptions about the background, training, interests, and abilities of the audience, it is also necessary that readers know what is expected of them. This book is about quantitative methods for the analysis of geologic data—the area of Earth science which some call ***geomathematics*** and others call ***mathematical geology***. Also included is an introduction to geostatistics, a subspecialty that has grown into an entire branch of applied statistics.

The orientation of the book is methodological, or "how-to-do-it." Theory is not emphasized for several reasons. Most geologists tend to be pragmatists, and are far more interested in results than in theory. Many useful procedures are *ad hoc* and have no adequate theoretical background at present. Methods which are theoretically developed often are based on statistical assumptions so restrictive that the procedures are not strictly valid for geologic data. Although elementary probability is discussed and many statistical tests described, the detailed development of statistical and geostatistical theory has been left to others.

Because the most complex analytical procedure is built up of a series of relatively simple mathematical manipulations, our emphasis is on operations. These operations are most easily expressed in matrix algebra, so we will study this subject, illustrating the operations with geological examples.

The first edition of this text (published in 1973) devoted a chapter to the FORTRAN computer language and most procedures in that edition were accompanied by short program listings in FORTRAN. When the second edition appeared in 1986, FORTRAN no longer dominated scientific programming and computer centers maintained extensive libraries of statistical and mathematical routines written in many computer languages. Large statistical packages implemented almost every procedure described in the text, so program listings were no longer necessary. Now at

the time of this third edition, there are many easy-to-use interactive programs to perform almost any desired statistical calculation; these programs have graphical interfaces and run on personal computers. In addition, there are inexpensive, specialized programs for geostatistics, for analysis of compositional data, and for other "nonstandard" procedures of interest to Earth scientists. Some of these are distributed free or at nominal cost as "shareware." Computation is no longer among the major problems facing researchers today; they must be concerned, rather, with interpretation and the appropriateness of their approach. As a consequence, this third edition contains many more worked examples and also includes an extensive library of problem sets accessible over the Internet.

The discussion in the following chapters begins with the basic topics of probability and elementary statistics, including the special steps necessary to analyze compositional data, or variables such as chemical analyses and grain-size categories that sum to a constant. The next topic is matrix algebra. Then we will consider the analysis of various types of geologic data that have been classified arbitrarily into three categories: (1) data in which the sequence of observations is important, (2) data in which the two-dimensional relationships between observations are important, and (3) multivariate data in which order and location of the observations are not considered.

The first category contains all classes of problems in which data have been collected along a continuum, either of time or distance. It includes time series, calculation of semivariograms, analysis of stratigraphic sections, and the interpretation of chart recordings such as well logs. The second category includes problems in which spatial coordinates or geographic locations of samples are important, *i.e.*, studies of shape and orientation, contour mapping, trend-surface analysis, geostatistics including kriging, and similar endeavors. The final category is concerned with clustering, classification, and the examination of interrelations among variables in which sample locations on a map or traverse are not considered. Paleontological, mineralogical, and geochemical data often are of this type.

The topics proceed from simple to complex. However, each successive topic is built upon its predecessors, so aspects of multiple regression, covered in Chapter 6, have been discussed in trend analysis (Chapter 5), which has in turn been preceded by curvilinear regression (Chapter 4). The basic mathematical procedure involved has been described under the solution of simultaneous equations (Chapter 3), and the statistical basis of regression has first been discussed in Chapter 2. Other techniques are similarly developed.

The first topic in the book is elementary statistics. The final topic is canonical correlation. These two subjects are separated by a wide gulf that would require several years to bridge following a typical course of study. Obviously, we cannot cover this span in a single book without omitting a tremendous amount of material. What has been sacrificed are all but the rudiments of statistical theory associated with each of the techniques, the details of all mathematical operations except those that are absolutely essential, and all the embellishments and refinements that typically are added to the basic procedures. What has been retained are the fundamental algorithms involved in each analysis, discussions of the relations between quantitative techniques and example applications to geologic problems, and references to sources for additional details.

My contention is that a quantitative approach to geology can yield a fruitful return to the investigator; not so much, perhaps, by "proving" a geological hypothesis or demonstrating its validity, but by gaining insights from the critical examination of phenomena that is prerequisite to any quantitative procedure. Numerical analysis requires that collection of data be carefully controlled, with consideration given to extraneous influences. As a consequence, the investigator may acquire a closer familiarity with the objects of study than could otherwise be attained. Certainly a paleontologist who has made careful measurements on a large collection of randomly selected fossil specimens has a far greater and more accurate understanding of the natural variation of these organisms than does the paleontologist who relies on informal examination. The rigor and objectivity required by quantitative methodologies can compensate in part for insight and experience which otherwise must be gained by many years of work. At the same time, the discipline necessary to perform quantitative research will hasten the growth and maturity of the scientist.

The measurement and analysis of data may lead to interpretations that are not obvious or apparent when other means of investigation are used. Multivariate methods, for example, may reveal clusterings of objects that are at variance with accepted classifications, or may show relationships between variables where none were expected. These findings require explanation. Sometimes a plausible explanation cannot be found; but in other instances, new theories may be suggested which would otherwise have been overlooked.

Perhaps the greatest worth of quantitative methodologies lies not in their capability to demonstrate what is true, but rather in their ability to expose what is false. Quantitative techniques can reveal the insufficiency of data, the tenuousness of assumptions, the paucity of information contained in most geologic studies. Unfortunately, upon careful and dispassionate analysis, many geological interpretations deteriorate into a collection of guesses and hunches based on very little data, of which most are of a contradictory or inconclusive nature.

If geology were an experimental science like chemistry or physics—in which observations can be verified by any competent worker—controversy and conflict might disappear. However, geologists are practitioners of an observational science, and the rigorous application of quantitative methods often reveals us for the imperfect observers that we are. Indeed, a decline into scientific skepticism is one of the dangers that often traps geomathematicians. These workers are often characterized by a suspicious and iconoclastic attitude toward geological platitudes. Sadly it must be confessed that such cynicism is often justified. Geologists are trained to see patterns and structure in nature. Geomathematical methods provide the objectivity necessary to avoid creating these patterns when they may exist only in the scientist's desire for order.

Statistics in Geology

All of the techniques of quantitative geology discussed in this book can be regarded as statistical procedures, or perhaps "quasi-statistical" or "proto-statistical" procedures. Some are sufficiently well developed to be used in rigorous tests of statistical hypotheses. Other procedures are *ad hoc*; results from their application must be judged on utilitarian rather than theoretical grounds. Unfortunately, there is no adequate general theory about the nature of geological populations, although geology can boast of some original contributions to the subject, such as the theory of regionalized variables. However, like statistical tests, geomathematical techniques are based on the premise that information about a phenomenon can be deduced from an examination of a small sample collected from a vastly larger set of potential observations on the phenomenon.

Consider subsurface structure mapping for petroleum exploration. Data are derived from scattered boreholes that pierce successive stratigraphic horizons. The elevation of the top of a horizon measured in one of these holes constitutes a single observation. Obviously, an infinite number of measurements of the top of this horizon could be made if we drilled unlimited numbers of holes. This cannot be done; we are restricted to those holes which have actually been drilled, and perhaps to a few additional test holes whose drilling we can authorize. From these data we must deduce as best we can the configuration of the top of the horizon between boreholes. The problem is analogous to statistical analysis; but unlike the classical statistician, we cannot design the pattern of holes or control the manner in which the data were obtained. However, we can use quantitative mapping techniques that are either closely related to statistical procedures or rely on novel statistical concepts. Even though traditional forms of statistical tests may be beyond our grasp, the basic underlying concepts are the same.

In contrast, we might consider mine development and production. For years mining geologists and engineers have carefully designed sampling schemes and drilling plans and subjected their observations to statistical analyses. A veritable blizzard of publications has been issued on mine sampling. Several elaborate statistical distributions have been proposed to account for the variation in mine values, providing a theoretical basis for formal statistical tests. When geologists can control the means of obtaining samples, they are quick to exploit the opportunity. The success of mining geologists and engineers in the assessment of mineral deposits testifies to the power of these methods.

Unfortunately, most geologists must collect their observations where they can. Logs of oil wells have been made at too great a cost to ignore merely because the well locations do not fit into a predesigned sampling plan. Paleontologists must be content with the fossils they can glean from the outcrop; those buried in the subsurface are forever beyond their reach. Rock specimens can be collected from the tops of batholiths in exposures along canyon walls, but examples from the roots of these same bodies are hopelessly deep in the Earth. The problem is seldom too much data in one place. Rather, it is too little data elsewhere. Our observations of the Earth are too precious to discard lightly. We must attempt to wring from them what knowledge we can, recognizing the bias and imperfections of that knowledge.

Many publications on the design of statistical experiments and sampling plans have appeared. Notable among these is the geological text by Griffiths (1967), which

is in large part concerned with the effect sampling has on the outcome of statistical tests. Although Griffiths' examples are drawn from sedimentary petrology, the methods are equally applicable to other problems in the Earth sciences. The book represents a rigorous, formal approach to the interpretation of geologic phenomena using statistical methods. Griffiths' book, unfortunately now out of print, is especially commended to those who wish to perform experiments in geology and can exercise strict control over their sampling procedures. In this text we will concern ourselves with those less tractable situations where the sample design (either by chance or misfortune) is beyond our control. However, be warned that an uncontrolled experiment (*i.e.*, one in which the investigator has no influence over where or how observations are taken) usually takes us outside the realm of classical statistics. This is the area of "quasi-statistics" or "proto-statistics," where the assumptions of formal statistics cannot safely be made. Here, the well-developed formal tests of hypotheses do not exist, and the best we can hope from our procedures is guidance in what ultimately must be a human judgment.

Measurement Systems

A quantitative approach to geology requires something more profound than a headlong rush into the field armed with a personal computer. Because the conclusions reached in a quantitative study will be based at least in part on inferences drawn from measurements, the geologist must be aware of the nature of the number systems in which the measurements are made. Not only must the Earth scientist understand the geological significance of the recorded variables, the mathematical significance of the measurement scales used must also be understood. This topic is more complex than it might seem at first glance. Detailed discussions and references can be found in Stevens (1946), the book edited by Churchman and Ratoosh (1959) and, from a geologist's point of view, in Griffiths (1960).

A ***measurement*** is a numerical value assigned to an observation which reflects the magnitude or amount of some characteristic. The manner in which numerical values are assigned determines the ***scale of measurement***, and this in turn determines the type of analyses that can be made of the data. There are four measurement scales, each more rigorously defined than its predecessor, and each containing greater information. The first two are the nominal scale and the ordinal scale, in which observations are simply classified into mutually exclusive categories. The final two scales, the interval and ratio, are those we ordinarily think of as "measurements" because they involve determination of the magnitudes of an attribute.

The ***nominal scale*** of measurement consists of a classification of observations into mutually exclusive categories of equal rank. These categories may be identified by names, such as "red," "green," and "blue," by labels such as "A," "B," and "C," by symbols such as ✸, ☼, and ●, or by numbers. However, numbers are used only as identifiers. There can be no connotation that 2 is "twice as much" as 1, or that 5 is "greater than" 4. Binary-state variables are a special type of nominal data in which symbolic tags such as 1 and 0, "yes" and "no," or "on" and "off" indicate the presence or absence of a condition, feature, or organism. The classification of fossils as to type is an example of nominal measurement. Identification of one

fossil as a brachiopod and another as a crinoid implies nothing about the relative importance or magnitude of the two.

The number of observations occurring in each state of a nominal system can be counted, and certain nonparametric tests can be performed on nominal data. A classic example we will consider at length is the occurrence of heads or tails in a coin-flipping experiment. Heads and tails constitute two categories of a nominal scale, and our data will consist of the number of observations that fall into them. A geologic equivalent of this problem consists of the appearance of feldspar and quartz grains along a traverse across a thin section. Quartz and feldspar form mutually exclusive categories that cannot be meaningfully ranked in any way.

Sometimes observations can be ranked in a hierarchy of states. Mohs' hardness scale is a classic example of a ranked or ***ordinal scale.*** Although the minerals on the scale, which extends from one to ten, increase in hardness with higher rank, the steps between successive states are not equal. The difference in absolute hardness between diamond (rank ten) and corundum (rank nine) is greater than the entire range of hardness from one to nine. Similarly, metamorphic rocks may be ranked along a scale of metamorphic grade, which reflects the intensity of alteration. However, the steps between grades do not represent a uniform progression of temperature and pressure.

As with the nominal scale, a quantitative analysis of ordinal measurements is restricted primarily to counting observations in the various states. However, we can also consider the manner in which different ordinal classes succeed one another. This is done, for example, by determining if states tend to be followed an unusual number of times by greater or lesser states on the ordinal scale.

The ***interval scale*** is so named because the length of successive intervals is a constant. The most commonly cited example of an interval scale is that of temperature. The increase in temperature between 10° and 20° C is exactly the same as the increase between 110° and 120° C. However, an interval scale has no natural zero, or point where the magnitude is nonexistent. Thus, we can have negative temperatures that are less than zero. The starting point for the Celsius (centigrade) scale was *arbitrarily set* at a point coinciding with the freezing point of water, whereas the starting point on the Fahrenheit scale was chosen as the lowest temperature reached by an equal mixture of snow and salt. To convert from one interval scale to another, we must perform two operations: a multiplication to change the scale, and an addition or subtraction to shift the arbitrary origin.

Ratio scales have not only equal increments between steps, but also a true zero point. Measurements of length are of this type. A 2-in. long shell is twice the length of a 1-in. shell. A shell with zero length does not exist, because it has no length at all. It is generally agreed that "negative lengths" are not possible. To convert from one ratio scale to another, such as from inches to centimeters, we must only perform the single operation of multiplication.

Ratio scales are the highest form of measurement. All types of mathematical and statistical operations may be performed with them. Although interval scales in theory convey less information than ratio scales, for most purposes the two can be used in the same manner. Almost all geological data consist of continuously distributed measurements made on ratio or interval scales, because these include the basic physical properties of length, volume, mass, and the like. In subsequent chapters, we will not distinguish between the two measurement scales, and they

may occur intermixed in the same problem. An example occurs in trend-surface analysis where an independent variable may be measured on a ratio scale while the geographic coordinates are on an interval scale, because the coordinate grid has an arbitrary origin.

A False Feeling of Security

Perhaps this chapter should be concluded with a precautionary note. If you pursue the following topics, you will become involved with mathematical methods that have a certain aura of exactitude, that express relationships with apparent precision, and that are implemented on devices that have a popular reputation for infallibility. Computers can be used very effectively as devices of intimidation. The presentation of masses of numbers, all expressed to eight decimal places, overwhelms the minds of many people and numbs their natural skepticism. A geologic report couched in mathematical jargon and filled with computer output usually will bluff all but a few critics, and those who understand and comment often do so in equally obtuse terms. Hence, both the report and criticism pass over the heads of most of the intended audience. The greatest danger, however, is to researchers themselves. If they fall sway to their own computers, they may cease to critically examine their data and the interpretative methods. Hypnotized by numbers, he or she may be led to the most ludicrous conclusions, totally blind to any reality beyond the computer screen. Keep in mind the little phrase posted on the wall of every computation center: "GIGO—Garbage In, Garbage Out."

The first chapter in the first edition of this book began and ended with quotations; these were repeated in the second edition. I have no reason to remove them now, as they are as relevant today as they were then. An anonymous critic left the following rhyme on my desk almost 30 years ago. It remains posted on my wall to this day.

What could be cuter
Than to feed a computer
With wrong information
But naive expectation
To obtain with precision
A Napoleonic decision?

— Major Alexander P. de Seversky

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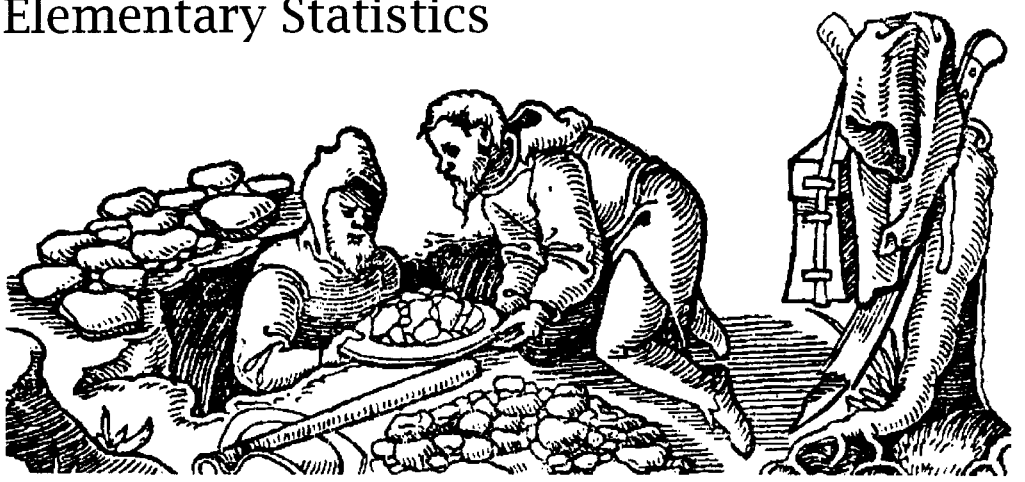
Chapter 2
Elementary Statistics



Geologists' direct observations of our world are confined to the outer part of the Earth's crust, yet they must attempt to understand the nature of the Earth's core and mantle and the deeper parts of the crust. Furthermore, the processes that modify the Earth, such as mountain building and continental evolution, are generally beyond the geologists' capabilities for direct manipulation. No other scientists, with the exception of astronomers, are more removed from the bulk of their study material and less able to experiment on their subject.

Geology, to a major extent, remains a science that is principally concerned with observation. Because geologists depend heavily on observations, particularly observations in which there is a large portion of uncertainty, statistics should play an important role in their research. Although the term "statistics" once referred simply to the collection of numerical facts such as baseball scores, it has come to include the analysis of data, and especially the uncertainty associated with such data. Statistical problems, whether perceived or not, occur wherever there are elements of chance. Geologists need to be conscious of these problems, and of some of the statistical tools that are available to help solve the problems.

Probability

Although many descriptions and definitions of statistics have been written, it perhaps may be best considered as the determination of the probable from the possible. In any circumstance, there are a variety (sometimes an infinity) of possible outcomes. All these have an associated probability that describes their frequency of occurrence. From an analysis of probabilities associated with events, future behavior or past states of the object or event under study may be estimated.

All of us have an intuitive concept of probability. For example, if asked to guess whether it will rain tomorrow, most of us would reply with some confidence that rain is likely or unlikely, or perhaps in rare circumstances, that it is certain to rain, or certain not to rain. An alternative way of expressing our estimate would be to

use a numerical scale, as for example a percentage scale. If we state that the chance of rain tomorrow is 30%, then we imply that the chance of it not raining is 70%.

Scientists usually express probability as an arbitrary number ranging from 0 to 1, or an equivalent percentage ranging from 0 to 100%. If we say that the probability of rain tomorrow is 0, we imply that we are absolutely certain that it will not rain. If, on the other hand, we state that the probability of rain is 1, we are absolutely certain that it will. Probability, expressed in this form, pertains to the likelihood of an event. Absolute certainty is expressed at the ends of this scale, 0 and 1, with different degrees of uncertainty in between. For example, if we rate the probability of rain tomorrow as 1/2 (and therefore of no rain as 1/2), we express our view with a maximum degree of uncertainty; the likelihood of rain is equal to that of no rain. If we rate the probability of rain as 3/4 (1/4 probability of no rain), we express a smaller degree of uncertainty, for we imply that it is three times as likely to rain as it is not to rain.

Our estimates of the likelihood of rain may be based on many different factors, including a subjective "feeling" about the matter. We may utilize the past behavior of a phenomenon such as the weather to provide insight into its probable future behavior. This "relative frequency" approach to probability is intuitively appealing to geologists, because the concept is closely akin to uniformitarianism. Other methods of defining and arriving at probabilities may be more appropriate in certain circumstances. In carefully prescribed games of chance, the probabilities attached to a specific outcome can be calculated exactly by combinatorial mathematics; we will use this concept of probability in our initial discussions because of its relative simplicity. An entire branch of statistics treats probabilities as subjective expressions of the "degree of belief" that a particular outcome will occur. We must rely on the subjective opinions of experts when considering such questions as the probability of failure of a new machine for which there is no past history of performance. The subjective approach is widely used (although seldom admitted to) in the assessment of the risks associated with petroleum and mineral exploration, where relative-frequency based estimates of geologic conditions and events are difficult to obtain (Harbaugh, Davis, and Wendebourg, 1995). The implications contained in various concepts of probability are discussed in books by von Mises (1981) and Fisher (1973). Fortunately, the mathematical manipulations of probabilities are identical regardless of the source of the probabilities.

The chance of rain is a discrete probability; it either will or will not rain. A classic example of discrete probability, used almost universally in statistics texts, pertains to the outcome of the toss of an unbiased coin. A single toss has two outcomes, heads or tails. Each is equally likely, so the probability of obtaining a head is 1/2. This does not imply that every other toss will be a head, but rather that, in the long run, heads will appear one-half of the time. Coin tossing is, then, a clear-cut example of discrete probability. The event has two states and must occupy one or the other; except for the vanishingly small possibility that the coin will land precisely on edge, it must come up either heads or tails.

An interesting series of probabilities can be formed based on coin tossing. If the probability of obtaining heads is 1/2, the probability of obtaining two heads in a row is $1/2 \cdot 1/2 = 1/4$. Perhaps we are interested in knowing the probabilities of obtaining three heads in a row; this will be $1/2 \cdot 1/2 \cdot 1/2 = 1/8$. The logic behind this progression is simple. On the first toss, our chances are 1/2 of obtaining a head. If we do, our chances of obtaining a second head are again 1/2, because the

second toss is not dependent in any way on the first. Likewise, the third toss is independent of the two preceding tosses, and has an associated probability of 1/2 for heads. So, we have "one-half of one-half of one-half" of a chance of getting all three heads.

Suppose instead that we are interested in the probability of obtaining only one head in three tosses. All possible outcomes, denoting heads as H and tails as T, are:

HHH	HTH	TTT
HHT	THH	[THT]
[HTT]	[TTH]	

Bracketed combinations are those that satisfy our requirements that they contain only one head. Because there are eight possible combinations, the probability of getting only one head in three tosses is 3/8.

What we have found is the number of possible ***combinations*** of three things (either heads or tails), taken one item at a time. This can be generalized to the number of possible combinations of n items taken r at a time. Symbolically, this is represented as $\binom{n}{r}$.

It can be demonstrated that the number of possible combinations of n items, taken r items at a time, is

$$\binom{n}{r} = \frac{n!}{r!(n-r)!} \tag{2.1}$$

The exclamation points stand for ***factorial*** and mean that the number preceding the exclamation point is multiplied by the number less one, then by the number less two, and so on:

$$n! = n \cdot (n-1) \cdot (n-2) \cdot (n-3) \cdot \ldots \cdot \tag{2.2}$$

The value of 3! is $3 \cdot 2 \cdot 1 = 6$. In our coin-flipping problem,

$$\binom{3}{1} = \frac{3!}{1!(3-1)!} = \frac{3 \cdot 2 \cdot 1}{1 \cdot (2 \cdot 1)} = \frac{6}{2} = 3$$

That is, there are three possible combinations that will contain one head. By this equation, how many possible combinations are there that contain exactly two heads?

$$\binom{3}{2} = \frac{3!}{2!(3-2)!} = \frac{3 \cdot 2 \cdot 1}{2 \cdot 1(1)} = \frac{6}{2} = 3$$

HHH	[HTH]	TTT
[HHT]	[THH]	THT
HTT	TTH	

These combinations are bracketed above in our collection of possible outcomes.

Next, how many possible combinations of three tosses contain exactly three heads?

$$\binom{3}{3} = \frac{3!}{3!(3-3)!} = \frac{3 \cdot 2 \cdot 1}{3 \cdot 2 \cdot 1(1)} = 1$$

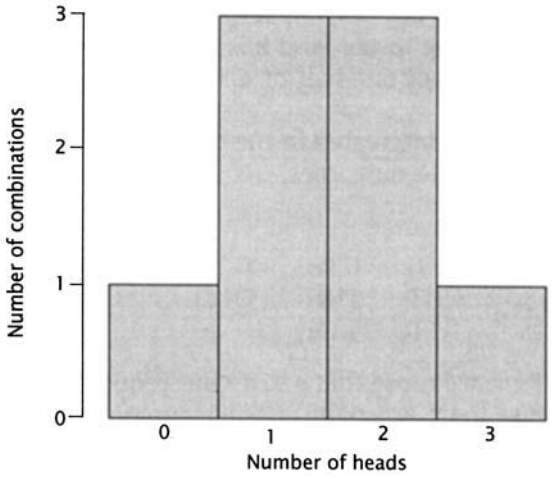


Figure 2–1. Bar graph showing the number of different ways to obtain a specified number of heads in three flips of a coin.

Note that 0! is defined as being one, not zero. Finally, the remaining possibility is the number of combinations that contain no heads:

$$\binom{3}{0} = \frac{3!}{0!(3-0)!} = \frac{3 \cdot 2 \cdot 1}{1(3 \cdot 2 \cdot 1)} = 1$$

Thus, with three flips of a coin, there is one way we can get no heads, three ways we can get one head, three ways we can get two heads, and one way we can get all heads. This can be shown in the form of a bar graph as in **Figure 2–1**.

We can count the number of total possible combinations, which is eight, and convert the frequencies of occurrence into probabilities. That is, the probability of getting no heads in three flips is one correct combination [TTT] out of eight possible, or 1/8. Our histogram now can be redrawn and expressed in probabilities, giving the discrete probability distribution shown in **Figure 2–2**. The total area under the distribution is 8/8, or 1. We are thus certain of getting some combination on the three tosses; the shape of the distribution function describes the likelihood of getting any specific combination. The coin-flipping experiment has four characteristics:

1. There are only two possible outcomes (call them "success" and "failure") for each trial or flip.
2. Each trial is independent of all others.
3. The probability of a success does not change from trial to trial.
4. The trials are performed a fixed number of times.

The probability distribution that governs experiments such as this is called the ***binomial distribution***. Among its geological applications, it may be used to forecast the probability of success in a program of drilling for oil or gas. The four characteristics listed above must be assumed to be true; such assumptions seem most reasonable when applied to "wildcat" exploration in relatively virgin basins. Hence, the binomial distribution often is used to predict the outcomes of drilling programs in frontier areas and offshore concessions.

Under the assumptions of the binomial distribution, each wildcat must be classified as either a discovery ("success") or a dry hole ("failure"). Successive wildcats

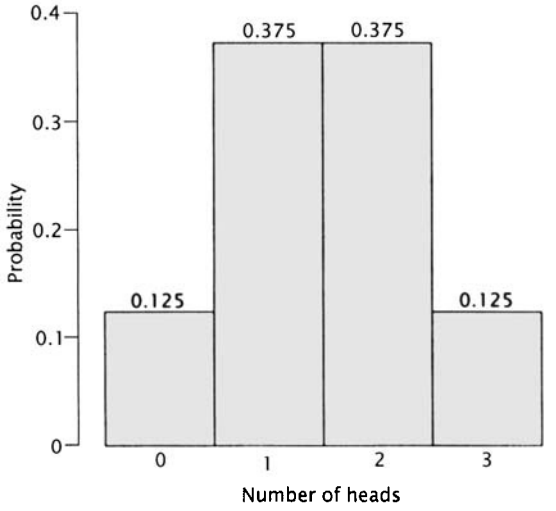


Figure 2–2. Discrete distribution giving the probability of obtaining specified numbers of heads in three flips of a coin.

are presumed to be independent; that is, success or failure of one hole will not influence the outcome of the next hole. (This assumption is difficult to justify in most circumstances, as a discovery usually will affect the selection of subsequent drilling sites. A protracted succession of dry holes will also cause a shift in an exploration program.) The probability of a discovery is assumed to remain unchanged. (This assumption is reasonable at the initiation of exploration, but becomes increasingly tenuous during later phases when a large proportion of the fields in a basin have been discovered.) Finally, the binomial is appropriate when a fixed number of holes will be drilled during an exploratory program, or during a single time period (perhaps a budget cycle) for which the forecast is being made.

The probability p that a wildcat hole will discover oil or gas can be estimated using industry-wide success ratios that have been observed during drilling in similar regions, using the success ratio of the particular company making the evaluation, or simply by making a subjective "guess." From p, the binomial model can be developed as it relates to exploratory drilling in the following steps:

1. The probability that a hole will result in a discovery is p.
2. Therefore, the probability that a hole will be dry is $1 - p$.
3. The probability that n successive wildcats will all be dry is

$$P = (1 - p)^n$$

4. The probability that the nth hole drilled will be a discovery but the preceding $(n - 1)$ holes will all be dry is

$$P = (1 - p)^{n-1}p$$

5. The probability of one discovery in a series of n wildcat holes is

$$P = n(1 - p)^{n-1}p$$

since the discovery can occur on *any* of the n wildcats.

6. The probability that $(n - r)$ dry holes will be drilled, followed by r discoveries, is

$$P = (1 - p)^{n-r}p^r$$

7. However, the $(n - r)$ dry holes and the r discoveries may be arranged in $\binom{n}{r}$ combinations or, equivalently, in $n!/(n - r)!r!$ different ways. So, the probability that r discoveries will be made in a drilling program of n wildcats is

$$P = \frac{n!}{(n-r)!r!}(1-p)^{n-r}p^r \tag{2.3}$$

This is an expression of the binomial distribution, and gives the probability that r successes will occur in n trials, when the probability of success in a single trial is p.

The binomial equation can be solved to determine the probability of occurrence of any particular combination of successes and failures, for any desired number of trials and any specified probability. These probabilities have already been computed and tabulated for many combinations of n, r, and p. Using either the equation or published tables such as those in Hald (1952), many interesting questions can be investigated. For example, suppose we wish to develop the probabilities associated with a five-hole exploration program in a virgin basin where the success ratio is anticipated to be about 10%. What is the probability that the entire exploration program will be a total failure, with no discoveries? Such an outcome is called "gambler's ruin" for obvious reasons, and the binomial expression has the terms

$$n = 5$$
$$r = 0$$
$$p = 0.10$$
$$P = \binom{5}{0} \cdot 0.10^0 \cdot (1 - 0.10)^5$$
$$= \frac{5!}{5!0!} \cdot 1 \cdot 0.90^5$$
$$= 1 \cdot 1 \cdot 0.59 = 0.59$$

The probability that no discoveries will result from the exploratory effort is almost 60%.

If only one hole is a discovery, it may pay off the costs of the entire exploration effort. What is the probability that one well will come in during the five-hole exploration campaign?

$$P = \binom{5}{1} \cdot 0.10^1 \cdot (1 - 0.10)^4$$
$$= \frac{5!}{4!1!} \cdot 0.10 \cdot 0.90^4$$
$$= 5 \cdot 0.10 \cdot 0.656 = 0.328$$

Using either the binomial equation or a table of the binomial distribution, the probabilities associated with all possible outcomes of the five-hole drilling program can be found. These are shown in **Figure 2–3.**

Other discrete probability distributions can be developed for those experimental situations where the basic assumptions are different. Suppose, for example, an

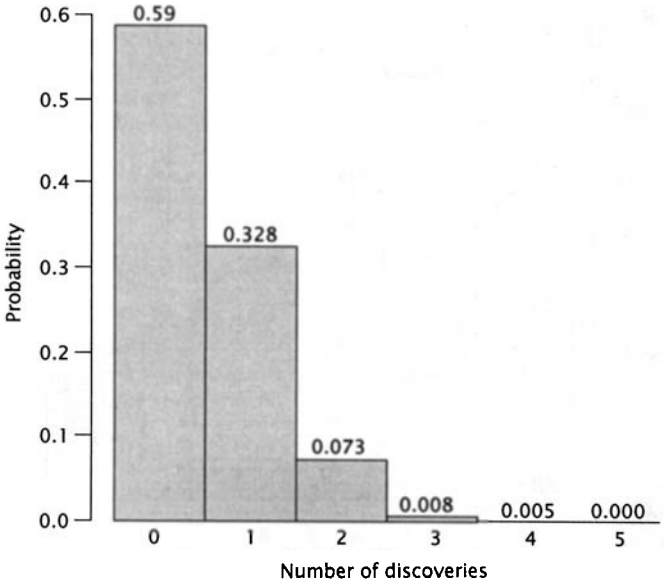


Figure 2–3. Discrete distribution giving the probability of making n discoveries in a five-hole drilling program when the success ratio (probability of a discovery) is 10%.

exploration company is determined to discover two new fields in a virgin basin it is prospecting, and will drill as many holes as required to achieve its goal. We can investigate the probability that it will require $2, 3, 4, \ldots$, up to n exploratory holes before two discoveries are made. The same conditions that govern the binomial distribution may be assumed, except that the number of "trials" is not fixed.

The probability distribution that governs such an experiment is called the ***negative binomial***, and its development is very similar to that of the binomial distribution. As in that example, p is the probability of a discovery and r is the number of "successes" or discovery wells. However, n, the number of trials, is not specified. Instead, we wish to find the probability that x dry holes will be drilled before r discoveries are made. The negative binomial has the form

$$P = \binom{r + x - 1}{x} (1 - p)^x p^r \tag{2.4}$$

Note the similarity between this equation and Equation (2.3); the term $r + x - 1$ appears because the last hole drilled in a sequence must be the rth success. Expanding Equation (2.4) gives

$$P = \frac{(r + x - 1)!}{(r - 1)!\,x!} (1 - p)^x p^r \tag{2.5}$$

If the regional success ratio is assumed to be 10%, the probability that a two-hole exploration program will meet the company's goal of two discoveries can be calculated:

$$P = \frac{(2 + 0 - 1)!}{(2 - 1)!0!} \cdot (1 - 0.10)^0 \cdot 0.10^2$$

$$= \frac{1!}{1!0!} \cdot 0.90^0 \cdot 0.10^2$$

$$= 1 \cdot 1 \cdot 0.01 = 0.01$$

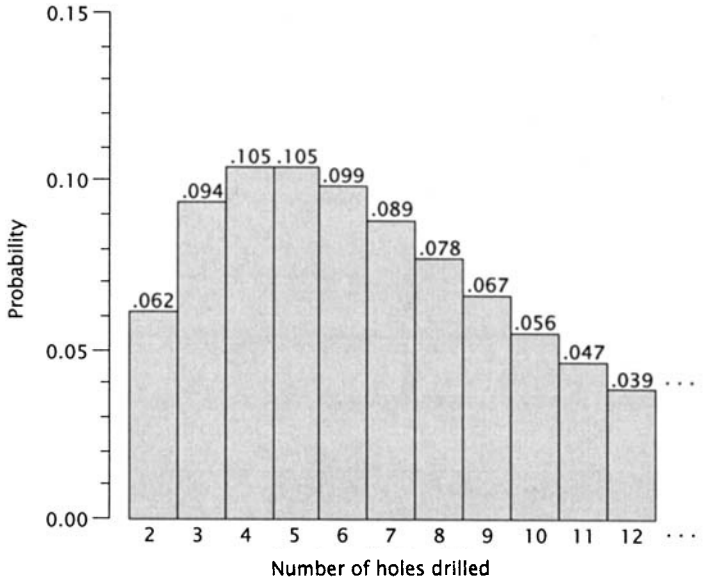


Figure 2–4. Discrete distribution for exactly two successes in a drilling program of n exploratory holes when the probability of a discovery is 25%.

The probabilities attached to other drilling programs having different numbers of holes or probabilities of success can be found in a similar way. The possibility that five holes will be required to achieve two successes when the regional success ratio is 25% is

$$P = \frac{(2+3-1)!}{(2-1)!3!} \cdot (1-0.25)^3 \cdot 0.25^2$$
$$= \frac{24}{1 \cdot 6} \cdot 0.422 \cdot 0.062 = 0.105$$

We can calculate the probabilities attached to a succession of possible outcomes and plot the results in the form of a distribution, just as we have done previously. **Figure 2–4** is a negative binomial probability distribution for a drilling program where the probability of a discovery on any hole is 25% and the drilling program will continue until exactly two discoveries have been made. Obviously, this distribution must start at two, since this is the minimum number of holes that might be required, and continues without limit (in the event of extremely bad luck!); we show the distribution only up to 12 holes.

The probabilities calculated are low because they relate to the likelihood of obtaining two successes and exactly x dry holes. It may be more useful to consider the distribution of the probability that more than x dry holes must be drilled before the goal of r discoveries is achieved. This is found by first calculating the negative binomial distribution in ***cumulative form*** in which each successive probability is added to the preceding probabilities; the cumulative distribution gives the probability that the goal of two successes will be achieved in $(x + r)$ or fewer holes as shown in **Figure 2–5**. If we subtract each of these probabilities from 1.0 we obtain the desired probability distribution (**Fig. 2–6**). The negative binomial will appear again in Chapter 5, as it constitutes an important model for the distribution of points in space.

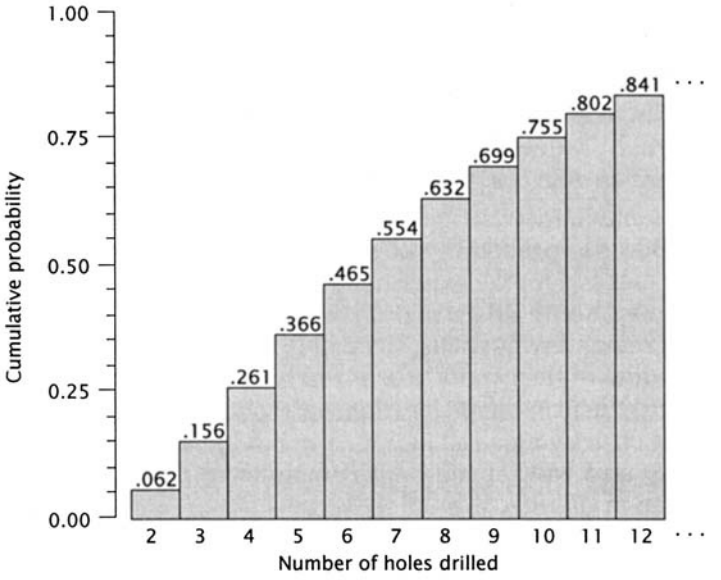


Figure 2–5. Discrete distribution giving the cumulative probability that two discoveries will be made by or before a specified hole when the probability of a discovery is 25%.

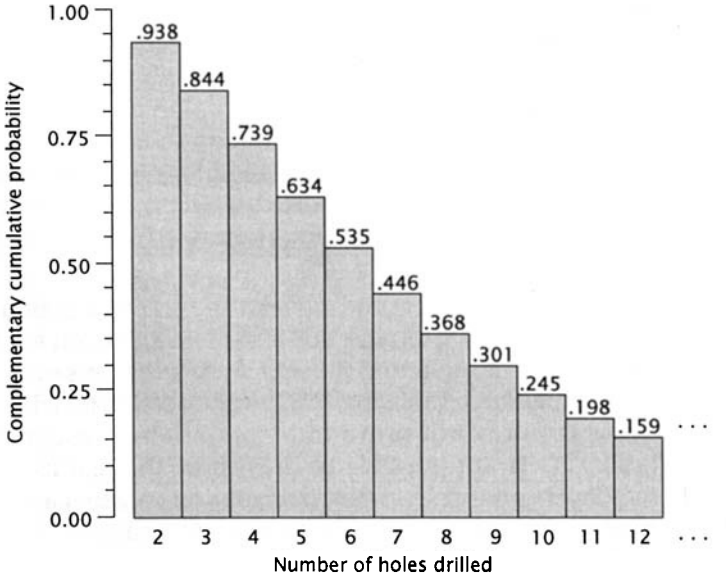


Figure 2–6. Discrete distribution giving the probability that more than a specified number of holes must be drilled to make two discoveries when the probability of a discovery is 25%.

There are other discrete probability distributions that apply to experimental situations similar to those appropriate for the binomial. These include the ***Poisson distribution***, which can be used instead of the binomial when p, the probability of success, is very small. The Poisson distribution will be discussed in Chapter 4, where it will be applied to the analysis of rare, random events in time (such as earthquakes or volcanic eruptions), and in Chapter 5, where it will serve as a model

for objects located randomly in space. The ***geometric distribution*** is a special case of the negative binomial, appropriate when interest is focused on the number of trials prior to the initial success. The ***multinomial distribution*** is an extension of the binomial where more than two mutually exclusive outcomes are possible. These topics are extensively developed in most books on probability theory, such as those by Parzen (1960) or Ash (1970).

An important characteristic of all of the discrete probability distributions just discussed is that the probability of success remains constant from trial to trial. Statisticians discuss simple experiments called ***sampling with replacement*** in which this assumption holds strictly true. A typical experiment would involve an urn filled with red and white balls; if a ball is selected at random, the probability it will be red is equal to the proportion of red balls originally in the urn. If the ball is then returned to the urn, the proportions of the two colors remain unchanged, and the probability of drawing a red ball on a second trial remains unchanged as well. The probability also will remain approximately constant if there are a very large number of balls in the urn, even if those selected are not returned, because their removal causes an infinitesimal change in the proportions among those remaining. This latter condition usually is assumed to prevail in many geological situations where discrete probability distributions are applied. In our binomial probability example, the "urn" consists of the geologic basin where exploration is occurring, and the red and white balls correspond to undiscovered reservoirs and barren areas. As long as the number of undrilled locations is large, and the number of prospects that have been drilled (and hence "removed from the urn") is small, the assumption of constant probability of discovery seems reasonable. However, if a sampling experiment is performed with a small number of colored balls initially in the urn and those taken from the urn are not returned, the probabilities obviously change with each draw. Such an experiment is called ***sampling without replacement***, and is governed by the discrete ***hypergeometric distribution***. Geologic problems where its use is appropriate are not common, but McCray (1975) presents an example from geophysical exploration for petroleum.

In some circumstances it is possible to know the size of the population within which discoveries will be made. Suppose an offshore concession contains ten well-defined seismic features that seem to represent structures caused by movement of salt at depth. From experience in nearby offshore tracts, it is believed that about 40% of such seismic features will prove to be productive structures. Because of budgetary limitations, it is not possible to drill all of the features in the current exploration program. The hypergeometric distribution can be used to estimate the probabilities that specified numbers of discoveries will be made if only some of the identified prospects are drilled.

The binomial distribution is not appropriate for this problem because the probability of a discovery changes with each exploratory hole. If there are four reservoirs distributed among the ten seismic features, the discovery of one reservoir increases the odds against finding another because there are fewer remaining to be discovered. Conversely, drilling a dry hole on a seismic feature increases the probability that the remaining untested features will prove productive, because one nonproductive feature has been eliminated from the population.

Calculating the hypergeometric probability consists simply of finding all of the possible combinations of producing and dry features within the population, and then enumerating those combinations that yield the desired number of discoveries.

The probability of making x discoveries in a drilling program of n holes, when sampling from a population of N prospects of which S are believed to contain reservoirs, is

$$P = \frac{\binom{S}{x}\binom{N-S}{n-x}}{\binom{N}{n}} \tag{2.6}$$

This is the number of combinations of the reservoirs taken by the number of discoveries, times the number of combinations of barren anomalies taken by the number of dry holes, all divided by the number of combinations of all the prospects taken by the total number of holes in the drilling program.

The hypergeometric probability distribution can be applied to our offshore concession that contains ten seismic features, of which four are likely to be structures containing reservoirs. Unfortunately, we cannot know in advance of drilling which four of the ten features will prove productive. If the current season's exploration budget permits the drilling of only four of the prospects, we can determine the probabilities attached to the various possible outcomes.

What is the probability that the drilling program will be a total failure, with no discoveries among the four features tested?

$$P = \frac{\binom{4}{0}\binom{6}{4}}{\binom{10}{4}} = \frac{1 \cdot 15}{210} = 0.071$$

The probability of gambler's ruin is approximately 7%. What is the probability that one discovery will be made?

$$P = \frac{\binom{4}{1}\binom{6}{3}}{\binom{10}{4}} = \frac{4 \cdot 20}{210} = 0.381$$

The probability that one discovery will be made is 38%.

A histogram can be prepared which shows the probabilities attached to all possible outcomes in this exploration situation (**Fig. 2–7**). Note that the probability of some success is (1.00 – 0.07), or 93%.

The preceding examples have addressed situations where there are only two possible outcomes: a hole is dry, or oil is discovered. If oil is found, the well cannot be dry, and *vice versa*. Events in which the occurrence of one outcome precludes the occurrence of the other outcome are said to be ***mutually exclusive***. The probability that one event or the other happens is the sum of their separate probabilities; that is, p (*discovery* ***or*** *dry hole*) = p (*discovery*) + p (*dry hole*). This is called the ***additive rule of probability***.

Events are not necessarily mutually exclusive. For example, we may be drilling an exploratory hole for oil or gas in anticipation of hitting a porous reservoir sandstone in what we have interpreted as an anticlinal structure from seismic data. The

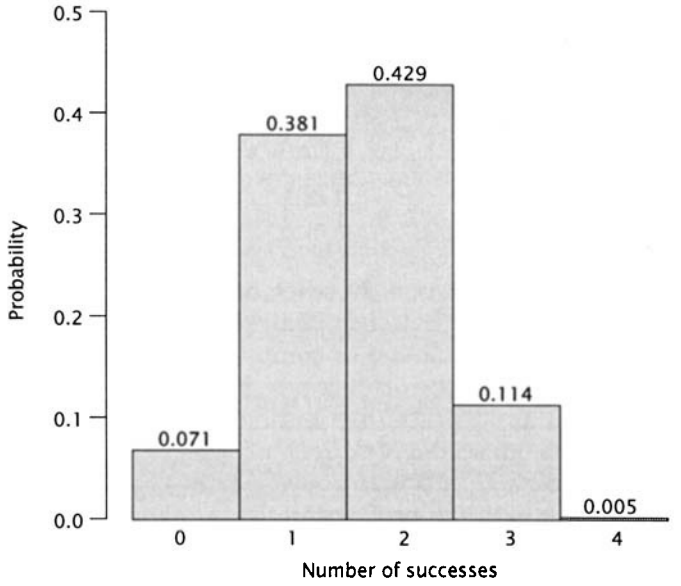


Figure 2–7. Discrete distribution for the probability of n discoveries in drilling four out of ten prospects when four prospects contain oil.

two outcomes, *hit porous sandstone* and *drill into an anticline*, are not mutually exclusive as we hope that both can occur simultaneously. Since the presence of a sandstone is governed by factors that operated at the time of deposition, and since the occurrence of an anticlinal fold is presumed to be related to tectonic conditions at a later time, the two outcomes are unrelated, or ***independent***. If two events are not mutually exclusive but *are* independent, the ***joint probability*** that they will occur simultaneously is the product of their separate probabilities of occurrence. That is, p (*hit sandstone* ***and*** *drill anticline*) = p (*hit sandstone*) × p (*drill anticline*). This is the ***multiplicative rule of probability***.

Two events may be related in some way, so that the outcome of one is dependent in part on the outcome of the other. The joint probability of such events is said to be ***conditional***. Such events are extremely important in geology, because we may be able to observe one event directly, but the other event is hidden. If the two are conditional, the occurrence of the observable event tells us something about the likely state of the hidden event. For example, the upward movement of magma in chambers beneath a volcano such as Mt. St. Helens in Washington is believed to cause a harmonic tremor, a particular type of earthquake. We cannot directly observe an active magma chamber, but we can observe and record the seismic activity associated with a volcano. If a conditional relationship exists between these two events, the occurrence of harmonic tremors may help predict eruptions. If p (*tremor*) is the probability that a harmonic tremor occurs and p (*eruption*) is the probability of a subsequent volcanic eruption, then p (*tremor* ***and*** *eruption*) $\neq$ p (*tremor*) × p (*eruption*) if the two events have a conditional relationship.

The conditional probability that an eruption will occur, given that harmonic tremors have been recorded, is denoted p (*eruption* | *tremor*). In this instance the conditional probability of an eruption is greater than the unconditional probability, or p (*eruption*), which is simply the probability that an eruption will occur without any knowledge of other events. Other conditional probabilities may be lower than

the corresponding unconditional probabilities (the probability of finding a fossil, given that the terrain is igneous, is much lower than the unconditional probability of finding a fossil). Obviously, geologists exploit conditional probabilities in all phases of their work, whether this is done consciously or not.

The relationship between conditional and unconditional probabilities can be expressed by ***Bayes' theorem***, named for Thomas Bayes, an eighteenth century English clergyman who investigated the manner in which probabilities change as more information becomes available. Bayes' basic equation is:

$$p(A,B) = p(B|A)p(A) \tag{2.7}$$

which states that $p(A,B)$, the ***joint probability*** that both events A and B occur, is equal to the probability that B will occur given that A has already occurred, times the probability that A will occur. $p(B|A)$ is a conditional probability because it expresses the probability that B will occur conditional upon the circumstance that A has already occurred. If events A and B are related (or dependent), the fact that A has already transpired tells us something about the likelihood that B will then occur. Conversely, it is also true that

$$p(A,B) = p(A|B)p(B)$$

Therefore, the two can be equated, giving

$$p(B|A)p(A) = p(A|B)p(B)$$

which may be rewritten as

$$p(B|A) = \frac{p(A|B)p(B)}{p(A)} \tag{2.8}$$

This is a most useful relationship, because sometimes we know one form of conditional probability but are interested in the other. For example, we may determine that mining districts often are characterized by the presence of abnormal geomagnetic fields. However, we are more interested in the converse, which is the probability that an area will prove to be mineralized, conditional upon the presence of a magnetic anomaly. We can gather estimates of the conditional probability p (*anomaly* | *mineralization*) and the unconditional probability p (*mineralization*) from studies of known mining districts, but it may be more difficult to directly estimate p (*mineralization* | *anomaly*) because this would require the examination of geomagnetic anomalies that may not yet have been prospected.

If there is an all-inclusive number of events B_i that are conditionally related to event A, the probability that event A will occur is simply the sum of the conditional probabilities $p(A|B_i)$ times the probabilities that the events B_i occur. That is,

$$p(A) = \sum_{i=1}^{n} p(A|B_i)p(B_i) \tag{2.9}$$

If Equation (2.9) is substituted for $p(A)$ in Bayes' theorem, as given in Equation (2.8), we have the more general equation

$$p(B_i|A) = \frac{p(A|B_i)\,p(B_i)}{\sum_{i=1}^{n} p(A|B_i)\,p(B_i)} \tag{2.10}$$

A simple example involving two possible prior events, B_1 and B_2, will illustrate the use of Bayes' theorem. A fragment of a hitherto unknown species of mosasaur has been found in a stream bed in western Kansas, and a vertebrate paleontologist would like to send a student field party out to search for more complete remains. Unfortunately, the source of the fragment cannot be identified with certainty because the fossil was found below the junction of two dry stream tributaries. The drainage basin of the larger stream contains about 18 mi^2, while the basin drained by the smaller stream includes only about 10 mi^2. On the basis of just this information alone, we might postulate that the probability that the fragment came from one of the drainage basins is proportional to the area of the basin, or

$$p(B_1) = \frac{18}{28} = 0.64$$
$$p(B_2) = \frac{10}{28} = 0.36$$

However, an examination of a geologic report and map of the region discloses the additional information that about 35% of the outcropping Cretaceous rocks in the larger basin are marine, while almost 80% of the outcropping Cretaceous rocks in the smaller basin are marine. We may therefore postulate the conditional probability that, given a fossil is derived from basin B_i, it will be a marine fossil, as proportional to the percentage of the Cretaceous outcrop area in the basin that is marine, or for basin B_1

$$p(A|B_1) = 0.35$$

and for basin B_2

$$p(A|B_2) = 0.80$$

Using these probabilities and Bayes' theorem, we can assess the conditional probability that the fossil fragment came from basin B_1, given that the fossil is marine.

$$p(B_1|A) = \frac{p(A|B_1)\,p(B_1)}{p(A|B_1)\,p(B_1) + p(A|B_2)\,p(B_2)}$$
$$= \frac{(0.35)(0.64)}{(0.35)(0.64) + (0.80)(0.36)}$$
$$= 0.44$$

Similarly, the probability that the fossil came from the smaller basin is

$$p(B_2|A) = \frac{p(A|B_2)\,p(B_2)}{p(A|B_1)\,p(B_1) + p(A|B_2)\,p(B_2)}$$
$$= \frac{(0.80)(0.36)}{(0.35)(0.64) + (0.80)(0.36)}$$
$$= 0.56$$

Fortunately for the students who must search the area, it seems somewhat more likely that the fragment of marine fossil mosasaur came from the smaller basin than from the larger. However, the differences in probability are very small and, of course, depend upon the reasonableness of the assumptions used to estimate the probabilities.

Continuous Random Variables

To introduce the next topic we must return briefly to the binomial distribution. **Figure 2–2** shows the probability distribution for all possible numbers of heads in three flips of a coin. A similar experiment could be performed that would involve a much larger number of trials. **Figure 2–8**, for example, gives the probabilities associated with obtaining specified numbers of "successes" (or heads) in ten flips of a coin, and **Figure 2–9** shows the probability distribution that describes outcomes from an experiment involving 50 flips of a coin. All of the probabilities were obtained either from binomial tables or calculated using the binomial equation.

In each of these experiments, we have enumerated all possible numbers of heads that we could obtain, from zero up to three, to ten, or to 50. No other combinations of heads and tails can occur. Therefore, the sum of all the probabilities within each experiment must total 1.00, because we are absolutely certain to obtain a result from among those enumerated. We can conveniently represent this by setting the areas underneath histograms in **Figures 2–8** and **2–9** equal to 1.00, as was done in the histogram of **Figure 2–2**. The greater number of coin tosses can be accommodated only by making the histogram bars ever more narrow, and the histogram becomes increasingly like a smooth and continuous curve. We can imagine an ultimate experiment involving flips of an infinite number of coins, yielding a histogram having an infinite number of bars of infinitesimal width. Then, the histogram would be a continuous curve, and the horizontal axis would represent a continuous, rather than discrete, variable.

In the coin-tossing experiment, we are dealing with discrete outcomes—that is, specific combinations of heads and tails. In most experimental work, however, the possible outcomes are not discrete. Rather, there is an infinite continuum of possible results that might be obtained. The range of possible outcomes may be finite and in fact quite limited, but within the range the exact result that may appear cannot be predicted. Such events are called ***continuous random variables***. Suppose, for example, we measure the length of the hinge line on a brachiopod and find it to be 6 mm long. However, if we perform our measurement using a binocular microscope, we may obtain a length of 6.2 mm, by using an optical comparator we may measure 6.23 mm, and with a scanning electron microscope, 6.231 mm. A continuous variate can, in theory, be infinitely refined, which implies that we can always find a difference between two measurements, if we conduct the measurements at a fine enough scale. The corollary of this statement is that every outcome on a continuous scale of measurement is unique, and that the probability of obtaining a specific, exact result must be zero!

If this is true, it would seem impossible to define probability on the basis of relative frequencies of occurrence. However, even though it is impossible to observe a number of outcomes that are, for example, exactly 6.000...000 mm, it is entirely feasible to obtain a set of measurements that fall within an interval around this value. Even though the individual measurements are not precisely identical, they are sufficiently close that we can regard them as belonging to the same class. In effect, we divide the continuous scale into discrete segments, and can then count the number of events that occur within each interval. The narrower the class boundaries, the fewer the number of occurrences within the classes, and the lower the estimates of the probabilities of occurrence.

When dealing with discrete events, we are counting—a process that usually can be done with absolute precision. Continuous variables, however, must be measured

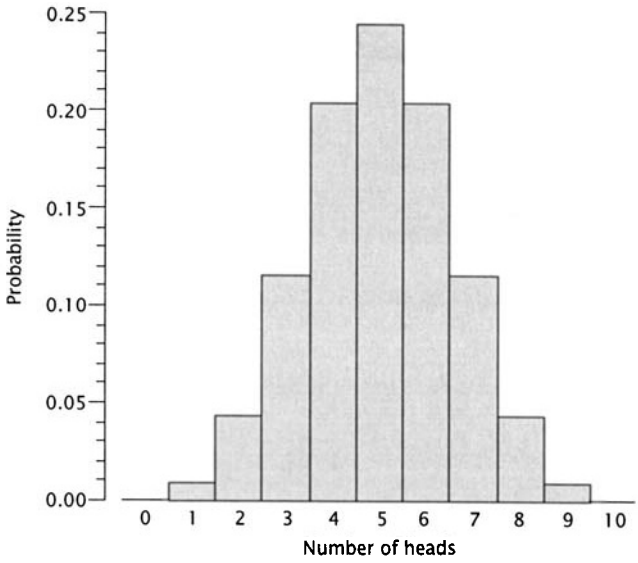


Figure 2–8. Discrete distribution giving the probability of obtaining specified numbers of heads in ten flips of a coin.

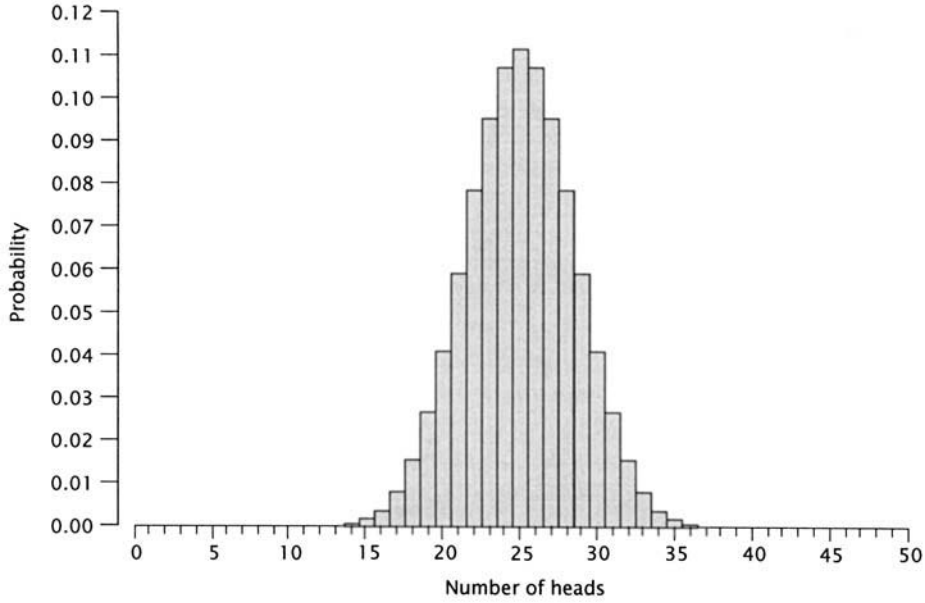


Figure 2–9. Discrete distribution giving the probability of obtaining specified numbers of heads in 50 flips of a coin.

by some physical procedure, and these inherently are limited in both their accuracy and precision. Repeated measurements made on the same object will display small differences whose magnitude may reflect both natural variation in the object, variation in the measurement process, and variation inadvertently caused by the person making the measurements. A single, exact, "true" value cannot be determined;

rather, we will observe a continuous distribution of possible values. This is a fundamental characteristic of a continuous random variable.

To further illustrate the nature of a continuous random variable, we can consider the problem of performing permeability tests on core samples. Permeabilities are determined by measuring the time required to force a certain amount of fluid, under standardized conditions, through a piece of rock. Suppose one test indicates a permeability of 108 md (millidarcies). Is this the "true" permeability of the sample? A second test run on the same specimen may yield a permeability of 93 md, and a third test may register 112 md. The permeability that is recorded on the instruments during any given run is affected by conditions which inevitably vary within the instrument from test to test, vagaries of flow and turbulence that occur within the sample, and inconsistencies in the performance of the test by the operator. No single test can be taken as an exactly correct measure of the true permeability. The various sources of fluctuation combine to yield a continuously random variable, which we are sampling by making repeated measurements.

Variation induced into measurements by inaccuracy of instrumentation is most apparent when repeated measurements are made on a single object or a test is repeated without change. This variation is called ***experimental error***. In contrast, variation may occur between members of a set if measurements or experiments are performed on a series of test objects. This is usually the variation that is of scientific interest. Sometimes the two types of variations are hopelessly mixed together, or ***confounded***, and the experimenter cannot determine what portion of the variability is due to variation between his test objects and what is due to error.

Rather than a single piece of rock, suppose we have a sizable length of core taken from a borehole through a sandstone body. We want to determine the permeability of the sandstone, but obviously cannot put 20 ft of core into our permeability apparatus. Instead, we cut small plugs from the larger core at intervals and determine the permeability of each. The variation we see is due in part to differences between the test plugs, but also results from differences in experimental conditions. Devising methods to estimate the magnitude of different sources of variation is one of the major tasks of statistics.

Repeated measurements on large samples drawn from natural populations may produce a characteristic frequency distribution. Most values are clustered around some central value, and the frequency of occurrence declines away from this central point. A graph of the distribution (**Fig. 2–10**) appears bell-shaped, and is called a ***normal distribution***. It often is assumed that random variables are normally distributed, and many statistical tests are based on this supposition.

As with all frequency distributions, we may define the total area underneath the normal curve as being equal to 1.00 (or if we wish, as 100%), so we can calculate the probability directly from the curve. You should note the similarity of the bell-shaped continuous curve shown in **Figure 2–10** to the histogram of the binomial distribution in **Figure 2–9**. However, in **Figure 2–10** there is an infinite number of subdivisions along the horizontal axis so the probability of obtaining one exact, specific event is essentially zero. Instead, we consider the probability of obtaining a result within a specified range. This probability is proportional to the area of the frequency curve bounded by these limits. If our specified range is wide, we are more likely to observe an event within them; if the range is extremely narrow, observing an event is extremely unlikely.

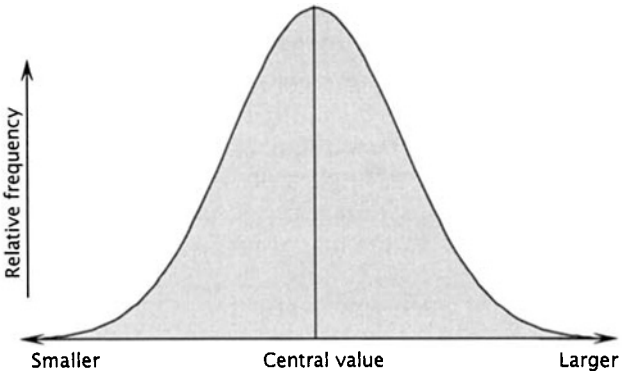


Figure 2–10. Plot of the normal frequency distribution.

Two terms have been introduced in preceding paragraphs without definition. These are "population" and "sample," two important concepts in statistics. A ***population*** consists of a well-defined set (either finite or infinite) of elements. Commonly, these elements are measurements of a specific nature made on items of a specified type. A ***sample*** is a subset of elements taken from a population. A finite population might consist of all oil wells drilled in Kansas in 1963. An example of an infinite geologic population might be all possible thin sections of the Tensleep Sandstone, or all possible shut-in tests on a well. Note in the latter example that the population includes not only the limited number of tests that have been run, but also all possible tests that could be run. Tests that actually were performed may be regarded as a sample of all potential tests.

Geologists typically attach a different meaning to the noun, "sample," than do statisticians. A geological sample, such as a "hand sample" of a rock, a "cuttings sample" from a well, or a "grab sample" or "channel sample" from a mine face, is a physical specimen and when represented by a quantitative or qualitative value would be called an observation or event by a statistician. What a statistician describes as a sample would likely be called a "collection" or "suite of samples" by a geologist. In this book, we will always use the noun "sample" in the statistical sense, meaning a set of observations taken from a population. The verb, "to sample," has essentially the same meaning for both geologists and statisticians and means the act of taking observations.

There are several practical reasons why we might wish to take samples. Many populations are infinite or so vast that it is only possible to examine a subset. Sometimes the measurements we make, such as chemical analyses, require the destruction of the material. By sampling, only a small part of the population is destroyed. Most geological populations extend deep into the Earth and are not accessible in their entirety. Finally, even if it were possible to observe an entire population, it might be more efficient to sample. There is always a point beyond which the increase in information gained from additional observations is not worth the increase in the cost of obtaining them.

Although all populations exhibit diversity, there is no real population whose elements vary without limit. Because any population has characteristic properties and the variation of its constituent members is limited, it is possible to select a relatively small, random sample that can adequately portray the traits of the population.

If observations with certain characteristics are systematically excluded from the sample, deliberately or inadvertently, the sample is said to be ***biased***. Suppose, for example, we are interested in the porosity of a particular sandstone unit. If we exclude all loose and crumbly rocks from our sample because their porosity is difficult to measure, we will alter the results of the study. It is likely that the range of porosities will be truncated at the high end, biasing the sample toward low values and giving an erroneously low estimate of the variation in porosity within the unit.

Samples should be drawn from populations in a random manner. This means that each item in the population has an equal opportunity to be included in the sample. A random sample will be unbiased, and as the sample size is increased, will provide an increasingly refined picture of the nature of the population. Unfortunately, obtaining a truly random sample may be impractical, as in the situation of sampling a geologic unit that is partially buried. Samples within the unit at depth do not have the same opportunity of being chosen as samples at outcrops. The problems of sampling in such circumstances are complex; some of the references at the end of this chapter discuss the effects of various sampling schemes and the relative merits of different sampling designs. However, many geologic problems involve the analysis of data collected without prior design. The interpretation of subsurface structure from drill-hole data is a prominent example.

Statistics

Distributions have certain characteristics, such as their midpoint; measures indicating the amount of "spread"; and measures of symmetry of the distribution. These characteristics are known as ***parameters*** if they describe populations, and ***statistics*** if they refer to samples. Statistics may be used to estimate parameters of parent populations and to test hypotheses about populations.

Although summary statistics are important, sometimes we can learn more by examining the distribution of the observations as shown on different plots and graphs. A familiar form of display is the ***histogram***, a bar chart in which a continuous variable is divided into discrete categories and the number or proportion of observations that fall into each category is represented by the areas of the corresponding bars. (As we have already seen, histograms are useful for showing discrete distributions but now we are interested in their application to continuous variables.) Usually the limits of categories are chosen so all of the histogram intervals will be the same width, so the heights of the bars also are proportional to the numbers of observations within the categories represented by the bars. If the vertical scale on the bar chart reads in number of observations, the graphic is called a ***frequency histogram.*** If the number of observations in each category are divided by the total number of observations, the scale reads in percent and the bar chart is a ***relative frequency histogram.*** Since a histogram covers the entire range of observations, the sum of the areas of all the bars will represent either the total number of observations or 100%. If the observations have been selected in an unbiased, representative manner, the sample histogram can be considered an approximation of the underlying probability distribution.

The appearance of a histogram is strongly affected by our choice of the number of categories and the starting value of the first category, especially if the sample contains only a few observations. Dividing the data into a small number of categories increases the average number in each and the histogram will be relatively

reproducible with repeated sampling. Unfortunately, such a histogram will contain little detail and may not be particularly informative. Increasing the number of categories reveals more details of the distribution, but because each category will contain fewer observations, the histogram will be less stable. The choice of origin for histogram categories also may influence the shape of the histogram. Interactive software allows the user to dynamically vary the width of the histogram intervals and move the origin, so alternatives can be easily evaluated. **Figure 2–11** shows four different histograms representing 125 airborne measurements of total radiation, recorded on the Istrian peninsula of Croatia. The data are contained in file CROATRAD.TXT at the Web sites (see Preface). If you have access to an interactive statistics package, you can experiment with these data to see the effects of changing the size and origin of the histogram categories. Examples shown in **Figure 2–11** are only a few of the possible histograms that could be constructed from these data.

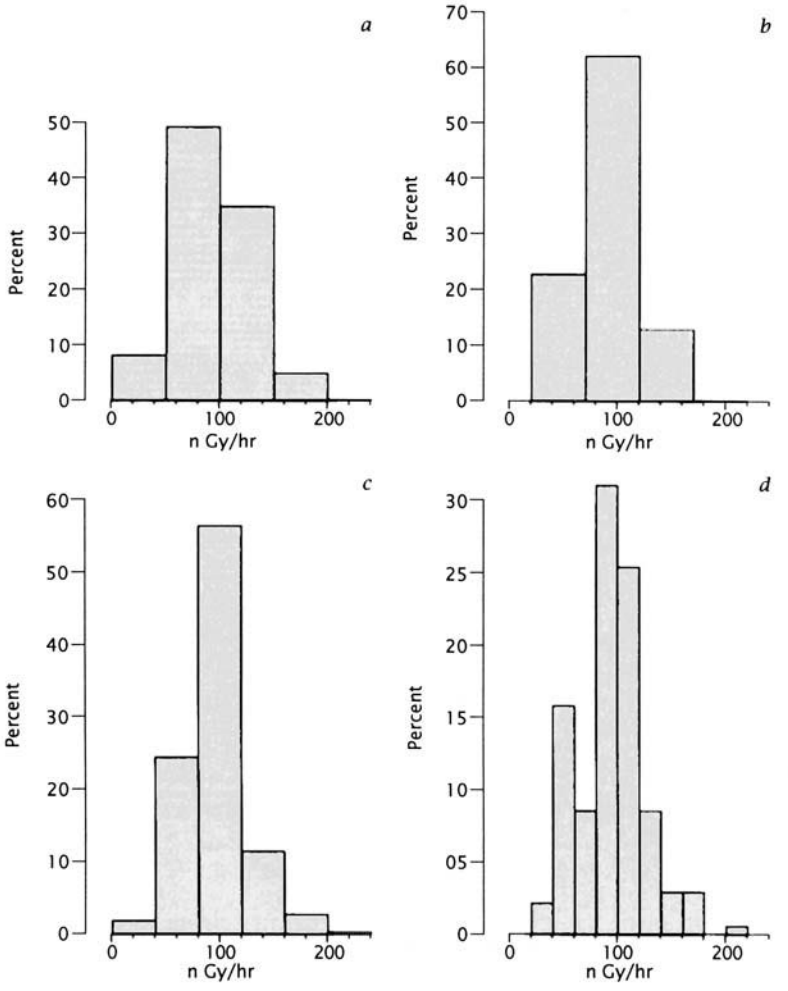


Figure 2–11. Histograms of airborne measurements of total radiation on the Istrian peninsula of Croatia, shown with different class intervals or histogram origins.

An alternative to a histogram is to show the data in the form of a ***cumulative plot***. We will illustrate the relation of this graphic to a conventional histogram

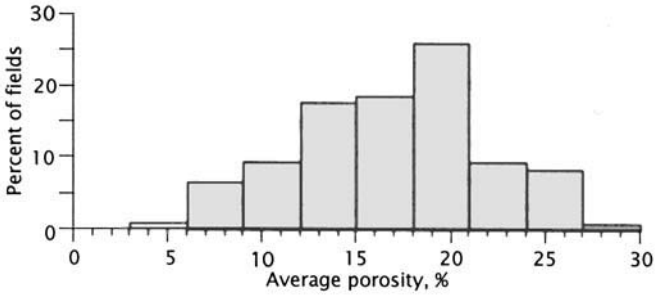


Figure 2–12. Histogram of field-wide average porosities of oil fields producing from the "D" and "J" sands in the Denver–Julesburg Basin of Colorado. Vertical axis is compressed for comparison with Figure 2–13.

using observations in file DJPOR.TXT, which gives the field-wide average porosities for 105 oil fields producing from the Cretaceous "D" and "J" sands in the Denver-Julesburg Basin of eastern Colorado. **Figure 2–12** is a histogram of these data in which the vertical axis is compressed for easier comparison with **Figure 2–13,** where each successive histogram bar begins at the top of the preceding bar. In effect, we have stacked the histogram bars so that the successive categories show the cumulative numbers or proportions of observations.

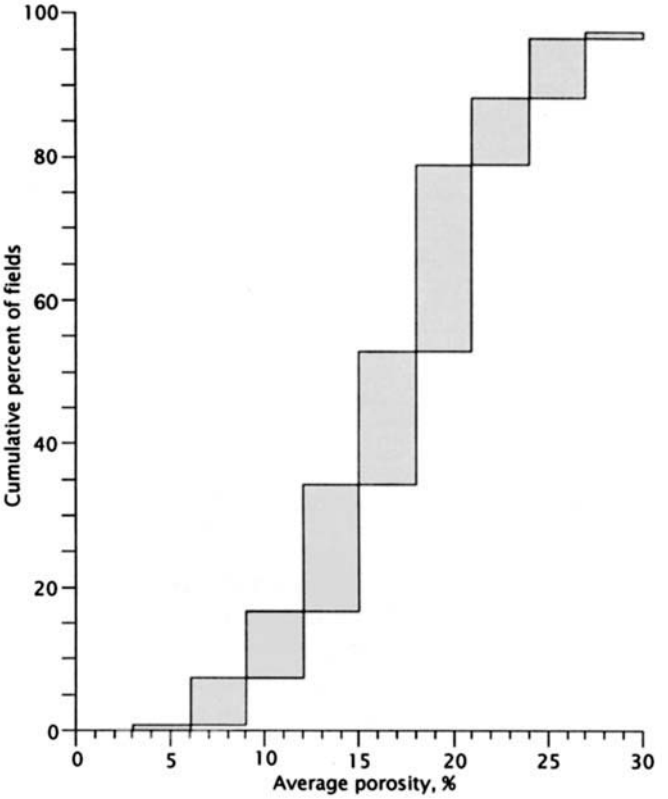


Figure 2–13. Histogram bars from Figure 2–12 stacked to form a cumulative distribution.

The great advantage of plotting data in cumulative form, however, comes about because we can show the individual observations directly, and avoid the loss of resolution that comes from grouping the observations into categories for a histogram. To do this, we must first rank the observations from smallest to largest, divide each observation's rank by the number of observations to convert it into a fraction, then multiply by 100 to express it as a percentile. That is,

$$\text{percentile of } x_i = 100 \left(\frac{\text{rank of } x_i}{n} \right) \tag{2.11}$$

where n is the number of observations. By graphing the percentile of each observation versus its value, we form a cumulative plot (**Fig. 2–14**). Note that both the cumulative histogram and the cumulative plot have a characteristic ogive form.

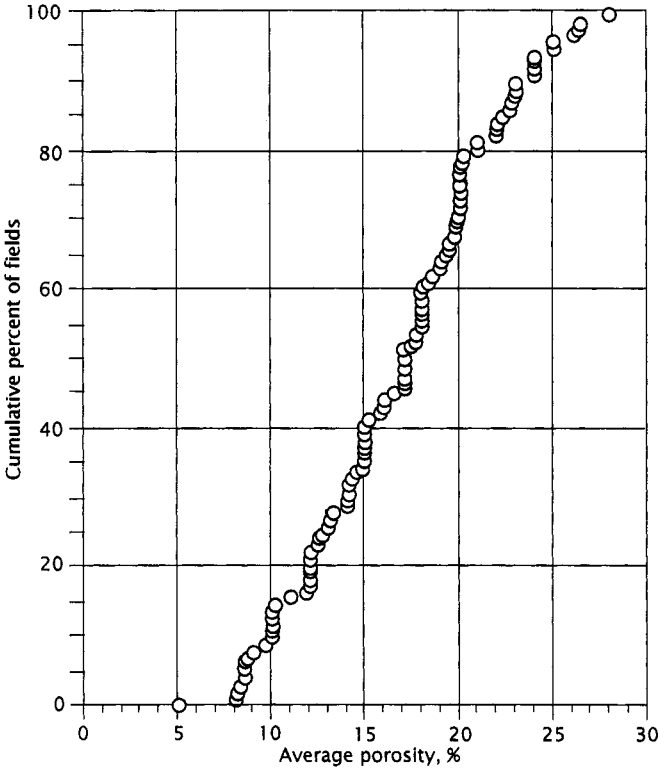


Figure 2–14. Cumulative plot of individual porosity measurements used to construct Figures 2–12 and 2–13.

Successive divisions of a distribution are called ***quantiles***. If we rank all observations in a sample and then divide the ranks into 100 equal-sized categories, each category is a ***percentile***. Suppose our sample contains 300 observations; the three smallest values constitute the first percentile. Each category is called a ***decile*** if the ranked sample is divided into ten equal categories, and a ***quartile*** if it is divided into four equal categories. Certain divisions of a distribution such as the 5th and 95th percentiles, the 25th and 75th percentiles (also called the 1st and 3rd quartiles), and the 50th percentile (also called the 5th decile, the 2nd quartile, or the median) are considered especially diagnostic and are indicated on the graphic plots we will consider next.

Box-and-whisker plots were devised by John Tukey (1977) to more effectively show the essential aspects of a sample distribution. There are many variants of the box-and-whisker plot, but all are graphs that show the spread of the central 50% of a distribution by a box whose lower limit is set at the first quartile and whose upper limit is set at the third quartile. The 50th percentile (second quartile or median) usually is indicated by a line across the box. The mean, or arithmetic average of the observations, may also be indicated by an asterisk or diamond. "Whiskers" are lines that extend from the ends of the box, usually to the 5th and 95th percentiles. Observations lying beyond these extremes may be shown as dots. **Figure 2–15** shows a histogram and several alternative box-and-whisker plots produced by several popular commercial programs. The data are 125 airborne measurements of radiation emitted by ^{137}Cs, recorded on the Istrian peninsula of Croatia. This component of total radiation (see **Fig. 2–11**) reflects fallout from the Chernobyl reactor accident in the Soviet Union during April of 1986. The data are given in file CROATRAD.TXT.

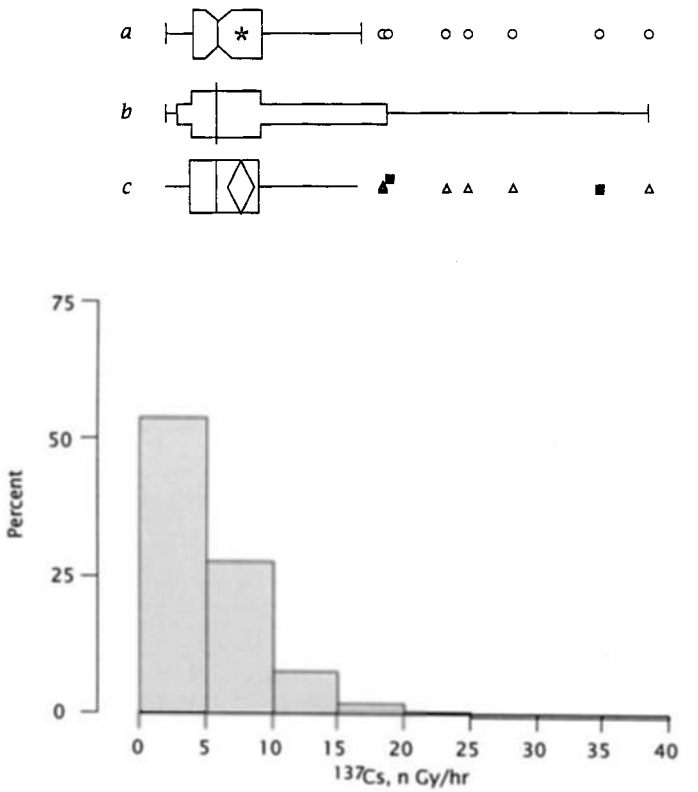


Figure 2–15. Histogram and alternative forms of box-and-whisker plots of airborne measurements of ^{137}Cs radiation recorded on the Istrian peninsula of Croatia.

Summary Statistics

The most obvious measure of a population or sample is some type of average value. Several measures exist, but only a few are used in practice. The ***mode*** is the value that occurs with the greatest frequency. In an asymmetric distribution such as that shown in **Figure 2–16**, the mode is the highest point on the frequency curve. The ***median*** is the value midway in the frequency distribution. In **Figure 2–16**, one-half of the area below the distribution curve is to the right of the median, one-half is to the left. The median is the 50th percentile, the 5th decile, or the 2nd quartile. The ***mean*** is another word for the arithmetic average, and is defined as the sum of all observations divided by the number of observations. The ***geometric mean*** is the nth root of the products of the n observations, or equivalently, the exponential of the arithmetic mean of the logarithms of the observations. In asymmetric frequency curves, the median lies between the mean and the mode. In symmetric curves such as the normal distribution, the mean, median, and mode coincide.

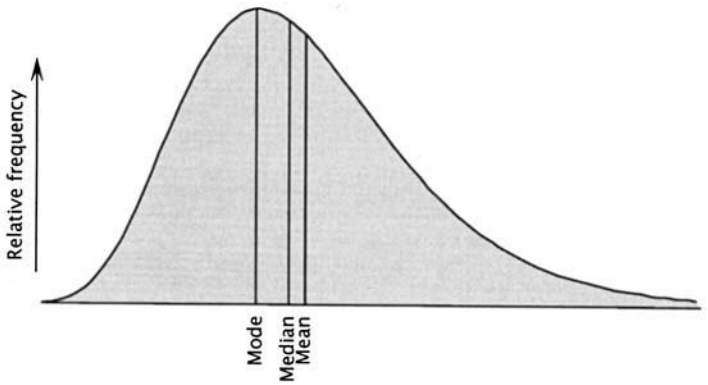


Figure 2–16. Asymmetric distribution showing relative positions of mean, median, and mode.

Certain symbols traditionally have been assigned to measures of distribution curves. Generally, the symbols for population distributions are Greek letters, and those for sample distributions are Roman. The sample mean, for example, is designated $\overline{X}$ and the population mean is μ (mu). A common objective in an investigation is to estimate some parameter of a population. A statistic we compute based on a sample taken from the population is used as an estimator of the desired parameter. The use of Greek and Roman symbols serves to emphasize the difference between parameters and the equivalent statistics.

The sample mean has two highly desirable properties that make it more useful as an estimator of the average or central value of a population than either the sample median or mode. First, the sample mean is an unbiased estimate of the population mean. A (sample) statistic is an unbiased estimate of the equivalent (population) parameter if the average value of the statistic, from a large series of samples, is equal to the parameter. Second, it can be demonstrated that, for symmetrical distributions such as the normal, the sample mean tends to be closer to the population mean than any other unbiased estimate (such as the median) based on the same sample. This is equivalent to saying that sample means are less variable

Table 2–1. Chromium content of an Upper Pennsylvanian shale from Kansas.

Replicate	Cr (ppm)
1	205
2	255
3	195
4	220
5	235
TOTAL =	1110
MEAN =	1110/5 = 222

than sample medians, hence they are more efficient in estimating the population parameter.

In geochemical analyses, it is common practice to make multiple determinations, or ***replicates***, of a single sample. The most nearly correct analytical value is taken to be the mean of the determinations. **Table 2–1** lists five values for chromium, in parts per million (ppm), obtained by spectrographic analysis of replicate splits of a Pennsylvanian shale specimen from southeastern Kansas. The table shows the steps in calculating the mean, whose equation is simply

$$\overline{X} = \frac{\sum_{i=1}^{n} x_i}{n} \tag{2.12}$$

Another characteristic of a distribution curve is the spread or dispersion about the mean. Various measures of this property have been suggested, but only two are used to any extent. One is the ***variance***, and the other is the square root of the variance, called the ***standard deviation***. Variance may be regarded as the average squared deviation of all possible observations from the population mean, and is defined by the equation

$$\sigma^2 = \frac{\sum_{i=1}^{n} (x_i - \mu)^2}{n} \tag{2.13}$$

The variance of a population, σ^2, is given by this equation. The variance of a sample is denoted by the symbol s^2. If the observations $x_1, x_2, \ldots, x_n$ are a random sample from a normal distribution, s^2 is an efficient estimate of σ^2.

The reason for using the average of squared deviations may not be obvious. It may seem, perhaps, more logical to define variability as simply the average of deviations from the mean, but a few simple trials will demonstrate that this value will always equal zero. That is,

$$\frac{\sum_{i=1}^{n} x_i - \overline{X}}{n} = 0 \tag{2.14}$$

Another choice might be the average absolute deviation from the mean, or ***mean deviation***, MD:

$$\text{MD} = \frac{\sum_{i=1}^{n} |x_i - \overline{X}|}{n} \tag{2.15}$$

The vertical bars denote that the absolute value (*i.e.*, without sign) of the enclosed quantity is taken. However, the mean deviation is less efficient than the sample

variance. If we take repeated samples, the mean deviations will be more variable than variances calculated from the same samples. Although not intuitively obvious, the variance has properties that make it far more useful than other measures of scatter.

Because variance is the average squared deviation from the mean, its units are the square of the units of the original measurements. A granite, for example, may have feldspar phenocrysts whose longest axes have an average length of 13.2 mm and a variance of 2.0 mm^2. Many people may find themselves reluctant to regard areas as an appropriate measurement unit for the dispersion of lengths! Fortunately, in most instances where we are concerned with variance, it is standardized or converted to a form independent of the measurement units. This is a topic discussed in greater detail elsewhere in this chapter.

To provide a statistic that describes dispersion or spread of data around the mean, and is in the units of measurement of the data, we can calculate the ***standard deviation.*** This is defined simply as the square root of variance and is symbolically written as σ for the population parameter and s for the sample statistic. In equation form,

$$\sigma = \sqrt{\sigma^2} = \sqrt{\frac{\sum_{i=1}^{n} (x_i - \mu)^2}{n}} \qquad (2.16)$$

A small standard deviation indicates that observations are clustered tightly around a central value. Conversely, a large standard deviation indicates that values are scattered widely about the mean and the tendency for central clustering is weak. This is illustrated in **Figure 2–17**, which shows two symmetric frequency curves having different standard deviations. Curve *a* represents the percent oil saturation (s_o) measured in cores from the producing zone of a northeastern Oklahoma oil field. Curve *b* is the same type of data from a field in West Texas. The mean oil saturation differs in the two fields, but the major difference between the curves reflects the fact that the Texas field has a much greater variation in oil saturation.

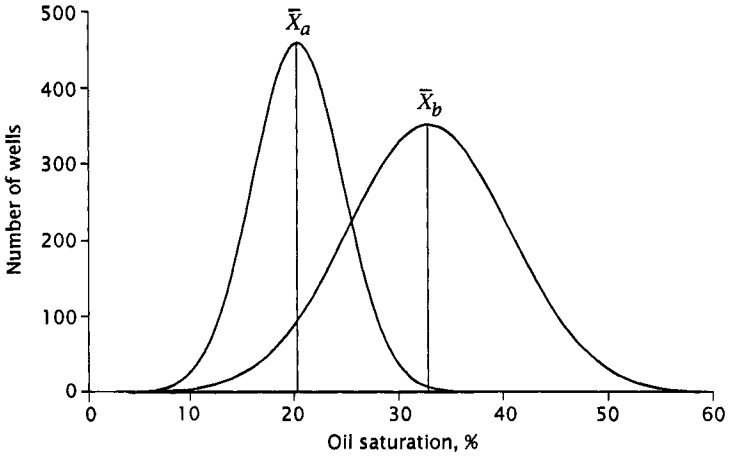


Figure 2–17. Distribution of percent oil saturation (s_o) measured on cores from a field (*a*) in northeastern Oklahoma and (*b*) in west Texas.

A most useful property of normal distributions is that areas under the curve, within any specified range, can be precisely calculated and expressed in terms of

standard deviations from the mean. For example, slightly over two-thirds (68.27%) of observations will fall within one standard deviation on either side of the mean of a normal distribution. Approximately 95% of all observations are included within the interval from +2 to −2 standard deviations, and more than 99% are covered by the interval lying three standard deviations on both sides of the mean. This is illustrated in **Figure 2–18.**

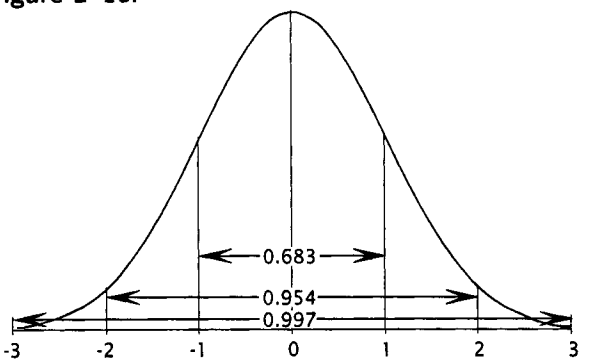


Figure 2–18. Areas enclosed by successive standard deviations of the standard normal distribution.

The distribution of measured oil saturations in cores from the northeastern Oklahoma field (**Fig. 2–17**, curve *a*) has a mean of 20.1% s_o and a standard deviation of 4.3% s_o. If we assume that the distribution is normal, we would expect about two-thirds of the cores tested to have oil saturations between about 16% s_o and 24% s_o. Examination of the original data shows that there are 1145 cores having saturations within this range, or about 68% of the data. Only 101 cores, or about 6% of the total number of observations, have saturations outside the 2σ range; that is, oil saturations less than 12% s_o or more than 29% s_o.

Equation (2.13) is called the definitional equation of variance. This equation is not often used for hand calculation, involving as it does n subtractions, n multiplications, and n summations. Instead, a formula suitable for computation with a calculator is used which is algebraically equivalent but easier to perform. This equation is

$$s^2 = \frac{\sum_{i=1}^{n} x_i^2 - n\overline{X}^2}{n-1} \tag{2.17}$$

or alternatively,

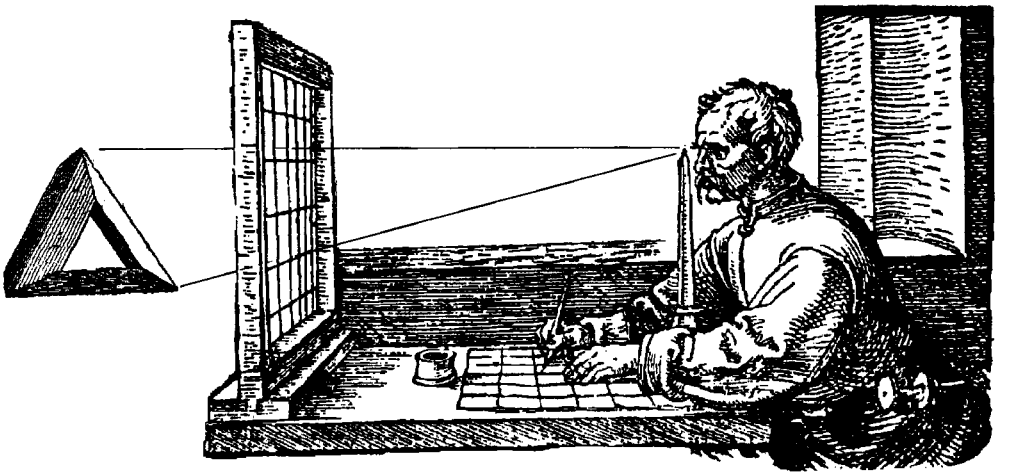
$$s^2 = \frac{n\sum_{i=1}^{n} x_i^2 - \left(\sum_{i=1}^{n} x_i\right)^2}{n(n-1)} \tag{2.18}$$

On hand calculators, $\sum x_i$ and $\sum x_i^2$ can be found simultaneously, thus reducing the number of operations by n. However, this formula requires subtracting two quantities, $\sum x_i^2$ and $(\sum x_i)^2$, and both may be very large and very nearly the same. Problems can arise if significant digits are truncated during this operation, so it is better to use the definitional equation to calculate variance in a computer program.

To compute variances and standard deviations, we generate intermediate quantities which can be used directly in many techniques we will discuss in following chapters. The ***uncorrected sum of squares*** is simply $\sum x_i^2$; the ***corrected sum of squares*** (SS) is defined as

$$SS = \sum_{i=1}^{n} \left(x_i - \overline{X}\right)^2 \tag{2.19}$$

Chapter 3
Matrix Algebra



This chapter is devoted to matrix algebra. Most of the methods we will discuss in subsequent chapters are based on matrix manipulations, especially as performed by computers. In this chapter, we will examine the mathematical operations that underlie such techniques as trend-surface analysis, principal components, and discriminant functions. These techniques are almost impossible to apply without the help of computers, because the calculations are complicated and must be performed repetitively. However, with matrix algebra we can express the basic principles involved in a manner that is succinct and easily understood. Once you master the rudiments of matrix algebra, you will be able to see the fundamental structure within the complex procedures we will examine later.

Most geologists probably have not taken a course in matrix algebra. This is unfortunate; the subject is not difficult and is probably one of the most useful tools in mathematics. College courses in matrix algebra usually are sprinkled liberally with theorems and their proofs. Such an approach is certainly beyond the scope of this short chapter, so we will confine ourselves to those topics pertinent to techniques that we will utilize later. Rather than giving derivations and proofs, the material will be presented by examples.

The Matrix

A ***matrix*** is a rectangular array of numbers, exactly the same as a table of data. In matrix algebra, the array is considered to be a single entity rather than a collection of individual values and is operated upon as a unit. This results in a great simplification of the statement of complicated procedures and relationships. Individual numbers within a matrix are called the ***elements*** of the matrix and are identified by subscripts. The first subscript specifies the row in which the element occurs and the second specifies the column. The individual elements of a matrix may be

measurements of variables, variances or covariances, sums of observations, terms in a series of simultaneous equations or, in fact, any set of numbers.

As an example, in Chapter 2 you were asked to compute the variances and covariances of trace-element data given in **Table 2–3**. Your answers can be arranged in the form of the matrix below.

$$\begin{bmatrix} \text{var}_{Cr} & \text{cov}_{Cr\,Ni} & \text{cov}_{Cr\,V} \\ \text{cov}_{Ni\,Cr} & \text{var}_{Ni} & \text{cov}_{Ni\,V} \\ \text{cov}_{V\,Cr} & \text{cov}_{V\,Ni} & \text{var}_{Ni} \end{bmatrix} = \begin{bmatrix} 570 & 537.5 & 663.75 \\ 537.5 & 562.5 & 718.75 \\ 663.75 & 718.75 & 1007.5 \end{bmatrix}$$

We can designate a matrix (perhaps containing values of several variables) symbolically by capital letters such as [X], **X**, (X), or ||X||. In a change from earlier editions of this book, we will adopt the commonly used boldface notation for matrices. Individual entries in a matrix, or its elements, are indicated by subscripted italic lowercase letters such as x_{ij}. Particularly in older books, you may encounter different conventions for denoting individual elements of a matrix. The symbol x_{ij} is the element in the ith row and the jth column of matrix **X**. For example, if **X** is the 3×3 matrix

$$\mathbf{X} = \begin{bmatrix} 1 & 4 & 7 \\ 2 & 5 & 8 \\ 3 & 6 & 9 \end{bmatrix}$$

x_{33} is 9, x_{13} is 7, x_{21} is 2, and so on. The ***order*** of a matrix is an expression of its size, in the sense of the number of rows and/or the number of columns it contains. So, the order of **X**, above, is 3. If the number of rows equals the number of columns, the matrix is ***square.*** Entries in a square matrix whose subscripts are equal (*i.e.*, $i = j$) are called the ***diagonal elements***, and they lie on the ***principal diagonal*** or ***major diagonal*** of the matrix. In the matrix of trace-element variances and covariances, the variances lie on the diagonal and the off-diagonal elements are the covariances. The diagonal elements in the matrix above are 1, 5, and 9. Although data arrays usually are in the form of rectangular matrices, often we will create square matrices from them by calculating their variances and covariances or other summary statistics. Many useful operations that can be performed on square matrices are not possible with nonsquare matrices. However, two forms of nonsquare matrices are especially important; these are the ***vectors***, $1 \times m$ (row vector) and $m \times 1$ (column vector).

Certain square matrices have special importance and are designated by name. A ***symmetric matrix*** is a square matrix in which all observations $x_{ij} = x_{ji}$, as for example

$$\begin{bmatrix} 1 & 2 & 3 \\ 2 & 4 & 5 \\ 3 & 5 & 6 \end{bmatrix}$$

The variance-covariance matrix of trace elements given above is another example of a square matrix that is symmetrical about the diagonal.

A ***diagonal matrix*** is a square, symmetric matrix in which all the off-diagonal elements are 0. If all of the diagonal elements of a diagonal matrix are equal, the matrix is a ***scalar matrix.*** Finally, a scalar matrix whose diagonal elements are equal to 1 is called an ***identity matrix*** or ***unit matrix.*** An identity matrix is almost always

indicated by **I**:

$$\mathbf{I} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

Elementary Matrix Operations

Addition and subtraction of matrices obey the rules of algebra of ordinary numbers, with one important additional characteristic. The two matrices being added or subtracted must be of the same order; that is, they must have the same number of rows and columns.

To perform the operation **C** = **A** + **B**, every element of **A** is added to its corresponding element in **B**. If the matrices are not of the same order, there will be leftover elements, and the operation cannot be completed. Subtraction, such as **C** = **A** − **B**, proceeds in exactly the same manner, with every element of **B** subtracted from its corresponding element in **A**.

Table 3–1. Bentonite production in Wyoming, 1964.

	Clay (100,000 tons)		
District	Drilling Mud	Foundry Clay	Miscellaneous
Eastern	105	63	5
Montana Border	218	80	2
Central	220	76	1

As an illustration, **Table 3–1** contains 1964 production figures for bentonite from three mining districts in Wyoming. Three major grades of clay were produced: clay for drilling mud; foundry clay; and a miscellaneous category that includes cattle feed binder, drug and cosmetic uses, and pottery clay. These data can be expressed in a 3 × 3 matrix, **A**:

$$\mathbf{A} = \begin{bmatrix} 105 & 63 & 5 \\ 218 & 80 & 2 \\ 220 & 76 & 1 \end{bmatrix}$$

Production figures for the following year may be expressed in the same manner, giving the matrix **B**:

$$\mathbf{B} = \begin{bmatrix} 84 & 102 & 4 \\ 240 & 121 & 1 \\ 302 & 28 & 0 \end{bmatrix}$$

Total production for the 2 years in the three districts is the sum, **C**, of the the matrices **A** and **B**:

$$\begin{matrix} \mathbf{A} & & \mathbf{B} & & \mathbf{C} \end{matrix}$$

$$\begin{bmatrix} 105 & 63 & 5 \\ 218 & 80 & 2 \\ 220 & 76 & 1 \end{bmatrix} + \begin{bmatrix} 84 & 102 & 4 \\ 240 & 121 & 1 \\ 302 & 28 & 0 \end{bmatrix} = \begin{bmatrix} 189 & 165 & 9 \\ 458 & 201 & 3 \\ 522 & 104 & 1 \end{bmatrix}$$

Similarly, the change in production can be found by subtracting:

$$\begin{matrix} \mathbf{B} & - & \mathbf{A} & = & \mathbf{D} \end{matrix}$$

$$\begin{bmatrix} 84 & 102 & 4 \\ 240 & 121 & 1 \\ 302 & 28 & 0 \end{bmatrix} - \begin{bmatrix} 105 & 63 & 5 \\ 218 & 80 & 2 \\ 220 & 76 & 1 \end{bmatrix} = \begin{bmatrix} -21 & 39 & -1 \\ 22 & 41 & -1 \\ 82 & -48 & -1 \end{bmatrix}$$

Note that **A** was subtracted from **B** simply to show increases in production as positive values.

As in ordinary algebra, $\mathbf{A} + \mathbf{B} = \mathbf{B} + \mathbf{A}$, and $(\mathbf{A} + \mathbf{B}) + \mathbf{C} = \mathbf{A} + (\mathbf{B} + \mathbf{C})$, provided all are $n \times m$ matrices. The order of subtraction is, of course, mandatory.

Transposition is a matrix operation in which rows become columns and columns become rows. Each element x_{ij} becomes the element x_{ji} in the transpose. The operation is indicated symbolically by $\mathbf{X}^{\mathbf{T}}$ or by $\mathbf{X}'$. So,

$$\mathbf{X} = \begin{bmatrix} 1 & 4 \\ 2 & 5 \\ 3 & 6 \end{bmatrix} \qquad \mathbf{X}^{\mathbf{T}} = \begin{bmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \end{bmatrix}$$

Note that the first row has become the first column of the transpose, and the second row has become the second column. In some of the calculations we will consider later, a row vector, **A**, becomes a column vector, $\mathbf{A}^{\mathbf{T}}$, when transposed, and *vice versa*. The row and column vectors

$$\mathbf{A} = \begin{bmatrix} 1 & 2 & 3 & 4 \end{bmatrix} \qquad \mathbf{A}^{\mathbf{T}} = \begin{bmatrix} 1 \\ 2 \\ 3 \\ 4 \end{bmatrix}$$

are the transpose of each other.

A matrix may be ***multiplied by a constant*** by multiplying each element in the matrix by the constant. For example

$$3 \times \begin{bmatrix} 1 & 4 \\ 2 & 5 \\ 3 & 6 \end{bmatrix} = \begin{bmatrix} 3 & 12 \\ 6 & 15 \\ 9 & 18 \end{bmatrix}$$

Strictly speaking, a matrix cannot be divided by a constant, but we can perform an equivalent operation. If we multiply a matrix by a value equal to the inverse of a constant, we obtain the same numerical result as if we divided each element of the matrix by the constant. The inverse of the constant, c, is indicated by c^{-1}, which represents $1/c$.

Table 3–2. Measurements of axes of pebbles (in inches) collected from glacial till.

	Axis		
Sample	*a*	*b*	*c*
1	3.4	2.2	1.8
2	4.6	4.3	4.2
3	5.4	4.7	4.7
4	3.9	2.8	2.3
5	5.1	4.9	3.8

As a simple example, consider **Table 3–2**, which contains measurements of the *a*-, *b*-, and *c*-axes of chert pebbles collected in a glacial till. The measurements were recorded in inches and we wish to convert them to millimeters. If the data are expressed in the form of the matrix **E**, we may multiply **E** by the constant 25.4 to obtain a matrix containing the measurements in millimeters:

$$25.4 \times \mathbf{E} = \mathbf{M}$$

$$25.4 \times \begin{bmatrix} 3.4 & 2.2 & 1.8 \\ 4.6 & 4.3 & 4.2 \\ 5.4 & 4.7 & 4.7 \\ 3.9 & 2.8 & 2.3 \\ 5.1 & 4.9 & 3.8 \end{bmatrix} = \begin{bmatrix} 86.36 & 55.88 & 45.72 \\ 116.84 & 109.22 & 106.68 \\ 137.16 & 119.38 & 119.38 \\ 99.06 & 71.12 & 58.42 \\ 129.54 & 124.46 & 96.52 \end{bmatrix}$$

Matrix Multiplication

Recall the coin-flipping problem from Chapter 2, where we considered the probability of obtaining a succession of heads if the probability of heads on one flip was 1/2. The probability that we would get three heads in a row was $1/2 \times 1/2 \times 1/2$, or $1/2^3$. We can develop an equivalent set of probabilities for lithologies encountered in a stratigraphic section. Suppose we have measured an outcrop and identified the units as sandstone, shale, or limestone. At every foot, the rock type can be categorized and the type immediately above noted. We would eventually build a matrix of frequencies similar to that below. This is called a ***transition frequency matrix*** and tells us, for example, that sandstone is followed by shale 18 times, but followed by limestone only 2 times. Similarly, limestone follows shale 41 times, succeeds itself 51 times, but follows sandstone only 2 times:

		To: Sandstone	Shale	Limestone
From:	Sandstone	59	18	2
	Shale	14	86	41
	Limestone	4	34	51

We can convert these frequencies to probabilities by dividing each element in a row by the total of the row. This will give the ***transition probability matrix*** shown below, from which the probability of proceeding from one state to another can be assessed. This subject will be considered in detail in a later chapter, where its use in time-series analysis will be examined. Now, however, we are interested in the matrix of probabilities, which is analogous to the single probability associated with the flip of a coin:

		To: Sandstone	Shale	Limestone
From:	Sandstone	0.74	0.23	0.03
	Shale	0.10	0.61	0.29
	Limestone	0.05	0.38	0.57

Just as we can find the probability of producing a string of heads in a coin-flipping experiment by powering the probability associated with a single flip, we

can determine the probability of attaining specified states at successive intervals by powering the transition probability matrix. That is, the probability matrix, **P**, after n steps through the succession is equal to $\mathbf{P}^n$. The nth power of a matrix is simply the matrix times itself n times. To perform this operation, however, we must know the special procedures of matrix multiplication.

The simplest form of multiplication involves two square matrices, **A** and **B**, of equal size, producing the product matrix, **C**. An easy method of performing this operation is to arrange the matrices in the following manner:

$$\begin{bmatrix} & & \\ & & \\ & & \end{bmatrix} \begin{bmatrix} b_{11} & b_{12} & b_{13} \\ b_{21} & b_{22} & b_{23} \\ b_{31} & b_{32} & b_{33} \end{bmatrix}$$

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} \begin{bmatrix} c_{11} & c_{12} & c_{13} \\ c_{21} & c_{22} & c_{23} \\ c_{31} & c_{32} & c_{33} \end{bmatrix}$$

To obtain the value of an element c_{ij}, multiply each element of row i of **A**, starting at the left, by each element of column j of **B**, starting at the top. All the products are summed to obtain the c_{ij} element of the answer. The steps in multiplication are demonstrated below on the two matrices,

$$\begin{bmatrix} 1 & 4 & 7 \\ 2 & 5 & 8 \\ 3 & 6 & 9 \end{bmatrix} \times \begin{bmatrix} 1 & 2 & 3 \\ 3 & 4 & 5 \\ 5 & 6 & 7 \end{bmatrix}$$

First, multiply a_{11} by $b_{11} = 1$,

$$\begin{bmatrix} \textcircled{1} & 4 & 7 \\ 2 & 5 & 8 \\ 3 & 6 & 9 \end{bmatrix} \times \begin{bmatrix} \textcircled{1} & 2 & 3 \\ 3 & 4 & 5 \\ 5 & 6 & 7 \end{bmatrix}$$

Then, a_{12} by $b_{21} = 12$,

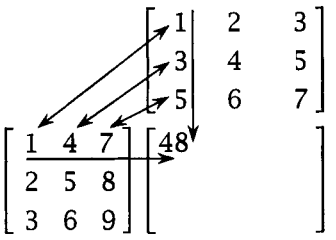
$$\begin{bmatrix} 1 & \textcircled{4} & 7 \\ 2 & 5 & 8 \\ 3 & 6 & 9 \end{bmatrix} \times \begin{bmatrix} 1 & 2 & 3 \\ \textcircled{3} & 4 & 5 \\ 5 & 6 & 7 \end{bmatrix}$$

Finally, a_{13} by $b_{31} = 35$,

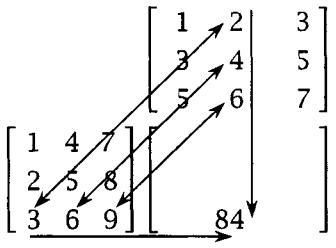
$$\begin{bmatrix} 1 & 4 & \textcircled{7} \\ 2 & 5 & 8 \\ 3 & 6 & 9 \end{bmatrix} \times \begin{bmatrix} 1 & 2 & 3 \\ 3 & 4 & 5 \\ \textcircled{5} & 6 & 7 \end{bmatrix}$$

The entry c_{11} is the sum of these three values, $1 + 12 + 35 = 48$. These steps can be summarized in the diagram below. Note that each entry c_{ij} in the product matrix results from multiplying and summing the products of elements in the ith row of matrix **A** by elements in the jth column of matrix **B**.

To find element c_{11}



To find element c_{32}



The completed matrix multiplication has the appearance

$$\begin{bmatrix} 1 & 4 & 7 \\ 2 & 5 & 8 \\ 3 & 6 & 9 \end{bmatrix} \begin{bmatrix} 1 & 2 & 3 \\ 3 & 4 & 5 \\ 5 & 6 & 7 \end{bmatrix} = \begin{bmatrix} 48 & 60 & 72 \\ 57 & 72 & 87 \\ 66 & 84 & 102 \end{bmatrix}$$

In general, if the order of multiplication is reversed to $\mathbf{B}\times\mathbf{A} = \mathbf{C}$, a different answer will be obtained:

$$\begin{bmatrix} 1 & 2 & 3 \\ 3 & 4 & 5 \\ 5 & 6 & 7 \end{bmatrix} \begin{bmatrix} 1 & 4 & 7 \\ 2 & 5 & 8 \\ 3 & 6 & 9 \end{bmatrix} = \begin{bmatrix} 14 & 32 & 50 \\ 26 & 62 & 98 \\ 38 & 92 & 146 \end{bmatrix}$$

In the operation $\mathbf{A} \times \mathbf{B} = \mathbf{C}$, the matrix **B** is said to be ***premultiplied*** by **A**. Similarly, the matrix **A** can be said to be ***postmultiplied*** by **B**. This is simply a verbal way of specifying the order of multiplication.

If two square matrices are multiplied, the product is a square matrix of the same size. However, if an $m \times n$ matrix is multiplied by an $n \times r$ matrix, the result is an $m \times r$ matrix. That is, the product matrix has the same number of rows as the premultiplier matrix on the left and the same number of columns as the postmultiplier matrix on the right. For example, premultiplying a 3×2 matrix by a 5×3 matrix results in a 5×2 matrix:

$$\begin{bmatrix} 1 & 2 & 4 \\ 2 & 1 & 2 \\ 3 & 1 & 1 \\ 2 & 3 & 1 \\ 1 & 2 & 0 \end{bmatrix} \times \begin{bmatrix} 3 & 4 \\ 2 & 1 \\ 0 & 1 \end{bmatrix} = \begin{bmatrix} 7 & 10 \\ 8 & 11 \\ 11 & 14 \\ 12 & 12 \\ 7 & 6 \end{bmatrix}$$

However, the 3×2 matrix cannot be postmultiplied by the 5×3 matrix because the number of columns (two) in the left matrix would not equal the number of rows (five) in the right matrix.

Multiplying a matrix by its transpose results in a square, symmetric matrix product whose size is determined by the order of multiplication. Typically, a data array consists of n rows and m columns, where n is much larger than m. If such an array is premultiplied by its transpose, the ***minor product matrix*** will be $m \times m$:

$$\begin{bmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \end{bmatrix} \times \begin{bmatrix} 1 & 4 \\ 2 & 5 \\ 3 & 6 \end{bmatrix} = \begin{bmatrix} 14 & 32 \\ 32 & 77 \end{bmatrix}$$

But reversing the order of multiplication yields the $n \times n$ ***major product matrix***:

$$\begin{bmatrix} 1 & 4 \\ 2 & 5 \\ 3 & 6 \end{bmatrix} \times \begin{bmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \end{bmatrix} = \begin{bmatrix} 17 & 22 & 27 \\ 22 & 29 & 36 \\ 27 & 36 & 45 \end{bmatrix}$$

The equation for the general case of matrix multiplication is

$$c_{ij} = \sum_{k=1}^{n} a_{ik} b_{kj} \tag{3.1}$$

In a series of multiplications, the sequence in which the multiplications are accomplished is not mandatory if the arrangement is not changed. That is,

$$\mathbf{A} \times \mathbf{B} \times \mathbf{C} = (\mathbf{A} \times \mathbf{B}) \times \mathbf{C} = \mathbf{A} \times (\mathbf{B} \times \mathbf{C})$$

Because powering is simply a series of multiplications, a square matrix can be raised to a power. So,

$$\mathbf{A}^2 = \mathbf{A} \times \mathbf{A}$$

and

$$\mathbf{A}^3 = \mathbf{A}^2 \times \mathbf{A} = \mathbf{A} \times \mathbf{A} \times \mathbf{A}$$

Note that nonsquare matrices cannot be powered, because the number of rows and columns of a rectangular matrix would not accord if the matrix were multiplied by itself.

As an example, we can power the array of transition probabilities discussed at the first of this section. In matrix form,

$$\mathbf{T} = \begin{bmatrix} 0.74 & 0.23 & 0.03 \\ 0.10 & 0.61 & 0.29 \\ 0.05 & 0.38 & 0.57 \end{bmatrix}$$

So,

$$\mathbf{T}^2 = \begin{bmatrix} 0.572 & 0.322 & 0.106 \\ 0.150 & 0.505 & 0.345 \\ 0.104 & 0.460 & 0.437 \end{bmatrix}$$

and

$$\mathbf{T}^3 = \begin{bmatrix} 0.461 & 0.368 & 0.171 \\ 0.178 & 0.474 & 0.348 \\ 0.144 & 0.470 & 0.385 \end{bmatrix}$$

If we continue to power the transition probability matrix, it converges to a stable configuration (called the ***stationary probability matrix***) in which each column of the matrix is a constant. These are the proportions of the specific lithologies represented by the columns. In this example, the proportions are 23% sandstone, 45% shale, and 32% limestone. We can see that the columns are converging on these values at the 10th power of **T**:

$$\mathbf{T}^{10} = \begin{bmatrix} 0.248 & 0.443 & 0.309 \\ 0.230 & 0.449 & 0.321 \\ 0.228 & 0.450 & 0.322 \end{bmatrix}$$

Square matrices also can be raised to a fractional power, most commonly to the one-half power. This is equivalent to finding the square root of the matrix. That is, $\mathbf{A}^{1/2}$ is a matrix, **X**, whose square is **A**:

$$\mathbf{A}^{1/2} = \mathbf{X}$$
$$\mathbf{X}^2 = \mathbf{X} \times \mathbf{X} = \mathbf{A}$$

Finding fractional powers of matrices can be computationally troublesome. Fortunately, in the applications we will consider, we will only need to find the fractional powers of diagonal matrices, which have special properties that make it easy to raise them to a fractional power. If we raise the diagonal matrix **A** to the one-half power, the result is a diagonal matrix whose nonzero elements are equal to the square roots of the equivalent elements in **A**. For example, if **A** is 3×3,

$$\begin{bmatrix} a_{11} & 0 & 0 \\ 0 & a_{22} & 0 \\ 0 & 0 & a_{33} \end{bmatrix}^{1/2} = \begin{bmatrix} \sqrt{a_{11}} & 0 & 0 \\ 0 & \sqrt{a_{22}} & 0 \\ 0 & 0 & \sqrt{a_{33}} \end{bmatrix}$$

As we defined it earlier, the identity matrix is a special diagonal matrix in which the diagonal terms are all equal to 1. The identity matrix has an extremely useful property; if a matrix is multiplied by an identity matrix, the resulting product is exactly the same as the initial matrix:

$$\mathbf{A} \times \mathbf{I} = \mathbf{A}$$

$$\begin{bmatrix} 1 & 4 & 7 \\ 2 & 5 & 8 \\ 3 & 6 & 9 \end{bmatrix} \times \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} = \begin{bmatrix} 1 & 4 & 7 \\ 2 & 5 & 8 \\ 3 & 6 & 9 \end{bmatrix}$$

Thus, the identity matrix corresponds to the 1 of ordinary multiplication. This property is especially important in operations in the following sections.

Inversion and Solution of Simultaneous Equations

Division of one matrix by another, in the sense of ordinary algebraic division, cannot be performed. However, by utilizing the rules of matrix multiplication, an operation can be performed that is equivalent to solving the equation

$$\mathbf{A} \times \mathbf{X} = \mathbf{B}$$

for the unknown matrix, **X**, when the elements of **A** and **B** are known. This is one of the most important techniques in matrix algebra, and it is essential for the solution of simultaneous equations such as those of trend-surface analysis and discriminant functions. The techniques of matrix inversion will be encountered again and again in the next chapters of this book.

The equation given above is solved by finding the inverse of matrix **A**. The ***inverse matrix*** (or ***reciprocal*** matrix) $\mathbf{A}^{-1}$ is one that satisfies the relationship $\mathbf{A} \times \mathbf{A}^{-1} = \mathbf{I}$. If both sides of a matrix equation are multiplied by $\mathbf{A}^{-1}$, the matrix **A** is effectively removed from the left side. At the same time, **B** is converted into a quantity that is the value of the unknown matrix **X**. The matrix **A** must be a square matrix. Beginning with

$$\mathbf{A} \times \mathbf{X} = \mathbf{B}$$

premultiply both sides by the inverse of **A**, or $\mathbf{A}^{-1}$:

$$\mathbf{A}^{-1} \times \mathbf{A} \times \mathbf{X} = \mathbf{A}^{-1} \times \mathbf{B}$$

Since $\mathbf{A}^{-1} \times \mathbf{A} = \mathbf{I}$ and $\mathbf{I} \times \mathbf{X} = \mathbf{X}$, the equation reduces to

$$\mathbf{X} = \mathbf{A}^{-1} \times \mathbf{B} \tag{3.2}$$

Thus, the problem of division by a matrix reduces to one of finding a matrix that satisfies the reciprocal relationship. In some situations, an inverse cannot be found because division by zero is encountered during the inversion process. A matrix with no inverse is called a ***singular matrix***, and presents problems beyond the scope of this chapter.

The inversion procedure may be illustrated by solving the following pair of simultaneous equations in matrix form. The unknown coefficients are $x_1 = 2$ and $x_2 = 3$. We will attempt to recover them by a process of matrix inversion and multiplication:

$$\begin{aligned} 4x_1 + 10x_2 &= 38 \\ 10x_1 + 30x_2 &= 110 \end{aligned}$$

This is a set of equations of the general type

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

where **A** is a matrix of coefficients, **X** is a column vector of unknowns, and **B** is a column vector of right-hand sides of the equations. In the specific set of equations given above, we have

$$\begin{bmatrix} 4 & 10 \\ 10 & 30 \end{bmatrix} \times \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 38 \\ 110 \end{bmatrix}$$

To solve the equation, the matrix **A** will be inverted and **B** will be multiplied by $\mathbf{A}^{-1}$ to give the solution for **X**.

It may not be apparent why the set of simultaneous equations can be set into the matrix form shown. You can satisfy yourself on this point, however, by multiplying the two terms, **AX**, to obtain the left-hand side of the simultaneous equation set:

$$\begin{bmatrix} 4 & 10 \\ 10 & 30 \end{bmatrix} \times \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 4x_1 + 10x_2 \\ 10x_1 + 30x_2 \end{bmatrix}$$

Working through this multiplication, you will see that all of the terms are associated with the proper coefficients. By the rules of matrix multiplication,

$$\begin{bmatrix} 4 & 10 \\ 10 & 30 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 4x_1 + 10x_2 \\ \end{bmatrix}$$

Then, multiplying the bottom row,

$$\begin{bmatrix} 4 & 10 \\ 10 & 30 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} \\ 10x_1 + 30x_2 \end{bmatrix}$$

We will solve the simultaneous equation set by first inverting the term **A**. Place the **A** matrix beside an identity matrix, **I**, and perform all operations simultaneously on both matrices. The purpose of each operation is to convert the diagonal elements of **A** to ones and the off-diagonal elements to zeros. This is done by dividing rows of the matrix by constants and subtracting (or adding) rows of the matrix from other rows:

1. $\begin{bmatrix} 4 & 10 \\ 10 & 30 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$ The matrix **A** is placed beside an identity matrix, **I**;
2. $\begin{bmatrix} 1 & 2.5 \\ 10 & 30 \end{bmatrix} \begin{bmatrix} 0.25 & 0 \\ 0 & 1 \end{bmatrix}$ row one is divided by 4, the first element in the row, to produce 1 at a_{11};
3. $\begin{bmatrix} 1 & 2.5 \\ 0 & 5 \end{bmatrix} \begin{bmatrix} 0.25 & 0 \\ -2.5 & 1 \end{bmatrix}$ 10 times row one is subtracted from row two to reduce a_{21} to 0;
4. $\begin{bmatrix} 1 & 2.5 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} 0.25 & 0 \\ -0.5 & 0.2 \end{bmatrix}$ row two is divided by 5 to give 1 at a_{22}, and
5. $\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} 1.5 & -0.5 \\ -0.5 & 0.2 \end{bmatrix}$ 2.5 times row two is subtracted from row one to reduce the final off-diagonal element to 0.

The matrix is now inverted. Work may be checked by multiplying the original matrix **A** by the inverted matrix, $\mathbf{A}^{-1}$, which should yield the identity matrix

$$\begin{bmatrix} 1.5 & -0.5 \\ -0.5 & 0.2 \end{bmatrix} \times \begin{bmatrix} 4 & 10 \\ 10 & 30 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

Because

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

the following identities hold:

$$\mathbf{A}^{-1}\mathbf{A}\mathbf{X} = \mathbf{A}^{-1}\mathbf{B}$$
$$\mathbf{I}\mathbf{X} = \mathbf{A}^{-1}\mathbf{B}$$
$$\mathbf{X} = \mathbf{A}^{-1}\mathbf{B}$$

By postmultiplying the inverted matrix $\mathbf{A}^{-1}$ by the matrix **B**, the unknown matrix, **X**, is solved,

$$\mathbf{A}^{-1} \quad \times \quad \mathbf{B} \quad = \quad \mathbf{X}$$

$$\begin{bmatrix} 1.5 & -0.5 \\ -0.5 & 0.2 \end{bmatrix} \times \begin{bmatrix} 38 \\ 110 \end{bmatrix} = \begin{bmatrix} 2 \\ 3 \end{bmatrix}$$

The column vector contains the unknown coefficients which we find to be equal to $x_1 = 2$ and $x_2 = 3$. You will recall that it was stated that these were the coefficients originally in the equation set, so we have recovered the proper values.

As an additional example of the solution of simultaneous equations by matrix inversion, we can set the equations below into matrix form and solve for x_1 and x_2 by inversion,

$$2x_1 + x_2 = 4$$
$$3x_1 + 4x_2 = 1$$

The steps in the inversion process can be written out briefly:

1. $\begin{bmatrix} 2 & 1 \\ 3 & 4 \end{bmatrix} \times \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 4 \\ 1 \end{bmatrix}$

2. $\begin{bmatrix} 2 & 1 \\ 3 & 4 \end{bmatrix}^{-1} = \begin{bmatrix} 4/5 & -1/5 \\ -3/5 & 2/5 \end{bmatrix}$

3. $\begin{bmatrix} 4/5 & -1/5 \\ -3/5 & 2/5 \end{bmatrix} \times \begin{bmatrix} 4 \\ 1 \end{bmatrix} = \begin{bmatrix} 3 \\ -2 \end{bmatrix}$

Therefore, the unknown coefficients are $x_1 = 3$ and $x_2 = -2$.

It may be noted that the procedure just described is almost exactly the same as the classical algebraic method of solving two simultaneous equations. In fact, the solution of simultaneous equations is probably the most important application of matrix inversion. The advantage of matrix manipulation over the "try it and see" approach of ordinary algebra is that it is more amenable to computer programming. Almost all of the techniques described in subsequent chapters of this book involve the solution of sets of simultaneous equations. These can be expressed conveniently in the form of matrix equations and solved in the manner just described.

Matrix inversion can, of course, be applied to square matrices of any size, and not just the 2×2 examples we have investigated so far. Demonstrate this to yourself by inverting the 3 × 3 matrix below:

$$\begin{bmatrix} 1 & 2 & 3 \\ 2 & 6 & 5 \\ 3 & 5 & 6 \end{bmatrix}$$

If we need the inverse of a diagonal matrix, the problem is much simpler. The inverse of a diagonal matrix is simply another diagonal matrix whose nonzero

elements are the reciprocals of the corresponding elements of the original matrix. Considering the 3×3 matrix, **A**,

$$\begin{bmatrix} a_{11} & 0 & 0 \\ 0 & a_{22} & 0 \\ 0 & 0 & a_{33} \end{bmatrix}^{-1} = \begin{bmatrix} 1/a_{11} & 0 & 0 \\ 0 & 1/a_{22} & 0 \\ 0 & 0 & 1/a_{33} \end{bmatrix}$$

Certain combinations of otherwise complicated operations become very simple when the matrices involved are diagonal matrices. For example, consider the multiplication

$$\mathbf{A}^{-1}\mathbf{A}^{1/2} = \mathbf{A}^{-1/2}$$

If **A** is 3×3, the product is

$$\begin{bmatrix} a_{11} & 0 & 0 \\ 0 & a_{22} & 0 \\ 0 & 0 & a_{33} \end{bmatrix}^{-1/2} = \begin{bmatrix} 1/\sqrt{a_{11}} & 0 & 0 \\ 0 & 1/\sqrt{a_{22}} & 0 \\ 0 & 0 & 1/\sqrt{a_{33}} \end{bmatrix}$$

In some applications, the inverse may not be required, but only the solutions to a set of simultaneous equations. In the handworked example, we wanted the values of the matrix **X** in the equation

$$\begin{bmatrix} 4 & 10 \\ 10 & 30 \end{bmatrix} \times \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 38 \\ 110 \end{bmatrix}$$

To find this, we inverted **A** and then postmultiplied $\mathbf{A}^{-1}$ by **B** to give **X**. We could have instead found **X** directly by operating on **B** as **A** was transformed into an identity matrix. To do this, we would utilize what is called an ***augmented matrix*** that has one more column than it has rows. The column vector, **B**, then occupies the $(n+1)$ column of the matrix, and the remaining $(n \times n)$ part is inverted. Repeating the same problem:

1. $\left[\begin{array}{cc|c} 4 & 10 & 38 \\ 10 & 30 & 110 \end{array}\right]$ Matrices **A** and **B** are combined in an $n \times (n+1)$ matrix.
2. $\left[\begin{array}{cc|c} 1.0 & 2.5 & 9.5 \\ 1.0 & 3.0 & 11.0 \end{array}\right]$ Row one is divided by 4 and row two is divided by 10.
3. $\left[\begin{array}{cc|c} 1.0 & 2.5 & 9.5 \\ 0.0 & 0.5 & 1.5 \end{array}\right]$ Row one is subtracted from row two.
4. $\left[\begin{array}{cc|c} 1.0 & 0 & 2.0 \\ 0.0 & 0.5 & 1.5 \end{array}\right]$ Row two is multiplied by 5 and the product is subtracted from row one.
5. $\left[\begin{array}{cc|c} 1.0 & 0.0 & 2.0 \\ 0.0 & 1.0 & 3.0 \end{array}\right]$ Row two is divided by 0.5.

So, the $(n+1)$ column of the augmented matrix contains the solution to the simultaneous equation set, and our original matrix has been replaced by an identity matrix.

Few mathematical procedures have received the attention given to matrix inversion. Dozens of methods have been devised to solve sets of simultaneous equations, and hundreds of programmed versions exist. Some are especially tailored to deal with special types of matrices, such as those containing many zero elements (such matrices are called ***sparse***) or possessing certain types of symmetry. Numerical computation packages for personal computers, such as MATHEMATICA® and MATLAB®, contain alternative algorithms that can be used to calculate the inverse of matrices. Some of these procedures, such as singular value decomposition (SVD), will find approximate inverses even when exact solutions do not exist.

Determinants

Before discussing our final topic, which is eigenvalues and eigenvectors and how they are obtained, we must examine an additional property of a square matrix called the ***determinant***. A determinant is a single number extracted from a square matrix by a series of operations, and is symbolically represented by det **A**, $|\mathbf{A}|$, or by

$$\begin{vmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{vmatrix}$$

It is defined as the sum of $n!$ terms of the form

$$(-1)^k a_{1i_1} a_{2i_2} \dots a_{ni_n} \tag{3.3}$$

where n is the number of rows (or columns) in the matrix, the subscripts $i_1, i_2, \dots, i_n$ are equal to $1, 2, \dots, n$, taken in any order, and k is the number of exchanges of two elements necessary to place the i subscripts in the order $1, 2, \dots, n$. Each term contains one element from each row and each column. The process of obtaining a determinant from a square matrix is called ***evaluating the determinant***.

We begin the process of evaluating the determinant by selecting one element from each row of the matrix to form a term or combination of elements. The elements in a term are selected in order from row $1, 2, \dots, n$, but each combination can contain only one element from each column. For example, we might select the combination $a_{12}a_{21}a_{33}$ from a 3×3 matrix. Note that the method of selection places the elements in proper order according to their first, or row, subscript. The term contains one and only one element from each row and each column. We must find all possible combinations of elements that can be formed in this way. If a matrix is $n \times n$, there will be $n!$ combinations which contain one element from each row and column, and whose first subscripts are in the order $1, 2, \dots, n$.

Since the order of multiplication of a series of numbers makes no difference in the product, that is, $a_{11}a_{22}a_{33} = a_{22}a_{11}a_{33} = a_{33}a_{22}a_{11}$ and so on, we can rearrange our combinations without changing the result. We wish to rearrange each combination until the second, or column, subscript of each element is in proper numerical order. The rearranging may be performed by swapping any two adjacent elements. As the operation is performed, we must keep track of the number of exchanges or transpositions necessary to get the second subscript in the correct order. If an even number of transpositions is required (*i.e.*, 0, 2, 4, 6, *etc.*), the product is given a positive sign. If an odd number of transpositions is necessary (1, 3, 5, 7, *etc.*), the product is negative.

In a 2×2 matrix

$$\begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix}$$

we can find two combinations of elements that contain one and only one element from each row and each column. These are $a_{11}a_{22}$ and $a_{12}a_{21}$.

The second subscripts in $a_{11}a_{22}$ are in correct numerical order and no rearranging is necessary. The number of transpositions is zero, so the sign of the product is positive. However, $a_{12}a_{21}$ must be rearranged to $a_{21}a_{12}$ before the second subscripts are in numerical order. This requires one transposition, so the product is negative. The determinant of a 2×2 matrix is therefore

$$\begin{vmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{vmatrix} = +a_{11}a_{22} - a_{12}a_{21}$$

For a numerical example, we will consider the matrix

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

The determinant is

$$\begin{vmatrix} 2 & 1 \\ 4 & 3 \end{vmatrix} = +(2 \times 3) - (1 \times 4) = 2$$

Next, let us consider a more complex example, a 3×3 determinant:

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

There are 3!, or $3 \times 2 \times 1 = 6$, combinations of elements in a 3×3 matrix that contain one element from each row and column and whose first subscripts are in the order 1, 2, 3. Start with the top row and pick an entry from each row. Be sure to choose in order from the first row, second row, third row, ... nth row, with no more than one entry from each column. All possible combinations that satisfy these conditions in a 3×3 matrix are

$$\begin{array}{ll} a_{11}a_{22}a_{33} & a_{11}a_{23}a_{32} \\ a_{12}a_{23}a_{31} & a_{12}a_{21}a_{33} \\ a_{13}a_{21}a_{32} & a_{13}a_{22}a_{31} \end{array}$$

To determine the signs of each of these terms, we must see how many transpositions are necessary to get the second subscripts in the order 1, 2, 3. For $a_{11}a_{22}a_{33}$, no transpositions are necessary, so $k = 0$ and the term is positive. Transpositions for the others and the resulting signs are given below:

$$a_{11}\,a_{23}\,a_{32} = a_{11}\,a_{32}\,a_{23} \qquad k = 1 \quad \text{sign} = -$$

$$a_{12}\,a_{23}\,a_{31} = a_{12}\,a_{31}\,a_{23} = a_{31}\,a_{12}\,a_{23} \qquad k = 2 \quad \text{sign} = +$$

$$a_{12}\,a_{21}\,a_{33} = a_{21}\,a_{12}\,a_{33} \qquad k = 1 \quad \text{sign} = -$$

$$a_{13}\,a_{21}\,a_{32} = a_{21}\,a_{13}\,a_{32} = a_{21}\,a_{32}\,a_{13} \qquad k = 2 \quad \text{sign} = +$$

$$a_{13}\,a_{22}\,a_{31} = a_{13}\,a_{31}\,a_{22} = a_{31}\,a_{13}\,a_{22} = a_{31}\,a_{22}\,a_{13} \qquad k = 3 \quad \text{sign} = -$$

Thus, there are three negative and three positive terms in the determinant. Summing according to the signs just found yields a single number, which is

$$+a_{11}a_{22}a_{33} - a_{11}a_{23}a_{32} + a_{12}a_{23}a_{31} - a_{12}a_{21}a_{33} + a_{13}a_{21}a_{32} - a_{13}a_{22}a_{31}$$

We can now try a matrix of real values:

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

The six terms possible are

$$\begin{aligned} (4 \times 4 \times 3) &= 48 \\ (4 \times 1 \times 0) &= 0 \\ (3 \times 1 \times 1) &= 3 \\ (3 \times 2 \times 3) &= 18 \\ (2 \times 2 \times 0) &= 0 \\ (2 \times 4 \times 1) &= 8 \end{aligned}$$

The first, third, and fifth of these require an even number of transpositions for proper arrangement of the second subscript and so are positive. The others require an odd number of transpositions and are therefore negative. Summing, we have

$$\det \mathbf{A} = +48 - 0 + 3 - 18 + 0 - 8 = 25$$

This method of evaluating a determinant is described by Pettofrezzo (1978). A more conventional approach (see, for example, Anton and Rorres, 1994) uses what is called the "method of cofactors," but the two can be shown to be equivalent.

We now have at our command a system for reducing a square matrix into its determinant, but no clear grasp of what a determinant "really is." Determinants arise in many ways, but they appear most conspicuously during the solution of sets of simultaneous equations. You may not have noticed them, however, because they have been hidden in the inversion process we have been using.

Consider the set of equations:

$$\begin{aligned} a_{11}x_1 + a_{12}x_2 &= b_1 \\ a_{21}x_1 + a_{22}x_2 &= b_2 \end{aligned}$$

Expressed in matrix form, this becomes

$$\begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \end{bmatrix}$$

and we have discussed how the vector of unknown x's can be solved by matrix inversion. However, with algebraic rearrangement, the unknowns also can be found by the equations

$$x_1 = \frac{b_1 a_{22} - a_{12} b_2}{a_{11} a_{22} - a_{12} a_{21}}$$

and

$$x_2 = \frac{a_{11} b_2 - b_1 a_{21}}{a_{11} a_{22} - a_{12} a_{21}}$$

You will note that the denominators are the same for both unknowns. They also are the determinants of the matrix **A**. That is,

$$|\mathbf{A}| = \begin{vmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{vmatrix} = a_{11}a_{22} - a_{12}a_{21}$$

Furthermore, the numerators can be expressed as determinants. For the equation of x_1, the numerator is the determinant of the matrix

$$|\mathbf{B}\,\mathbf{A}_{i2}| = \begin{vmatrix} b_1 & a_{12} \\ b_2 & a_{22} \end{vmatrix} = b_1a_{22} - b_2a_{21}$$

and for x_2, it is the determinant of

$$|\mathbf{A}_{1i}\,\mathbf{B}| = \begin{vmatrix} a_{11} & b_1 \\ a_{21} & b_2 \end{vmatrix} = a_{11}b_2 - a_{21}b_1$$

This procedure can be generalized to any set of simultaneous equations and provides one common method for their solution. This procedure for solving equations is called ***Cramer's rule.*** The rule states that the solution for any unknown x_i in a set of simultaneous equations is equal to the ratio of the two determinants. The denominator is the determinant of the coefficients (in our example, the a's). The numerator is the same determinant except that the ith column is replaced by the vector of right-hand terms (the vector of b's). Let us check the rule with an example used before:

$$\begin{bmatrix} 4 & 10 \\ 10 & 30 \end{bmatrix} \times \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 38 \\ 110 \end{bmatrix}$$

The denominators of the ratios for both unknown coefficients are the same:

$$\begin{vmatrix} 4 & 10 \\ 10 & 30 \end{vmatrix} = (4 \times 30) - (10 \times 10) = 20$$

The numerator of x_1 is the determinant

$$\begin{vmatrix} 38 & 10 \\ 110 & 30 \end{vmatrix} = (38 \times 30) - (110 \times 10) = 40$$

so $x_1 = 40/20 = 2$. For x_2, the numerator is the determinant

$$\begin{vmatrix} 4 & 38 \\ 10 & 110 \end{vmatrix} = (4 \times 110) - (10 \times 38) = 60$$

so $x_2 = 60/20 = 3$. These are the same unknowns we recovered by matrix inversion.

The determinant of an arbitrary square matrix such as the 3×3 example above may be a positive value, a negative value, or zero. If the matrix is symmetric (the variety of matrix we will encounter most often), its determinant cannot be negative. However, the distinction between a positive determinant and a zero determinant is very important because a matrix whose determinant is zero cannot be inverted by ordinary methods. That is, the matrix will be singular.

What circumstances will lead to singularity? The condition indicates that two or more rows (or columns) of the matrix are linear combinations or linear transformations of other rows; that is, the values in some rows (or columns) are dependent on values in other rows. For example, the determinant

$$\begin{vmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \\ 2 & 4 & 6 \end{vmatrix} = 0$$

is zero because the third row of the matrix is simply twice the first row. Similarly, the determinant

$$\begin{vmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \\ 5 & 7 & 9 \end{vmatrix} = 0$$

is zero because the third row is the sum of rows one and two. Of course, in real problems the source of singularity usually is not so obvious. Consider the data in file BALTIC.TXT, which gives the weight-percent of sand in five successive size fractions, measured on bottom samples collected in an area of the Baltic Sea. We can calculate correlations between the five sand size categories and place the results in a square, symmetric correlation matrix:

$$\begin{bmatrix} 1 & 0.243 & -0.301 & 0.096 & -0.261 \\ 0.243 & 1 & -0.969 & -0.562 & -0.422 \\ -0.301 & -0.969 & 1 & 0.340 & 0.253 \\ 0.096 & -0.562 & 0.340 & 1 & 0.691 \\ -0.261 & -0.422 & 0.253 & 0.691 & 1 \end{bmatrix}$$

It is not obvious that this matrix should be singular with a zero determinant, yet it is. The linear dependence comes about because the weight-percentages in the five size categories sum to 100 for each observation, so there are induced negative correlations between the size categories. (Actually, because of rounding during computations, you may compute a correlation matrix that is not exactly singular. Depending upon the numerical precision of the computer program, rather than exactly 0, you may observe a very small determinant such as −0.0002. A matrix with a determinant near zero is said to be ***ill-conditioned***.)

Finally, there is another special case of interest. An identity matrix has a determinant equal to 1.0. If several variables are completely independent of each other, their correlations will be near zero and they will form a correlation matrix that approximates an identity matrix. The determinant of such a matrix will be close to one, and its logarithm will be close to zero; this is the basis for one test of independence between variables.

Eigenvalues and Eigenvectors

The topic we will consider next usually is regarded as one of the most difficult topics in matrix algebra, the determination of eigenvalues and eigenvectors (also called "latent" and "proper" values and vectors). The difficulty is not in their calculation, which is cumbersome but no more so than many other mathematical procedures. Rather, difficulties arise in developing a "feel" for the meaning of these quantities, especially in an intuitive sense. Unfortunately, many textbooks provide no help in this regard, placing their discussions in strictly mathematical terms that may be difficult for nonmathematicians to interpret.

A lucid discussion and geometric interpretation of eigenvectors and eigenvalues was prepared by Peter Gould for the benefit of geography students at Pennsylvania State University. The following discussion leans heavily on his prepared notes and a subsequent article (Gould, 1967). We will consider a real matrix of coordinates of points in space and interpret the eigenvalues and associated functions as geometric properties of the arrangement of these points. This approach limits us, of course, to small matrices, but the insights gained can be extrapolated to larger systems even though hand computation becomes impractical. In this regard, it may be noted that we are entering a realm where the computational powers of even the largest computers may be inadequate to solve real problems.

Eigenvalues

Having worked through determinants, we can use them to develop eigenvalues. Consider a hypothetical set of simultaneous equations expressed in the following matrix form:

$$\mathbf{A}\mathbf{X} = \lambda\mathbf{X} \tag{3.4}$$

This equation states that the matrix of coefficients (the a_{ij}'s) times the vector of unknowns (the x_i's) is equal to some constant (λ) times the unknown vector itself. The problem is the same as in the solution of the simultaneous equation set

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

except now

$$\mathbf{B} = \lambda\mathbf{X}$$

Our concern is to find values of λ that satisfy this relationship. Equation (3.4) can be rewritten in the form

$$(\mathbf{A} - \lambda\mathbf{I})\,\mathbf{X} = 0 \tag{3.5}$$

where $\lambda\mathbf{I}$ is nothing more than an identity matrix (of the same size as **A**) times the quantity λ. That is,

$$\lambda\mathbf{I} = \begin{bmatrix} \lambda & 0 & 0 \\ 0 & \lambda & 0 \\ 0 & 0 & \lambda \end{bmatrix}$$

for a 3×3 matrix. Written in conventional form, the equivalent of the three simultaneous equations is

$$\begin{aligned} (a_{11} - \lambda)\,x_1 + a_{12}x_2 + a_{13}x_3 &= 0 \\ a_{21}x_1 + (a_{22} - \lambda)\,x_2 + a_{23}x_3 &= 0 \\ a_{31}x_1 + a_{32}x_2 + (a_{33} - \lambda)\,x_3 &= 0 \end{aligned} \tag{3.6}$$

Let us assume that there are solutions to these equations other than the trivial case where all the unknown x's = 0. Look back at Cramer's rule for the solution of simultaneous equations, in which the unknowns are expressed as the ratio of two determinants. Because the numerator in our present example would contain a column of zeros, the determinant of the numerator also will be zero. That is, the solution for the **X** vector is

$$\mathbf{X} = \frac{0}{|\mathbf{A}|}$$

Rewriting, this becomes

$$|\mathbf{A}|\,\mathbf{X} = 0 \tag{3.7}$$

If the vector **X** is not zero, it follows that the determinant of the matrix **A** must be zero, or

$$|\mathbf{A} - \lambda\mathbf{I}| = \begin{vmatrix} a_{11} - \lambda & a_{12} & a_{13} \\ a_{21} & a_{22} - \lambda & a_{23} \\ a_{31} & a_{32} & a_{33} - \lambda \end{vmatrix} = 0 \tag{3.8}$$

We usually know the coefficients, a_{ij}, of the matrix, so this equation can be used to determine the values of $\lambda\mathbf{I}$ that satisfy all of these various conditions. This is done by expanding the determinant to yield a polynomial equation. Looking first at a 2×2 determinant,

$$\begin{vmatrix} a_{11} - \lambda & a_{12} \\ a_{21} & a_{22} - \lambda \end{vmatrix} = 0$$

Expanding gives

$$(a_{11} - \lambda)(a_{22} - \lambda) - a_{21}a_{12} = 0$$

Multiplying out the first term,

$$(a_{11} - \lambda)(a_{22} - \lambda) = (a_{11}a_{22}) - (a_{11}\lambda) - (a_{22}\lambda) + \lambda^2$$

Thus we have

$$(a_{11}a_{22}) - (a_{21}a_{12}) - (a_{11}\lambda) - (a_{22}\lambda) + \lambda^2 = 0$$

Because we know the various values of the elements a_{ij}, we can collect all of these terms together in the form of an equation such as

$$\lambda^2 + \alpha_1\lambda + \alpha_2 = 0 \tag{3.9}$$

where the α's represent the sum of the numerical values of the appropriate a_{ij}'s. You should recognize that this is a quadratic equation of the general form

$$ax^2 + bx + c = 0$$

which can be solved for the unknown terms by factoring. The general solution to a quadratic equation is

$$x = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a} \tag{3.10}$$

If this seems unfamiliar, review the sections in an elementary algebra book that deal with factoring and quadratic equations. Now, we can try the procedures just outlined to find the eigenvalues of the 2×2 matrix:

$$\mathbf{A} = \begin{bmatrix} 17 & -6 \\ 45 & -16 \end{bmatrix}$$

First, we must set the matrix in the form

$$\mathbf{A} - \lambda\mathbf{I} = \begin{bmatrix} 17 - \lambda & -6 \\ 45 & -16 - \lambda \end{bmatrix}$$

Equating the determinant to zero,

$$\begin{vmatrix} 17 - \lambda & -6 \\ 45 & -16 - \lambda \end{vmatrix} = 0$$

we can expand the determinant

$$\begin{vmatrix} 17 - \lambda & -6 \\ 45 & -16 - \lambda \end{vmatrix} = (17 - \lambda)(-16 - \lambda) - (-6)(45) = 0$$

Multiplying out gives

$$-272 - 17\lambda + 16\lambda + \lambda^2 + 270 = 0$$

which can be collected to give

$$\lambda^2 - \lambda - 2 = 0$$

This can be factored into

$$(\lambda - 2)(\lambda + 1) = 0$$

So, the two eigenvalues associated with the matrix **A** are

$$\lambda_1 = +2 \qquad \lambda_2 = -1$$

This example was deliberately chosen for ease in factoring. We can try a somewhat more difficult example by using the set of simultaneous equations we solved earlier. This is the 2×2 matrix:

$$\mathbf{A} = \begin{bmatrix} 4 & 10 \\ 10 & 30 \end{bmatrix}$$

Repeating the sequence of steps yields the determinant

$$\begin{vmatrix} 4 - \lambda & 10 \\ 10 & 30 - \lambda \end{vmatrix} = 0$$

which is then expanded into

$$\begin{vmatrix} 4 - \lambda & 10 \\ 10 & 30 - \lambda \end{vmatrix} = (4 - \lambda)(30 - \lambda) - 100 = 0$$

or

$$\lambda^2 - 34\lambda + 20 = 0$$

There are no obvious factors in the quadratic equation, so we must apply the rule for a general solution:

$$x = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a} = \lambda = \frac{-(-34) \pm \sqrt{-34^2 - 4 \times 1 \times 20}}{2 \times 1} = \frac{34 \pm \sqrt{1076}}{2}$$

$$\lambda_1 = 33.4 \qquad \lambda_2 = 0.6$$

We can check our work by substituting the eigenvalues back into the determinant to see if it is equal to zero, within the error introduced by round-off:

$$\begin{vmatrix} 4 - 33.4 & 10 \\ 10 & 30 - 33.4 \end{vmatrix} = (-29.4)(-3.4) - (10)(10) = -0.04$$

and

$$\begin{vmatrix} 4 - 0.6 & 10 \\ 10 & 30 - 0.6 \end{vmatrix} = (3.4)(29.4) - (10)(10) = -0.04$$

So, the eigenvalues we have found are correct within two decimal places.

Before we leave the computation of eigenvalues of 2×2 matrices, we should consider one additional complication that may arise. Suppose we want the eigenvalues of the matrix

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

Expressed as a determinant equal to zero, we have

$$\begin{vmatrix} 2 - \lambda & 4 \\ -6 & 3 - \lambda \end{vmatrix} = 0$$

which expands to

$$\begin{vmatrix} 2 - \lambda & 4 \\ -6 & 3 - \lambda \end{vmatrix} = (2 - \lambda)(3 - \lambda) + 24 = 0$$

or

$$\lambda^2 - 5\lambda + 30 = 0$$

The roots of this equation are

$$\lambda_1, \lambda_2 = \frac{5 \pm \sqrt{25 - 120}}{2}$$

But this leads to equations involving the square roots of negative numbers:

$$\lambda_1 = \frac{5 + \sqrt{-95}}{2} = 2.5 + 4.9i$$

$$\lambda_2 = \frac{5 - \sqrt{-95}}{2} = 2.5 - 4.9i$$

These are complex numbers, containing both real parts and imaginary parts which include the imaginary number, $i = \sqrt{-1}$. Fortunately, a symmetric matrix always yields real eigenvalues, and most of our computations involving eigenvalues and eigenvectors will utilize covariance, correlation, or similarity matrices which are always symmetrical.

Next, we will consider the eigenvalues of the third-order matrix:

$$\begin{bmatrix} 20 & -4 & 8 \\ -40 & 8 & -20 \\ -60 & 12 & -26 \end{bmatrix}$$

The determinant of the matrix is set to zero, giving

$$\begin{vmatrix} 20-\lambda & -4 & 8 \\ -40 & 8-\lambda & -20 \\ -60 & 12 & -26-\lambda \end{vmatrix} = 0$$

Expanding out the determinant and combining terms yields

$$-\lambda^3 + 2\lambda^2 + 8\lambda = 0$$

This is a cubic equation having three roots that must be found. In this instance, the polynomial can be factored into

$$(\lambda - 4)(\lambda - 0)(\lambda + 2) = 0$$

and the roots are directly obtainable:

$$\lambda_1 = +4 \qquad \lambda_2 = 0 \qquad \lambda_3 = -2$$

Although the techniques we have been using are extendible to any size matrix, finding the roots of large polynomial equations can be an arduous task. Usually, eigenvalues are not found by solution of a polynomial equation, but rather by matrix manipulation methods that involve refinement of a successive series of approximations to the eigenvalues. These methods are practical only because of the great computational speed of digital computers. Utilizing this speed, a researcher can compress literally a lifetime of trial solutions and refinements into a few minutes.

We can now define another measure of the "size" of a square matrix. The ***rank*** of a square matrix is the number of independent rows (or columns) in the matrix and is equal to the number of nonzero eigenvalues that can be extracted from the matrix. A nonsingular matrix has as many nonzero eigenvalues as there are rows or columns in the matrix, so its rank is equal to its order. A singular matrix has one or more rows or columns that are dependent on other rows or columns, and consequently will have one or more zero eigenvalues; its rank will be less than its order.

Now that we have an idea of the manipulations that produce eigenvalues, we may try to get some insight into their nature. The rows of a matrix can be regarded as the coordinates of points in m-dimensional space. If we restrict our consideration to 2×2 matrices, we can represent this space as an illustration on a page and can view matrix operations geometrically.

Table 3–3. Concentrations of selected elements (in ppm) measured in soil samples collected in vineyards and associated terraces on the Istrian peninsula of Croatia.

Cr	Cu	Mg	V	Zn
125	25	6936	114	194
205	33	5368	143	212
171	25	5006	90	272
62	157	3600	59	129
137	88	3220	130	123
234	185	7450	162	264
270	52	4400	205	155
179	322	5000	150	135
113	29	8600	98	114
65	400	4000	60	40
80	225	2000	90	130
35	230	1000	100	50
176	30	3100	160	100
90	164	5000	105	105
52	200	9000	60	170
98	29	3100	89	87
130	59	7100	112	147
158	28	6400	143	133
69	30	7900	109	103
108	30	2300	136	84

We will use a series of 2×2 matrices calculated from data that might arise in an environmental study. **Table 3–3** lists trace-element concentrations for five elements measured on 20 soil samples collected in vineyards and adjacent terraces on the Istrian peninsula of Croatia (the data are contained in the file ISTRIA.TXT). For centuries, the growers have treated their grapes with "blue galicia," or copper sulfate, to prevent fungus. As a consequence, the soil is enriched in copper and other metals that are present as impurities in the crude sulfate compound.

Using the matrix operations we have already discussed, we will construct a matrix containing correlations between the concentrations of the different metals. The data in **Table 3–3** can be regarded as a 20×5 matrix, **M**. Define a row vector **V** having 20 elements, each equal to 1.0. The matrix multiplication, **VM**, will yield a five-element row vector containing the column totals of **M**. If we premultiply this row vector by $1/20$, it will contain the means of each of the five columns.

We can now subtract the means from each observation to convert the data into deviations. By premultiplying the vector of means by the transpose of **V**, we create a 20×5 matrix in which every row is the same as the vector of means. Subtracting this matrix from **M** yields **D**, the data in the form of deviations from their means:

$$\mathbf{D} = \mathbf{M} - \mathbf{V}^{\mathrm{T}} n^{-1} \mathbf{V}\mathbf{M}$$

Here, n is the number of rows in **M** (*i.e.*, the number of observations) and n^{-1} is the inverse of n, or $1/20$.

Premultiplying **D** by its transpose will yield a square 5×5 matrix whose individual entries are the sums of squares (along the diagonal) and cross products of the

five elements, corrected for their means. If we divide a corrected sum of squares by $n - 1$ we obtain the variance, and if we divide a corrected sum of products by $n - 1$ we obtain the covariance. These are the elements of the covariance matrix, **S**, which we can compute by

$$\mathbf{S} = (n-1)^{-1}\mathbf{D}^{\mathrm{T}}\mathbf{D}$$

A subset of **S** could serve our purposes (and the covariance matrix often is used in multivariate statistics), but the relationships will be clearer if we use the correlation matrix, **R**. Correlations are simply covariances of standardized variables; that is, observations from which the means have been removed and then divided by the standard deviation. In matrix **D**, the means have already been removed. We can, in effect, divide by the appropriate standard deviations if we create a 5×5 matrix, **C**, whose diagonal elements are the square roots of the variances found on the diagonal of **S**, and whose off-diagonal elements are all 0.0. If we invert **C** and premultiply by **D**, each element of **D** will be divided by the standard deviation of its column. Call the result **U**, a 20×5 matrix of standardized values;

$$\mathbf{U} = \mathbf{D}\mathbf{C}^{-1}$$

We can calculate the correlation matrix by repeating the procedure we used to find **S**, substituting **U** for **D**:

$$\mathbf{R} = (n-1)^{-1}\mathbf{U}^{\mathrm{T}}\mathbf{U}$$

$$\mathbf{R} = \begin{bmatrix} 1 & -0.312 & 0.141 & 0.85 & 0.595 \\ -0.312 & 1 & -0.201 & -0.33 & -0.28 \\ 0.141 & -0.201 & 1 & -0.029 & 0.456 \\ 0.85 & -0.33 & -0.029 & 1 & 0.242 \\ 0.595 & -0.28 & 0.456 & 0.242 & 1 \end{bmatrix}$$

To graphically illustrate matrix relationships, we must confine ourselves to 2×2 matrices, which we can extract from **R**. Copper and zinc are recorded in the second and fifth columns of **M**, and so their correlations are the elements $r_{i,j}$ whose subscripts are 2 and 5:

$$\mathbf{R}_{cu,zn} = \begin{bmatrix} r_{2,2} & r_{2,5} \\ r_{5,2} & r_{5,5} \end{bmatrix} = \begin{bmatrix} 1 & -0.28 \\ -0.28 & 1 \end{bmatrix}$$

If we regard the rows as vectors in X and Y, we can plot each row as the tip of a vector that extends from the origin. In **Figure 3–1**, the tip of each vector is indicated by an open circle, labeled with its coordinates. The ends of the two vectors lie on an ellipse whose center is at the origin of the coordinate system and which just encloses the tips of the vectors. The eigenvalues of the 2×2 matrix $R_{cu,zn}$ represent the magnitudes, or lengths, of the major and minor semiaxes of the ellipse. In this example, the eigenvalues are

$$\lambda_1 = 1.28 \qquad \lambda_2 = 0.72$$

Gould refers to the relative lengths of the semiaxes as a measure of the "stretchability" of the enclosing ellipse. The semiaxes are shown by arrows on **Figure 3–1**. The first eigenvalue represents the major semiaxis whose length from center to

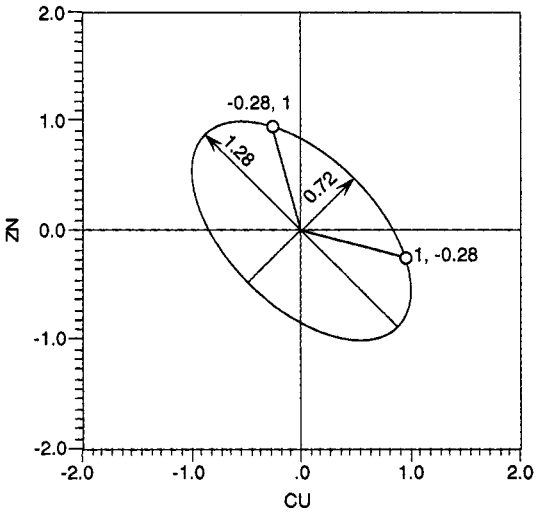


Figure 3–1. Ellipse defined by rows in matrix of correlations between copper and zinc. Eigenvectors of matrix correspond to principal semiaxes (arrows) of ellipse.

edge of the ellipse is 1.28 units. The second eigenvalue represents the length of the minor semiaxis, which is 0.72 units.

If the two vectors are closer together, the ratio between the semiaxes of the enclosing ellipse will change. For example, chromium and vanadium have very similar behavior in the vineyard soil samples, leading to a high correlation between the two. Their correlations are given by elements in the first and fourth rows and columns of **R**:

$$\mathbf{R}_{cr,v} = \begin{bmatrix} r_{1,1} & r_{1,4} \\ r_{4,1} & r_{4,4} \end{bmatrix} = \begin{bmatrix} 1 & 0.85 \\ 0.85 & 1 \end{bmatrix}$$

The rows of $\mathbf{R}_{cr,v}$ are plotted as vectors in **Figure 3–2**. The eigenvalues of this 2×2 matrix are

$$\lambda_1 = 1.85 \qquad \lambda_2 = 0.15$$

which define one very long major semiaxis and a short minor semiaxis. At the limit, we can imagine that two variables might behave in an identical fashion. Then, their rows in **R** would be so similar that they would be identical and the plotted vectors would coincide. That is,

$$\mathbf{R}_{x,y} = \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}$$

The enclosing ellipse would collapse to a straight line of semiaxis length $\lambda_1 = 2$ and a minor semiaxis of $\lambda_2 = 0$.

At the opposite extreme, two variables which are completely unrelated will have a correlation of near zero. Magnesium and vanadium show such behavior in the vineyard samples. They are represented by elements in the third and fourth rows and columns of **R**, and are shown plotted as vectors in **Figure 3–3**.

$$\mathbf{R}_{mg,v} = \begin{bmatrix} r_{3,3} & r_{3,4} \\ r_{4,3} & r_{4,4} \end{bmatrix} = \begin{bmatrix} 1 & -0.029 \\ -0.029 & 1 \end{bmatrix}$$

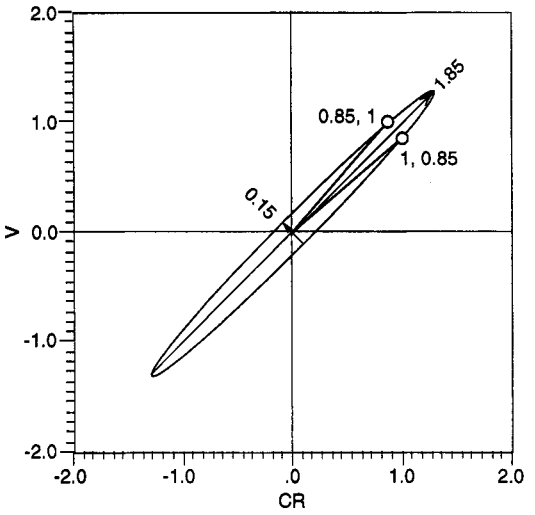


Figure 3–2. Elongated ellipse defined by rows in matrix of correlations between chromium and vanadium, which are highly correlated.

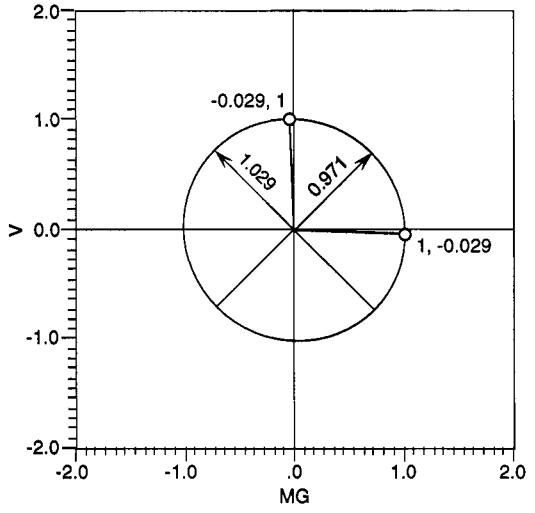


Figure 3–3. Nearly circular ellipse defined by rows in matrix of correlations between magnesium and vanadium, which have a correlation approaching zero.

The two eigenvalues of this matrix are

$$\lambda_1 = 1.029 \qquad \lambda_2 = 0.971$$

which are almost identical in size. As we can see, they define the major and minor semiaxes of an ellipse that is almost a circle, and both the semiaxes and the vectors are essentially radii. By definition, the axes of the ellipse are at right angles to each other, and the two plotted vectors also are almost orthogonal.

Some final notes on eigenvalues: You'll notice that the correlation matrices we've graphed are square, symmetrical about their diagonals, composed of real elements (that is, no imaginary numbers), and that the largest numbers in every row

are on the diagonal. As a consequence of these special conditions, the eigenvalues will always be real numbers that are equal to or greater than zero. As you can verify by checking these examples, the sum of the eigenvalues of a matrix is always equal to the sum of the diagonal elements, or the ***trace***, of the original matrix. In a correlation matrix, the diagonal elements are all equal to one, so the trace is simply the number of variables. The product of the eigenvalues will be equal to the determinant of the original matrix. Most (but not all) of the eigenvalue operations we will consider later will be applied to correlation or covariance matrices, so these special results will hold true in most instances. The methods just developed can be extended directly to $n \times n$ matrices, although the procedure becomes increasingly cumbersome with larger matrices.

Eigenvectors

We can examine the correlation matrices we calculated for the Istrian vineyard data to gain some insight into the geometrical nature of eigenvectors. First, consider the 2×2 matrix

$$\mathbf{R}_{cu,zn} = \begin{bmatrix} 1 & -0.28 \\ -0.28 & 1 \end{bmatrix}$$

with eigenvalues

$$\lambda_1 = 1.28 \qquad \lambda_2 = 0.72$$

Substituting the first eigenvalue into the original matrix gives

$$\begin{bmatrix} 1-1.28 & -0.28 \\ -0.28 & 1-1.28 \end{bmatrix} = \begin{bmatrix} -0.28 & -0.28 \\ -0.28 & -0.28 \end{bmatrix}$$

whose solution is the eigenvector

$$\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} -1 \\ 1 \end{bmatrix}$$

In **Figure 3–1**, we can interpret this eigenvector as the slope of the major semiaxis of the enclosing ellipse. If we regard the elements of the eigenvector as coordinates, the first eigenvector defines an axis which extends from the center of the ellipse into the second quadrant at an angle of 135°. The length is equal to the first eigenvalue, or 1.28.

Turning to the second eigenvalue, $\lambda_2 = 0.72$, the equation set is

$$\begin{bmatrix} 1-0.72 & -0.28 \\ -0.28 & 1-0.72 \end{bmatrix} = \begin{bmatrix} 0.28 & -0.28 \\ -0.28 & 0.28 \end{bmatrix}$$

whose solution gives the second eigenvector:

$$\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

In **Figure 3–1**, this will plot as the vector direction $1/1 = 45°$, perpendicular to the major semiaxis of the ellipse. Its magnitude or length is 0.72.

We can determine the eigenvalues for the matrix of correlations between chromium and vanadium in a similar fashion. The matrix is

$$\mathbf{R}_{cr,v} = \begin{bmatrix} 1 & 0.85 \\ 0.85 & 1 \end{bmatrix}$$

with eigenvalues

$$\lambda_1 = 1.85 \qquad \lambda_2 = 0.15$$

The first eigenvector is

$$\begin{bmatrix} 1 - 1.85 & 0.85 \\ 0.85 & 1 - 1.85 \end{bmatrix} = \begin{bmatrix} -0.85 & 0.85 \\ 0.85 & -0.85 \end{bmatrix}$$

$$\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

which defines a line having a slope of 45°. This axis bisects the angle between the two points and the center of the ellipse in **Figure 3–2.** The magnitude of the major semiaxis is equal to 1.85, the first eigenvalue of $\mathbf{R}_{cr,v}$. Similarly, we can show that the eigenvector associated with the second eigenvalue is

$$\begin{bmatrix} 1 - 0.15 & 0.85 \\ 0.85 & 1 - 0.15 \end{bmatrix} = \begin{bmatrix} 0.85 & 0.85 \\ 0.85 & 0.85 \end{bmatrix}$$

$$\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 1 \\ -1 \end{bmatrix}$$

This procedure can be applied to the matrix $\mathbf{R}_{mg,v}$ and the eigenvectors found will again define directions of 135° and 45°, as shown in **Figure 3–3.** By now you no doubt suspect that the eigenvectors of 2 × 2 symmetric matrices will always lie at these specific angles, and this is indeed the case. The eigenvectors of real, symmetric matrices are always orthogonal, or at right angles to each other. This is not true of eigenvectors of matrices in general, but only of symmetric matrices. In addition, the eigenvectors of two-dimensional symmetric matrices are additionally constrained to orientations that are multiples of 45°. Incidentally, if two vectors, **A** and **B**, are orthogonal, then $\mathbf{A}^T\mathbf{B} = 0$.

Eigenvalue and eigenvector techniques are directly extendible to larger matrices, even though the operations become tedious. As an example, we will consider the full 5 × 5 correlation matrix **R** for trace metals from Istrian vineyard soils. The five eigenvalues of this matrix are

$$\mathbf{\Lambda} = \begin{bmatrix} 2.453 & 1.233 & 0.789 & 0.465 & 0.061 \end{bmatrix}$$

and their associated eigenvectors are

$$\mathbf{V}_1 = \begin{bmatrix} 0.585 \\ -0.363 \\ 0.244 \\ 0.498 \\ 0.469 \end{bmatrix} \quad \mathbf{V}_2 = \begin{bmatrix} -0.248 \\ -0.075 \\ 0.736 \\ -0.490 \\ 0.389 \end{bmatrix} \quad \mathbf{V}_3 = \begin{bmatrix} 0.259 \\ 0.951 \\ 0.056 \\ 0.052 \\ 0.300 \end{bmatrix} \quad \mathbf{V}_4 = \begin{bmatrix} -0.014 \\ -0.149 \\ -0.628 \\ -0.398 \\ 0.652 \end{bmatrix} \quad \mathbf{V}_5 = \begin{bmatrix} -0.727 \\ 0.062 \\ -0.023 \\ 0.593 \\ 0.339 \end{bmatrix}$$

Each eigenvector can be regarded as a set of coordinates in five-dimensional space that defines the "direction" of a semiaxis of a hyperellipsoid. The length of each semiaxis is given by the corresponding eigenvalue. The first semiaxis is twice as long as the second, which is almost twice the length of the third. The fourth axis is very short, and the fifth axis is almost nonexistent; the hyperellipse defined by the correlation matrix, **R**, is really only a three-dimensional disk embedded in a space of five dimensions.

The slope of a line drawn from the origin of a graph through a point is defined by the ratio between the two coordinates of the point, and not by the actual magnitudes of the coordinates. Similarly, the absolute magnitudes of the elements in eigenvectors are not significant, only the ratios between the elements. An eigenvector can be scaled by multiplying by any arbitrary constant, and it will still define the same direction in multidimensional space. Different computer programs may return different eigenvectors for the same matrix; the eigenvectors simply have been scaled in different ways. Most programs ***normalize***, or scale each eigenvector so the sum of the squares of each element in a vector will be equal to 1.0. Others scale each eigenvector so the sum of its elements will be equal to its eigenvalue. Although such results appear to be different, the ratios between pairs of elements in the eigenvectors remain the same, and the vectors they define point in the same "direction." Also, you may note that the pattern of signs on the elements of the eigenvectors seems to be different for two otherwise identical sets of eigenvectors. This merely means that one set of vectors has been multiplied by (-1), reversing its "direction" but not changing its orientation in multivariate space.

Increasingly, computer programs for multivariate analysis employ alternative techniques for obtaining eigenvalues and eigenvectors. Rather than reducing a rectangular data matrix to a symmetrical, square correlation or covariance matrix and then extracting the desired eigenvalues and eigenvectors as we have done, these programs obtain results directly from the data matrix by ***singular value decomposition*** (SVD). An excellent description of SVD is given by Jackson (1991); Press and others (1992) provide a more compact presentation, as well as computer program listings. We will delay a discussion of this procedure until Chapter 6, where we can provide a motivation for our interest. Now, we merely note that an $n \times m$ rectangular matrix, **X**, can be decomposed into three other matrices:

$$\mathbf{X} = \mathbf{W}\mathbf{\Lambda}^{1/2}\mathbf{V}^{\mathrm{T}}$$

where **W** contains the eigenvectors of the major product matrix, $\mathbf{X}\mathbf{X}^{\mathrm{T}}$. **V** contains the eigenvectors of the minor product matrix, $\mathbf{X}^{\mathrm{T}}\mathbf{X}$, and $\mathbf{\Lambda}$ is an $m \times m$ diagonal matrix whose diagonal elements are the eigenvalues of either $\mathbf{X}\mathbf{X}^{\mathrm{T}}$ or $\mathbf{X}^{\mathrm{T}}\mathbf{X}$ (they will be identical except that $\mathbf{X}^{\mathrm{T}}\mathbf{X}$ will have $n - m$ extra eigenvalues, all equal to zero).

If you have worked through the small examples in this chapter, you can readily appreciate that the computational labor involved in dealing with large matrices can be formidable, even though the underlying, individual mathematical steps are simple. A modest data set such as ISTRIA.TXT will present a challenge to those who attempt to analyze the data by hand. Fortunately, there are many powerful computational tools available at modest cost (at least for student versions), and they run on almost any type of personal computer. A numerical computation package such as MATLAB®, Mathcad®, or MATHEMATICA®, and even some statistical packages,

such as S-PLUS©, will provide all of the mathematical computation power you are likely to need for applications in the Earth sciences. We have attempted to present, in as painless a manner as possible, the rudiments of beginning matrix algebra. As stated at the conclusion of Chapter 2, statistics is too large a subject to be covered in one chapter, or even one book. Matrix algebra also is an impossibly large subject to encompass in these few pages. However, you should now have some insight into matrix methods that will enable you to understand the computational basis of techniques we will cover in the remainder of this book.

EXERCISES

Exercise 3.1

File BHTEMP.TXT contains 15 bottomhole temperatures (BHT's) measured in the Mississippian interval in wells in eastern Kansas. The measurements are in degrees Fahrenheit. Convert the vector of temperatures to degrees Celsius using matrix algebra.

Exercise 3.2

The following two matrices are defined:

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

Compute the matrix products, $\mathbf{AB}$ and $\mathbf{BA}$. Two matrices which exhibit the property that will be apparent are said to be ***commutative***. Demonstrate that for commutative matrices, $\mathbf{A}^{-1}\mathbf{B}^{-1} = (\mathbf{AB})^{-1}$.

Consider the following two matrices,

$$\mathbf{C} = \begin{bmatrix} 2 & 1 & 0 \\ 3 & 4 & 0 \\ 0 & 0 & 2 \end{bmatrix} \qquad \mathbf{D} = \begin{bmatrix} 1 & -1 & 3 \\ 7 & 1 & 2 \\ 5 & 0 & 1 \end{bmatrix}$$

Compare the determinant, $|\mathbf{CD}|$, of the matrix product to the product, $|\mathbf{C}| \cdot |\mathbf{D}|$, of the determinants of the two matrices. The result you obtain is general. Determine if $|\mathbf{C}| + |\mathbf{D}| = |\mathbf{C} + \mathbf{D}|$. This result also is general. For the matrices $\mathbf{C}$ and $\mathbf{D}$, demonstrate that $(\mathbf{CD})^{\mathbf{T}} = \mathbf{D}^{\mathbf{T}}\mathbf{C}^{\mathbf{T}}$. Using matrix $\mathbf{C}$, show that $(\mathbf{C}^{-1})^{\mathbf{T}} = (\mathbf{C}^{\mathbf{T}})^{-1}$.

Exercise 3.3

File MAGNETIT.TXT contains the proportions of olivine, magnetite, and anorthite estimated by point-counting thin sections from 15 hand specimens collected at a magnetite deposit in the Laramie Range of Wyoming. The specific gravity is 3.34 for olivine, 2.76 for anorthite, and 5.20 for magnetite. Using matrix algebra, estimate the specific gravity of the 15 samples.

Exercise 3.4

Coordinates can be rotated by a matrix multiplication in which the premultiplier is a 2×2 matrix of sines and cosines of the angle of rotation,

$$\begin{bmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{bmatrix}$$

where θ is the desired angle of rotation. Data in file PROSPECT.TXT were taken from a surveyor's notebook describing the outline of a gold prospect in central Idaho. Coordinates are given in meters from an arbitrary origin at the southwest corner of the property and were measured relative to magnetic north. The magnetic declination in this area is 18°30′ east of true north. Convert the surveyor's measurements to coordinates relative to true north.

Exercise 3.5

Petrophysical well logs are strip charts made after the drilling of a well by lowering a sonde down the hole and recording physical properties versus depth in the well. Measurements include various electrical and sonic characteristics of the rocks, and both natural and induced radioactivity. The measured values reflect the composition of the rocks and the fluids in the pore space.

File KANSALT.TXT contains data for depths between 980 and 1030 ft below the surface in A.E.C. Test Hole No. 2, drilled in 1970 in Rice County, Kansas. At this depth, the well penetrated the Hutchinson Salt member of the Permian Wellington Formation, which was under investigation as a possible nuclear waste disposal site. The Wellington Formation is composed entirely of varying proportions of halite, anhydrite, and shale. Pure samples of these end members have distinct physical properties, so appropriate log responses can be used to estimate the relative amounts of halite, anhydrite, or shale at every foot within the Wellington Formation. A more detailed discussion of these data is given in Doveton (1986).

Table 3–4. Physical properties measured on pure samples of halite, anhydrite, and "shale" (clay minerals). From Gearhart-Owen (1975).

	Halite	Anhydrite	Shale
Apparent grain density (ρ_b), g/cc	2.03	2.98	2.43
Sonic transit time (Δ_t), μsec/ft	67	50	113

Two useful petrophysical properties are the apparent density (in grams per cubic centimeter) as measured by gamma-ray absorption and sonic transit time (in microseconds per foot). Laboratory-determined values for pure halite, anhydrite, and shale are given in **Table 3–4**. The apparent density and the sonic transmission time of a mixture of these three constituents can be calculated as the sum of the products of the densities and transit times for pure constituents times the proportions of the constituents. That is,

$$\rho_b = 2.03V_h + 2.98V_a + 2.43V_{sh}$$

$$\Delta_t = 67V_h + 50V_a + 113V_{sh}$$

where V_h, V_a, and V_{sh} are the proportions of halite, anhydrite, and shale. However, we want to reverse these equations, and for given values of ρ_b and Δ_t that we read from the well logs, estimate the proportions of the three constituents of the rock. Since three unknowns must be estimated, it seems we will require three equations and, hence, measurements of three log properties. However, because the proportions of halite, anhydrite, and shale must sum to one, we can use this constraint to provide the necessary third equation.

$$1 = V_h + V_a + V_{sh}$$

The three equations can be set into matrix form as

$$\mathbf{L} = \mathbf{CV}$$

$$\begin{bmatrix} \rho_b \\ \Delta_t \\ 1 \end{bmatrix} = \begin{bmatrix} 2.03 & 2.98 & 2.43 \\ 67 & 50 & 113 \\ 1 & 1 & 1 \end{bmatrix} \begin{bmatrix} V_h \\ V_a \\ V_{sh} \end{bmatrix}$$

However, what we really want to do is solve for **V**, given values of **L** taken from the well logs. This means that **C** must be moved to the other side of the equal sign, which we can do by multiplying both sides of the equation by its inverse, $\mathbf{C}^{-1}$. Then,

$$\begin{bmatrix} 2.03 & 2.98 & 2.43 \\ 67 & 50 & 113 \\ 1 & 1 & 1 \end{bmatrix}^{-1} \begin{bmatrix} \rho_b \\ \Delta_t \\ 1 \end{bmatrix} = \begin{bmatrix} V_h \\ V_a \\ V_{sh} \end{bmatrix}$$

Perform the necessary matrix inversion and multiplications to determine the proportions of halite, anhydrite, and shale in the 50-ft interval of the Hutchinson Salt. Plot the record of lithologic compositions in the form of a lithologic strip log. Ten of these estimates have been used in Chapter 2 (**Table 2.9**) to demonstrate the effects of closure on the calculation of correlations among closed variables.

[Hint: **L**, as given in file KANSALT.TXT, is a 2×50 matrix of ρ_b and Δ_t log responses. It must be converted to a 3×50 matrix by adding a column of 1's in order for the dimensions of the matrix multiplication to be correct. What does this column of 1's represent?]

Exercise 3.6

The state of stress in the subsurface can be represented in a 3×3 matrix, $\boldsymbol{\Sigma}$, whose diagonal elements represent normal stresses and whose off-diagonal elements represent shear stresses. The meanings of the nine elements of the stress matrix can be seen by imagining a cube in a Cartesian coordinate system in which the X-axis points to the east, the Y-axis points to the north, and the Z-axis points up. The symbol σ_{xx} represents the normal stress directed onto the east or west face of the cube; it will be a positive value if the stress is compressional and a negative value if the stress is tensional. There is a similar meaning for σ_{yy} and σ_{zz}. The symbol σ_{xy} represents the shear stress on the east or west face of the cube, acting parallel to the Y-axis. A shear stress is positive if the compressional or tensional component agrees in sign with the direction of force. That is, both components of shear

point in a positive coordinate direction, or both components point in a negative coordinate direction. Otherwise, the shear stress is negative. In order for the cube to be in rotational equilibrium, shear stresses on adjacent faces must balance; so, for example, $\sigma_{xy} = \sigma_{yx}$. This means that the stress matrix is symmetric about the diagonal:

$$\begin{bmatrix} \sigma_{xx} & \sigma_{xy} & \sigma_{xz} \\ \sigma_{xy} & \sigma_{yy} & \sigma_{yz} \\ \sigma_{xz} & \sigma_{yz} & \sigma_{zz} \end{bmatrix}$$

Turcotte and Schubert (1982) provide a more detailed discussion of stress in the subsurface and the measurement of stress components.

By finding the eigenvalues and eigenvectors of the 3×3 stress matrix, we can rotate the imaginary cube into a coordinate system in which all the shear stresses will be zero. The eigenvalues represent the magnitudes of the three orthogonal stresses. Their associated eigenvectors point in the directions of the stresses. The largest eigenvalue, λ_1, represents the maximum normal stress and the smallest, λ_3, represents the minimum normal stress. The maximum shear stress is given by $(\lambda_1 - \lambda_3)/2$ and occurs along a plane oriented perpendicular to a line that bisects the angle between the directions of maximum and minimum normal stress (that is, between the first and third eigenvectors). In a homogenous, isotropic material, failure (*i.e.*, faulting) will tend to occur along this plane. The orientation of this plane can be determined from the elements of the first eigenvector. In the conventional notation used by geologists, the strike of the first eigenvector is $\tan^{-1}(v_{12}/v_{11})$ and its dip is

$$\tan^{-1}\left(v_{13}\Big/\sqrt{v_{11}^2 + v_{12}^2}\right)$$

(Here, v_{ij} refers to the jth element of the ith eigenvector.) The strike and dip of the second and third eigenvectors can be found in the same manner.

Three-dimensional stress measurements have been made in a pillar in a deep mine, yielding the following stress matrix:

$$\begin{bmatrix} 61.2 & 4.1 & -8.2 \\ 4.1 & 51.5 & -3.0 \\ -8.2 & -3.0 & 32.3 \end{bmatrix}$$

The data are given in megapascals (MPa) and were recorded by strain gauges placed so the measurements have the same orientation as our imaginary cube (X increasing to the east, Y to the north, and Z increasing upward). Find the principal stresses and their associated directions. What is the maximum shear stress and what is the strike and dip of the plane on which this stress occurs?

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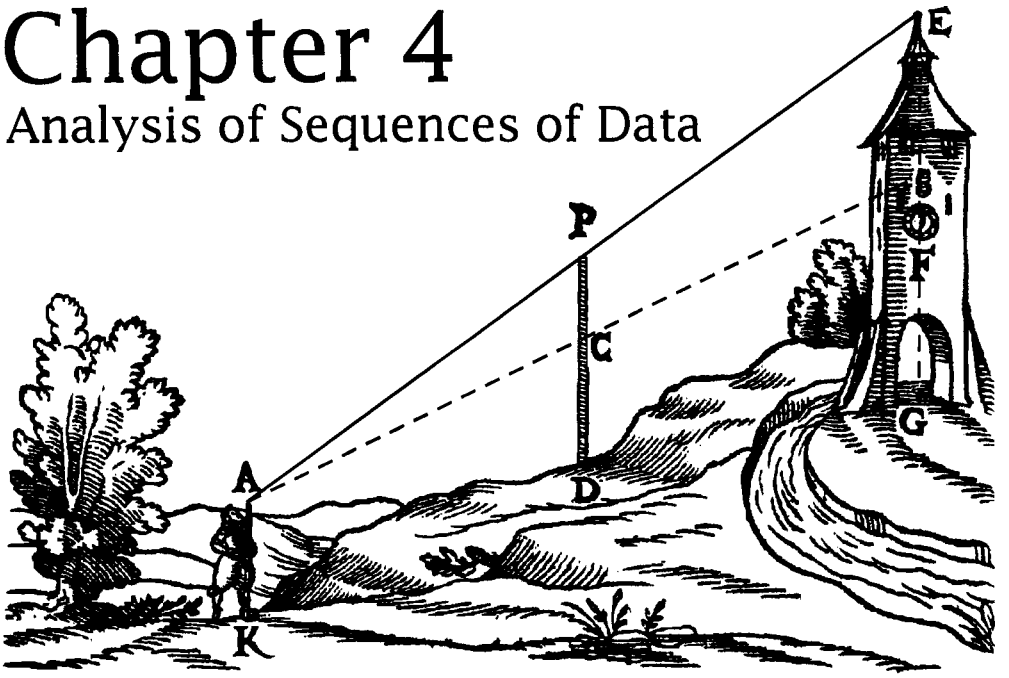
Chapter 4
Analysis of Sequences of Data



In this chapter we will consider ways of examining data that are characterized by their position along a single line. That is, they form a sequence, and the position at which a data point occurs within the sequence is important. Data sets of this type are common in geology, and include measured successions of lithologies, geochemical or mineralogical assays along traverses or drill holes, electric logs of oil wells, and chart recordings from instruments. Also in this general category are measurements separated by the flow of time, such as a sequence of water quality determinations at a river station, or the production history of a flowing gas well. Techniques for examining data having a single positional characteristic traditionally are considered part of the field of time-series analysis, although we will take the broader view that time and space relationships can be considered interchangeably.

Geologic Measurements in Sequences

Before proceeding to some geological examples and appropriate methods of examination, we must consider the nature of different types of sequences apt to be encountered by geologists. At one extreme, we may have a record which is quite precise, both in the variable which is measured and in the scale along which successive observations are located. Examples might include an electrical resistivity log from a borehole, or the production history of a commercial well. In the former, the variable is a measured attribute expressed in ohms (Ω) and the scale is measured in feet. In the latter example, the variable again is a measured attribute, barrels (bbl) of oil, and the scale is measured in days, months, or years. There are two important characteristics in either record. First, the variable being measured is expressed in units of an interval or ratio scale; 1000 bbl of oil is twice as large a quantity as 500 bbl, and a measurement of 10 Ω is ten times the resistance of 1 Ω. Second, the scales along which the data points are located also are expressed

in units having magnitude. A depth of 3000 ft in a well is ten times a depth of 300 ft, and the decade between the years 1940 and 1950 has the same duration as the interval between 1950 and 1960. These may seem obvious or even trivial points to emphasize, but as we shall see, not all geologic sequences have such well-behaved characteristics.

At the opposite extreme, we can consider a stratigraphic sequence consisting of the lithologic states encountered in a sedimentary succession. Such a sequence might be a cyclothem of limestone-shale-limestone-shale-sandstone-coal-shale-limestone, from bottom to top. We are interested in the significance of the succession, but we cannot put a meaningful scale on the sequence itself. Obviously, the succession of lithologies represents changes that occurred through time, but we have no way of estimating the time scale involved. We could use thickness, but this may change dramatically from location to location even though the sequence is not altered. If thickness is considered, it may obscure our examination of the succession, which is the subject of our interest. Thus, the fact that limestone is the third state in the section and coal is the sixth has no significance that can be expressed numerically (that is, position 6 is not "twice" position 3). Likewise, the lithologic states of the units cannot be expressed on a numerical scale. We might code the sequences just given as 1 – 2 – 1 – 2 – 3 – 4 – 2 – 1, where limestone is equated to 1, shale is 2, sandstone is 3, and coal is 4, but such a convention is purely arbitrary and expresses no meaningful relations between the states. It is obvious that this sequence poses different problems to the analyst than do the first examples.

There also are intermediate possibilities. For example, we may be interested in some measurable attribute contained in successive stages of a sequence. Perhaps we have measured the boron content of each lithologic unit in the cyclothem just discussed. We can utilize a distance scale of feet between samples and consider this a problem related to depth or distance. Alternatively, we can consider the relationship between the boron measurements and the sequence of states.

A closely related problem is the analysis of a sequence characterized by the presence or absence of some variable or variables at points along a line. We might be interested, for example, in the repeated recurrence of certain environment-dependent microfossils in the chips recovered during the drilling of a well. Another class of problems may be typified by the succession of mineral grains encountered on traverses across a thin section. In this case, we can use millimeters as a convenient spatial scale, but we have no way of evaluating whether olivine rates a higher number than plagioclase.

Data having the characteristic of being arranged along a continuum, either of time or space, often are referred to as forming a series, sequence, string, or chain. The nature of the data and the chain determine the questions that we can consider. Obviously, we cannot extract information about time intervals from stratigraphic succession data, because the time scale accompanying the succession is not known. We often substitute spatial scales for a time scale in stratigraphic problems, but our conclusions are no better than our fundamental assumptions about the length of time required to deposit the interval we have measured.

Table 4–1 is a classification of the various data-analysis techniques discussed in this chapter. We can consider two types of sequences. In the first, the distance between observations varies and must be specified for every point. In the second, the points are assumed to be equally and regularly spaced; the numerical value of the spacing does not enter into the analyses except as a constant. A subset of

Table 4–1. Techniques discussed in this chapter classified by the nature of the variable and its spacing along a line. Locations are explicit if X is specified for every Y; locations are implicit if X is implied by the order of observations.

Nature of Variables	Explicit Location in Time or Space	Implicit Location in Time or Space
Interval or Ratio Data	Interpolation Regression Splines	Zonation Seriation Autocorrelation Cross-correlation Semivariograms Periodograms Spectral Density
Nominal or Ordinal Data	Series of Events	Markov Chains Runs Tests

this category does not consider the spacing at all, and only the sequence of the observations is important.

The techniques also may be classified on the type of observations they require. Some necessitate interval or ratio observations; the variate must be measured on a scale and expressed in real numbers. Other methods accept nominal or ordinal data, and observations need only to be categorized in some fashion. In the methods discussed in this chapter, the classes are not ranked; that is, state A is not "greater" or "larger" in some sense than states B or C. Nominal data may be represented by integers, alphabetic characters, or symbols.

In the remainder of this chapter, we are going to examine the mathematical techniques required to analyze data in sequences. The methods described here do not exhaust the possibilities by any means. Rather, these are a collection of operations that have proved valuable in quantitative problem-solving in the Earth sciences, or that seem especially promising. Other methods may be more appropriate or powerful in specific situations or for certain data sets. However, a familiarity with the techniques discussed here will provide an introduction to a diverse field of analytical tools. Unfortunately, many of these methods were developed in scientific specialties alien to most geologists, and the description of an application in radar engineering, stock market analysis, speech therapy, or cell biology may be difficult to relate to a geologic problem. Some of the methods involve nonparametric statistics, and these are not widely considered in introductory statistics courses. Because of the general unfamiliarity of most Earth scientists with developments in the numerical analysis of data sequences, we have thought it best to present a potpourri of techniques and approaches. As you can see from **Table 4.1**, these cover a variety of sequences of different types, and are designed to answer different kinds of questions. None of the techniques can be considered exhaustively in this short space, but from the examples and applications presented, one or another may suggest themselves to the geologist with a problem to solve. The list of Selected Readings can then provide a discussion of a specific subject in more detail.

These methods provide answers to the following broad categories of questions: Are the observations random, or do they contain evidence of a trend or pattern? If a trend exists, what is its form? Can cycles or repetitions be detected and measured?

Can predictions or estimations be made from the data? Can variables be related or their effectiveness measured? Although such questions may not be explicitly posed in each of the following discussions, you should examine the nature of the methods and think about their applicability and the type of problems they may help solve. The sample problems are only suggestions from the many that could be used.

Geologists are concerned not only with the analysis of data in sequences, but also with the comparison of two or more sequences. An obvious example is stratigraphic correlation, either of measured sections or petrophysical well logs. A geologist's motive for numerical correlation may be a simple desire for speed, as in the production of geologic cross-sections from digitized logs stored in data banks. Alternatively, he may be faced with a correlation problem where the recognition of equivalency is beyond his ability. Subtle degrees of similarity, too slight for unaided detection, may provide the clues that will allow him to make a decision where none is otherwise possible. Numerical methods allow the geologist to consider many variables simultaneously, a powerful extension of his pattern-recognition facilities. Finally, because of the absolute invariance in operation of a computer program, mathematical correlation provides a challenge to the human interpreter. If a geologist's correlation disagrees with that established by computer, it is the geologist's responsibility to determine the reason for the discrepancy. The forced scrutiny may reveal complexities or biases not apparent during the initial examination. This is not to say that the geologist should unthinkingly bend his interpretation to conform with that of the computer. However, because modern programs for automatic correlation are increasingly able to mimic (and extend) the mental processes of a human interpreter, their output must be considered seriously.

Most techniques for comparing two or more sequences can be grouped into two broad categories. In the first of these, the data sequences are assumed to match at one position only, and we wish to determine the degree of similarity between the two sequences. An example is the comparison of an X-ray diffraction chart with a set of standards in an attempt to identify an unknown mineral. The chart and standards can be compared only in one position, where intensities at certain angles are compared to intensities of the standards at the same angles. Nothing is gained, for example, by comparing X-ray intensity at $20°2\theta$ with the intensity at $30°2\theta$ on another chart. Although the correspondence may be high, it is meaningless.

The fact that data such as these are in the form of sequences is irrelevant, because each data point is considered to be a separate and distinct variable. The intensity of diffracted radiation at $20°2\theta$ is one variable, and the intensity at $30°2\theta$ is another. We will consider methods for the comparisons of such sequences in greater detail in Chapter 6, when we discuss multivariate measures of similarity and problems of classification and discrimination. In this class of problems, an observation's location in a sequence merely serves to identify it as a specific variable, and its location has no other significance.

In contrast, some of the techniques we will discuss in this chapter regard data sequences as samples from a continuous string of possible observations. There is no *a priori* reason why one position of comparison should be better than any other. These methods of cross comparison superficially resemble the mental process of geologic correlation, but have the limitation that they assume the distance or time scales of the two sequences being compared are the same. In historic time series and sequences such as Holocene ice cores, this assumption is valid. In other

circumstances such as stratigraphic correlation, equivalent thicknesses may not represent equivalent temporal intervals and the problem of cross comparison is much more complex.

As we emphasized in Chapter 1, the computer is a powerful tool for the analysis of complex problems. However, it is mindless and will accept unreasonable data and return nonsense answers without a qualm. A bundle of programs for analyzing sequences of data can readily be obtained from many sources. If you utilize these as a "black box" without understanding their operation and limitations, you may be led badly astray. It is our hope in this chapter that the discussions and examples will indicate the areas of appropriate application for each method, and that the programs you use are sufficiently straightforward so that their operation is clear. However, in the final analysis, the researcher must be his own guide. When confronted with a problem involving data along a sequence, you may ask yourself the following questions to aid in planning your research:

(a) What question(s) do I want to answer?
(b) What is the nature of my observations?
(c) What is the nature of the sequence in which the observations occur?

You may quickly discover that the answer to the first question requires that the second and third be answered in specific ways. Therefore, you avoid unnecessary work if these points are carefully thought out before your investigation begins. Otherwise, the manner in which you gather your data may predetermine the techniques that can be used for interpretation, and may seriously limit the scope of your investigation.

Interpolation Procedures

Many of the following techniques require data that are equally spaced; the observations must be taken at regular intervals on a traverse or line, or equally spaced through time. Of course, this often is not possible when dealing with natural phenomena over which you have little control. Many stratigraphic measurements, for example, are recorded bed-by-bed rather than foot-by-foot. This also may be true of analytical data from drill holes, or from samples collected on traverses across regions which are incompletely exposed. We must, therefore, estimate the variable under consideration at regularly spaced points from its values at irregular intervals. Estimation of regularly spaced points will also be considered in Chapter 5, when we discuss contouring of map data. Most contouring programs operate by creating a regular grid of control points estimated from irregularly spaced observations. The appearance and fidelity of the finished map is governed to a large extent by the fineness of the grid system and the algorithm used to estimate values at the grid intersections. We are now considering a one-dimensional analogy of this same problem.

The data in **Table 4–2** consist of analyses of the magnesium concentration in stream samples collected along a river. Because of the problems of accessibility, the samples were collected at irregular intervals up the winding stream channel. Sample localities were carefully noted on aerial photographs, and later the distances between samples were measured.

Although there are many methods whereby regularly spaced data might be estimated from these data, we will consider only two in detail. The first and most obvious technique consists of simple ***linear interpolation*** between data points to

Table 4–2. Measurements of magnesium concentration in stream water at 20 locations; distances are from stream mouth to sample locations.

Distance (m)	Magnesium (ppm)	Distance (m)	Magnesium (ppm)
0.0	6.44	11,098	2.86
1820	8.61	11,922	1.22
2542	5.24	12,530	1.09
2889	5.73	14,065	2.36
3460	3.81	14,937	2.24
4586	4.05	16,244	2.05
6020	2.95	17,632	2.23
6841	2.57	19,002	0.42
7232	3.37	20,860	0.87
10,903	3.84	22,471	1.26

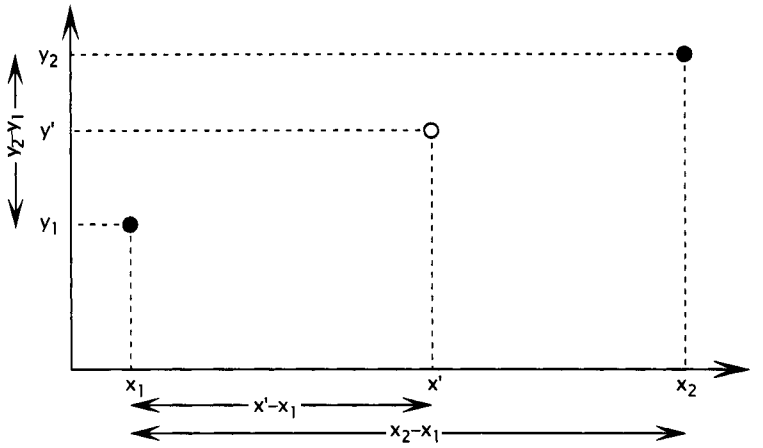


Figure 4–1. Linear interpolation between two data points along a sequence.

estimate intermediate points. This approach is illustrated in **Figure 4–1**. Assume y_1 and y_2 are observed values at points x_1 and x_2; we wish to estimate the value of y' at point x'. If we assume that a straight linear relation exists between sample points, intermediate values can be calculated from the geometric relationship

$$y' = \frac{(y_2 - y_1)(x' - x_1)}{x_2 - x_1} + y_1 \qquad (4.1)$$

Expressed in other words, the difference between values of two adjacent points is assumed to be a function of the distance separating them. The value of a point halfway between two observations is exactly intermediate between the values of the two enclosing points. The nearer a point is to an observation, the closer its value is to that of the observation. The manganese values from stream samples listed in **Table 4–2** are shown in graphical form in **Figure 4–2 a**, and interpolated to regular 1000-m intervals in **Figure 4–2 b**.

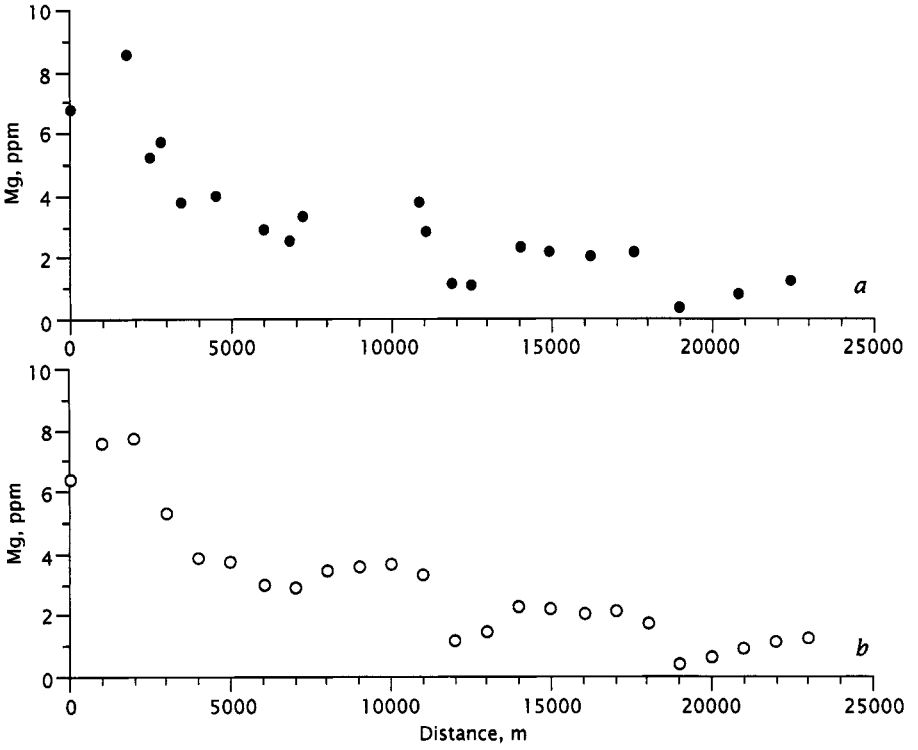


Figure 4–2. Magnesium concentration (parts per million) in water at 20 stream locations, measured in meters from stream mouth. (*a*) Original field measurements. (*b*) Values interpolated at 1000-m intervals.

Although linear interpolation is simple, it possesses certain drawbacks in many applications. If the number of equally spaced points is approximately the same as the number of original points, and the original points are somewhat uniformly spaced, the technique will give satisfactory results. However, if there are many more original points than interpolated points, most of the original data will be ignored because only two surrounding points determine an interpolated value. If the original data possess a large random component which causes values to fluctuate widely, interpolated points may also fluctuate unacceptably. Both of these objections may be met by techniques that consider more than two of the original values, perhaps by fitting a linear function that extends over several adjacent values. Wilkes (1966) devotes an entire chapter to various interpolation procedures.

If the original data are sparse and several values must be estimated between each pair of observations, linear interpolation will perform adequately, provided the idea of uniformity of slope between points is reasonable. In any problem where points are interpolated between observations, however, you must always remember that you cannot create data by estimation using any method. The validity of your result is controlled by the density of the original values and no amount of interpolation will allow refinement of the analysis beyond the limitations of the data. For example, we could estimate the magnesium content of the river at 500-m intervals, or even at every 5 m, but it is obvious that these new values would provide no additional information on the distribution of the metal in the stream.

We will next consider a method that produces equally spaced estimates of a variable and considers all observations between successive points of estimation.

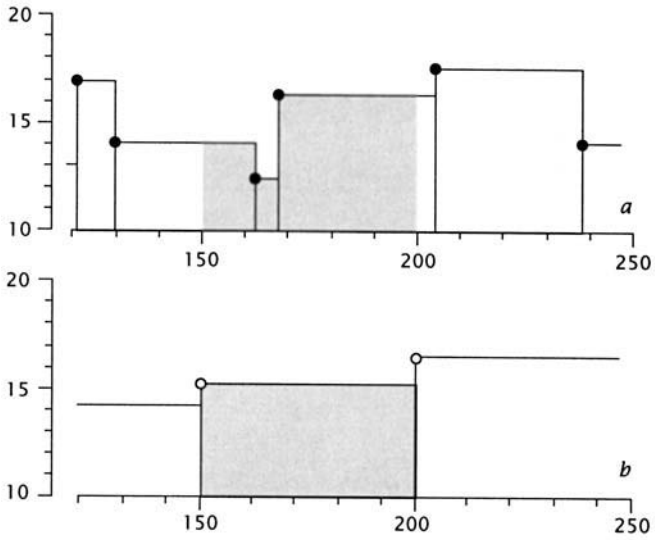


Figure 4–3. (*a*) Data sequence considered as a step function or "rectangular curve." (*b*) Equally spaced sequence created by rectangular integration. Shaded intervals in (*a*) and (*b*) have the same areas.

The technique is called ***rectangular integration.*** If we regard the original data as a rectangular curve or step function in which the interval from one observation to the succeeding observation has a constant value, a data set might have the form shown in **Figure 4–3 a**. If we wish to create an equally spaced approximation to this distribution, we can generate another step function of rectangles of equal length whose areas equal the total areas of the original rectangles. This is shown graphically in **Figure 4–3 b**, with the resulting sequence of equally spaced values derived from the data in part **a**. The shaded area under the curve is the same in both illustrations. This procedure has the advantage of considering all data within an interval in estimating a point. Also, because the area under the estimated curve is equal to the area under the original curve, observations used in the estimation of a point are weighted proportionally to the length of interval they represent.

Calculation of an estimate by rectangular integration is easy in theory but presents a somewhat difficult programming challenge. Starting at one estimated point, the distance to the next observation must be calculated, multiplied by the magnitude of the observation to give the rectangular area, and the process repeated through all successive observations up to the next estimated point. That point is determined by summing the areas just found and dividing by the equally spaced interval to give the estimated value. The initial estimated point in a sequence is taken as the same as the first preceding data point.

An obvious difference in the two interpolation procedures is apparent when original data are sparse and more than one point must be estimated between two observations. Using linear interpolation, values will be created which lie on a straight line between two surrounding data points. In contrast, rectangular integration will create estimates that are equal to the first observation.

In the study of a metamorphic halo around an intrusive, a diamond-drill core was taken perpendicular to the intrusive wall. The entire core was split and all garnet crystals exposed on the split surface were removed, individually crushed, and

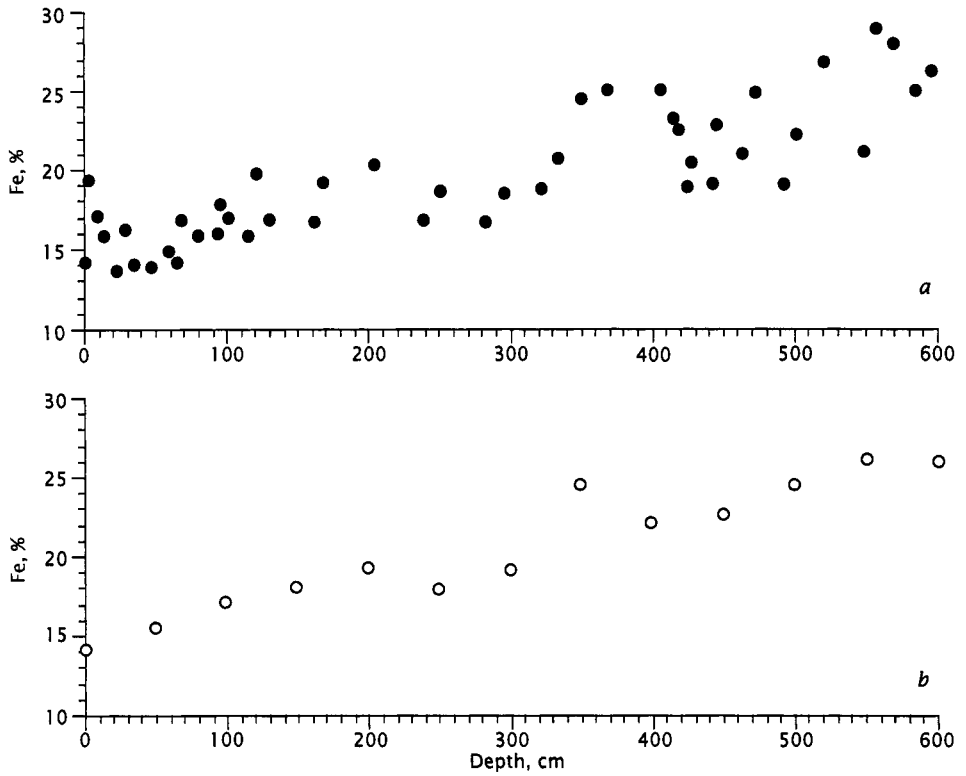


Figure 4–4. Iron content, in percent Fe_2O_3, of garnets taken from diamond-drill core through metamorphic halo. (*a*) Original measurements. (*b*) Values integrated to 50-cm intervals.

analyzed for iron content by a rapid spectrochemical method. Both the spacing between successive crystals and their iron content fluctuate through a wide range. Data from this core are shown in **Figure 4–4 a** and are given in file GARNETS.TXT. A generalized picture of compositional changes is desired, but the data seem too erratic for direct interpretation. As a preparatory step to further analysis, the data may be approximated by equally spaced estimates. The desired interval is 50 cm. Here we are presented with a situation that is different from the river data; observations are more abundant than estimates and we wish to preserve as much of the original information as possible. Rectangular integration seems more appropriate in this instance than linear interpolation. **Figure 4–4 b** shows the result of interpolating iron concentration to 50-cm intervals by rectangular integration. It may be instructive to compare these results with those from linear interpolation and to compare both with the overlying original data to see how much detail is lost by the two approximation processes.

In geology, equal spacing procedures have been most widely used to pretreat stratigraphic data (measured sections, drilling-time logs, and similar records) prior to filtering or time-trend analysis. Time-series methods, such as autocorrelation and spectral analysis, require equally spaced data. Time-series techniques are inherently more powerful than other analytical methods for examining sequential data, and their use has become widespread. However, they require long strings of data, which has restricted their application to geophysics, well-log analysis, and

the study of stratigraphic sequences and diamond-drill cores through ore deposits. Some work also has been done on mineral successions along traverses across thin sections. These applications will be considered in greater detail later in this chapter.

Markov Chains

In many geologic investigations, data sequences may be created that consist of ordered successions of mutually exclusive states. An example is a point-count traverse across a thin section, where the states are the minerals noted at succeeding points. Measured stratigraphic sections also have the form of series of lithologies, as may drill holes through zoned ore bodies where the rocks encountered are classified into different types of ore and gangue. Observations along a traverse may be taken at equally spaced intervals, as in point counting, or they may be taken wherever a change in state occurs, as is commonly done in the measurement of stratigraphic sections. In the first instance, we would expect runs of the same state; that is, several successive observations could conceivably fall in the same category. This obviously cannot happen if observations are taken only where states change.

Table 4–3. Stratigraphic succession shown in Figure 4–4 coded into four mutually exclusive states of sandstone (A), limestone (B), shale (C), and coal (D); observations taken at 1-ft intervals.

Top					
C	*C*	*B*	*C*	*A*	*A*
C	*C*	*B*	*C*	*A*	*A*
C	*C*	*B*	*C*	*A*	*A*
A	*A*	*B*	*C*	*C*	*A*
A	*A*	*B*	*A*	*C*	*A*
A	*C*	*C*	*A*	*D*	*A*
A	*C*	*C*	*A*	*C*	*C*
A	*D*	*C*	*A*	*C*	Bottom
A	*D*	*B*	*A*	*D*	
C	*C*	*B*	*C*	*D*	
C	*C*	*C*	*C*	*C*	

Sometimes we are interested in the nature of transitions from one state to another, rather than in the relative positions of states in the sequence. We can employ techniques that sacrifice all information about the position of observations within the succession, but that provide in return information on the tendency of one state to follow another. The data in **Table 4–3** represent the stratigraphic section shown in **Figure 4–5**, in which the sedimentary rock has been classified at successive points spaced 1 ft apart. The lithologies include four mutually exclusive states—sandstone, limestone, shale, and coal, arbitrarily designated A, B, C, and D, respectively. A 4×4 matrix can be constructed, showing the number of times a given rock type is succeeded, or overlain, by another. A matrix of this type is called a ***transition frequency matrix*** and is shown below. The measured stratigraphic section contains 63 observations, so there are $(n - 1) = 62$ transitions. The matrix is read "from rows to columns," meaning, for example, that a transition from state

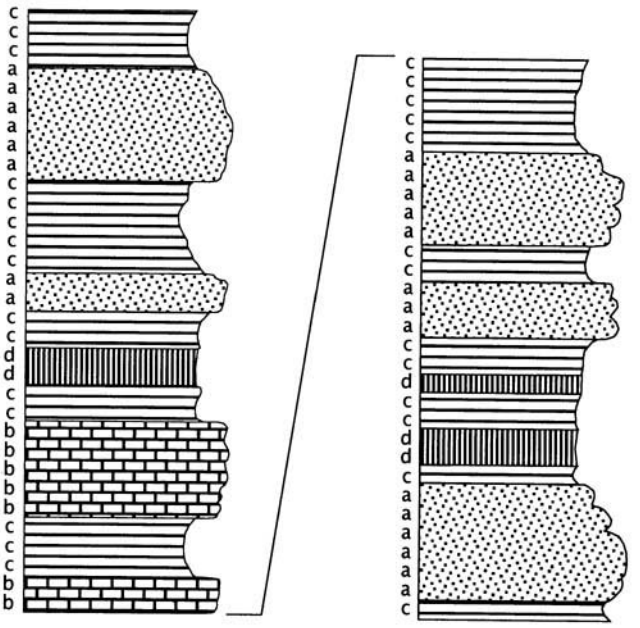


Figure 4–5. Measured stratigraphic column in which lithologies have been classified into four mutually exclusive states of sandstone (*a*), limestone (*b*), shale (*c*), and coal (*d*).

A to state *C* is counted as an entry in element $a_{1,3}$ of the matrix. That is, if we read from the row labeled *A* to the column labeled *C*, we see that we move from state *A* into state *C* five times in the sequence. Similarly, there are five transitions from state *C* to state *A* in the sequence; this number appears as the matrix element defined by row *C* and column *A*. The transition frequency matrix is a concise way of expressing the incidence of one state following another:

		to				Row Totals	
		A	*B*	*C*	*D*		
from	*A*	18	0	5	0	23	
	B	0	5	2	0	7	
	C	5	2	18	3	28	
	D	0	0	3	2	5	
Column Totals		23	7	28	5	63	Grand Total

Note that the row totals and the column totals will be the same, provided the section begins and ends with the same state; otherwise two rows and columns will differ by one. Also note that, unlike most matrices we have calculated before, the transition frequency matrix is asymmetric and in general $a_{i,j} \neq a_{j,i}$.

The tendency for one state to succeed another can be emphasized in the matrix by converting the frequencies to decimal fractions or percentages. If each element in the *i*th row is divided by the total of the *i*th row, the resulting fractions express the relative number of times state *i* is succeeded by the other states. In a probabilistic sense, these are estimates of the conditional probability, $p(j|i)$, the probability

that state j will be the next state to occur, *given* that the present state is i. [We here introduce the unconventional but equivalent notation, $p\,(i \rightarrow j)$, which can be read as the probability that state i will be followed by state j. This alternative notation will be useful later.]

		to				Row Totals
		A	*B*	*C*	*D*	
from	*A*	0.78	0	0.22	0	1.00
	B	0	0.71	0.29	0	1.00
	C	0.18	0.07	0.64	0.11	1.00
	D	0	0	0.60	0.40	1.00

Here, for example, we see that if we are in state C at one point, the probability is 64% that the lithology 1 ft up will also be state C. The probability is 18% that the lithology will be state A, 7% that it will be state B, and 11% that it will be state D. Since the four states are mutually exclusive and exhaustive, the lithology must be one of the four and so their sum, given as the row total, is 100%.

If we divide the row totals of the transition frequency matrix by the total number of transitions, we obtain the relative proportions of the four lithologies that are present in the section. This is called the ***marginal*** (or ***fixed***) ***probability vector***:

A	0.37
B	0.11
C	0.44
D	0.08

You will recall from Chapter 2 (Eq. 2.7) that the joint probability of two events, A and B, is

$$p(A,B) = p(B|A)p(A)$$

rearranging,

$$p(B|A) = \frac{p(B,A)}{p(A)}$$

So, the probability that state B will follow, or overlie, state A is the probability that both state A and B occur, divided by the probability that state A occurs. If the occurrence of states A and B are independent, or unconditional,

$$p(A,B) = p(A)\,p(B)$$

and

$$p(B|A) = \frac{p(A)\,p(B)}{p(A)} = p(B)$$

That is, the probability that state B will follow state A is simply the probability that state B occurs in the section, which is given by the appropriate element in the fixed probability vector. If the occurrences of all the states in the section are independent, the same relationship holds for all possible transitions; so, for example,

$$p(B|A) = p(B|B) = p(B|C) = p(B|D) = p(B)$$

This allows us to predict what the transition probability matrix should look like if the occurrence of a lithologic state at one point in the stratigraphic interval were

completely independent of the lithology at the immediately underlying point. The expected transition probability matrix would consist of rows that were all identical to the fixed probability vector. For our stratigraphic example, this would appear as

		to A	B	C	D	Row Totals
from	A	0.37	0.11	0.44	0.08	1.00
	B	0.37	0.11	0.44	0.08	1.00
	C	0.37	0.11	0.44	0.08	1.00
	D	0.37	0.11	0.44	0.08	1.00

We can compare this expected transition probability matrix to the transition probability matrix we actually observe to test the hypothesis that all lithologic states are independent of the immediately preceding states. This is done using a χ^2 test, first converting the probabilities to expected numbers of occurrences by multiplying each row by the corresponding total number of occurrences:

Expected Transition Probabilities				Totals	Expected Frequencies			
0.37	0.11	0.44	0.08	× 23 =	8.5	2.5	10.1	1.8
0.37	0.11	0.44	0.08	× 7 =	2.6	0.8	3.1	0.6
0.37	0.11	0.44	0.08	× 28 =	10.4	3.1	12.3	2.2
0.37	0.11	0.44	0.08	× 5 =	1.9	0.6	2.2	0.4

The χ^2 test is similar in form to the test equation (Eq. 2.65) described in Chapter 2. Each element in the transition frequency matrix constitutes a category, with both an observed and an expected number of transitions. These are compared by

$$\chi^2 = \sum \frac{(O - E)^2}{E} \tag{4.2}$$

where O is the observed number of transitions from one state to another, and E is the number of transitions expected if the successive states are independent. The test has $(m-1)^2$ degrees of freedom, where m is the number of states (a degree of freedom is lost from each row because the probabilities in the rows sum to 1.00). As with other types of χ^2 tests, each category must have an expected frequency of at least five transitions. This is not the case in this example, but we can still make a conservative test of independence by calculating the test statistic using the four categories whose expected frequency is greater than five. The remaining categories can be combined until their expected frequencies exceed five.

The categories include the transitions $A \rightarrow A$, $A \rightarrow C$, $C \rightarrow A$, and $C \rightarrow C$. Combined categories can be formed of all elements in the B row, all elements in the D row, and the combination of transitions $A \rightarrow B$, $A \rightarrow D$, $C \rightarrow B$ and $C \rightarrow D$. The resulting χ^2 statistic is

$$\chi^2 = \frac{(18-8.5)^2}{8.5} + \frac{(5-10.4)^2}{10.4} + \frac{(5-10.1)^2}{10.1} + \frac{(18-12.3)^2}{12.3}$$
$$+ \frac{(7-7.0)^2}{7.0} + \frac{(5-5.0)^2}{5.0} + \frac{(5-9.8)^2}{9.8}$$
$$= 20.99$$

The critical value of χ^2 for nine degrees of freedom and a 5% level of significance is 16.92; the test value comfortably exceeds this, so we may conclude that the hypothesis of independence of successive states is not correct. There is a statistically significant tendency for certain states to be preferentially followed by certain other states.

A sequence in which the state at one point is partially dependent, in a probabilistic sense, on the preceding state is called a ***Markov chain*** (named after the Russian statistician, A.A. Markov). A sequence having the Markov property is intermediate between deterministic sequences and completely random sequences. Our stratigraphic section exhibits *first-order* Markov properties; that is, the statistical dependency exists between points and their immediate predecessors. Higher order Markov properties can exist as well. For example, a second-order Markov sequence exhibits a significant conditional relationship between points that are two steps apart.

From the transition probability matrix we can estimate what the lithology will be 2 ft (that is, two observations) above a given point. Suppose we start in limestone (state *B*). The following probabilities estimate the lithology to be encountered at the next point upward:

State *A (sandstone)*	0%
State *B (limestone)*	71%
State *C (shale)*	29%
State *D (coal)*	0%

Suppose the next point actually falls in a shale; we can then determine the probable lithology of the following point:

State *A (sandstone)*	18%
State *B (limestone)*	7%
State *C (shale)*	64%
State *D (coal)*	11%

So, the probability that the lithologic sequence will be *limestone* → *shale* → *limestone* is

$$p(B \rightarrow C) \times p(C \rightarrow B) = 29\% \times 7\% = 2\%$$

However, there is another way to reach the limestone state in two steps. The sequence *limestone* → *limestone* → *limestone* is also possible. The probability attached to this sequence is

$$p(B \rightarrow B) \times p(B \rightarrow B) = 71\% \times 71\% = 50\%$$

Since the other transitions *limestone* → *sandstone* and *limestone* → *coal* have zero probability, these two sequences are the only possible ones which lead from limestone and back again in two steps. The probability that the lithology two steps above a limestone will also be a limestone, regardless of the intervening lithology, is the sum of all possibilities. That is,

$$\begin{aligned} p(B \rightarrow A \rightarrow B) &= 0\% \\ p(B \rightarrow B \rightarrow B) &= 50\% \\ p(B \rightarrow C \rightarrow B) &= 2\% \\ p(B \rightarrow D \rightarrow B) &= 0\% \\ \text{Total} &= 52\% \end{aligned}$$

The same reasoning can be applied to determine the probability of any lithology two steps hence, from any starting lithology. However, all of the various sequences do not have to be worked out individually, because the process of multiplying and summing is exactly that used for matrix multiplication. If the transition probability matrix is multiplied by itself (that is, the matrix is squared), the result is the second-order transition probability matrix describing the second-order Markov properties of the succession:

$$\begin{bmatrix} 0.78 & 0 & 0.22 & 0 \\ 0 & 0.71 & 0.29 & 0 \\ 0.18 & 0.07 & 0.64 & 0.11 \\ 0 & 0 & 0.60 & 0.40 \end{bmatrix}^2 = \begin{bmatrix} 0.64 & 0.02 & 0.31 & 0.02 \\ 0.05 & 0.52 & 0.39 & 0.03 \\ 0.26 & 0.09 & 0.54 & 0.11 \\ 0.11 & 0.04 & 0.62 & 0.23 \end{bmatrix}$$

Note that the rows of the squared matrix also sum to 100%.

The existence of a significant second-order property can be checked in exactly the same manner as we checked for independence between successive states, by using a χ^2 test. If you repeat the test performed earlier, but using the second-order transition probability matrix, you should find that the sequence has no significant second-order properties.

We can estimate the probable state to be encountered at any step in the future simply by powering the transition probability matrix the appropriate number of times. If the matrix is raised to a sufficiently high power, it reaches a stable state in which the rows all become equal to the fixed probability vector, or in other words, becomes an independent transition probability matrix and will not change with additional powering.

You will note in the example that the highest transition probabilities are from one state to itself, particularly from sandstone to sandstone, from limestone to limestone, and from shale to shale. It is obvious that these transition probabilities are related to the thicknesses of the stratigraphic units being sampled and the distance between the sample points. For example, the frequencies along the main diagonal of the transition frequency matrix would be doubled while off-diagonal frequencies remained unchanged if observations were made every half-foot. This would greatly enhance the Markovian property, but in a specious manner. Selecting the appropriate distance between sampling points can be a vexing problem; if observations are too closely spaced, the transition matrix reflects mainly the thickness of the more massive stratigraphic units. If the spacing is too great, thin units may be entirely missed.

Embedded Markov chains

The difficulty of selecting an appropriate sampling interval can be avoided if observations are taken only when there is a change in state. A stratigraphic section, for example, would be recorded as a succession of beds, each one of a different lithology than the immediately preceding bed. **Table 4–4** contains the record of successive rock types penetrated by a well drilled in the Midland Valley of Scotland (these data are contained in file MIDLAND.TXT). The well was drilled through 1600 ft of Coal Measures of Carboniferous age, consisting of interbedded shales, siltstones, sandstones, and coal beds or root zones. These sediments are interpreted as having been deposited in a delta plain environment subject to repeated flooding, so we would expect that certain lithologies would occur in preferred relations to

Table 4–4. Successive lithologic states encountered in a drill hole through the Coal Measures in the Midland Valley of Scotland (after Doveton, 1971); mutually exclusive states are barren shale (*A*), shale with fossils of nonmarine bivalves (*B*), siltstone (*C*), sandstone (*D*), and coal or root zone (*E*); read across rows. Data are in file MIDLAND.TXT.

Top →

B E A E A D A C D C D C A B E A D C D C D C A E
D C A D C A E C D C B E A D C D C D C A B A E D
C A E C A D E A D A C A B E A D C A E C D C A B
A E A D E A D C E A C D C D C D C A B E A B A B
A B E A B A C A C A B A B E A C D C D C D C A C
B E A C A C B E C A D C A C D C E A C D A C D C
B A B E A C D C A B A B E A D A C E A D A D C A
E A C D A E A E A C D C E C A B C E C A D B E A
D C D E A D A C A B E A B A B E A B A B E C A C
D A E A C D C D C A C A C E A C D C D C A B E A
D E A C D C D E C D C E A C A E A C A E A C A B
C D A E A C D C E A C B E A C A E A D A B E A C
D E A D C A B E A D C D E A D C D A E A C D C A
D A E A D A D C A C E D A B D B A E A C A E C D
C D C D A E A E C D A B E A B E A E A C D E A D
A D E C D C A E A E A C D A E C D B E A D C D C
A D A B A B E A D B A E A → Bottom

others. The data are taken from one of a large number of wells studied by Doveton (1971).

The four-state transition frequency matrix for the section in the Scottish well is given below. One obvious difference between this matrix and the one we have considered previously is that all the diagonal terms must be zero, since a state cannot succeed itself. The transition probability matrix, computed by dividing each element of the transition frequency matrix by the appropriate row total, shares this same characteristic. Sequences in which transitions from a state to itself are not permitted are called ***embedded Markov chains***, and their analysis presents special problems that have not always been appreciated by geologists studying stratigraphic records.

		to					Row Totals
		A	*B*	*C*	*D*	*E*	
from	*A*	0	13	36	19	52	120
	B	29	0	5	4	0	38
	C	35	2	0	45	12	94
	D	29	1	44	0	3	77
	E	26	23	9	9	0	67
Column Totals		119	39	94	77	67	397 Grand Total

The lithologic states have been coded as (*A*) unfossiliferous shale and mudstone, (*B*) shales containing nonmarine bivalves, (*C*) siltstone, (*D*) sandstone, and (*E*) coals and root zones. The corresponding transition probability matrix is

		to				
	A	B	C	D	E	Row Totals
A	0	0.11	0.30	0.16	0.43	1.00
B	0.76	0	0.13	0.11	0	1.00
from C	0.37	0.02	0	0.48	0.13	1.00
D	0.38	0.01	0.57	0	0.04	1.00
E	0.40	0.34	0.13	0.13	0	1.00

The marginal probability vector is

A	0.30
B	0.10
C	0.24
D	0.19
E	0.17

A χ^2 test, identical to Equation (4.2), can be used to check for the Markov property in an embedded sequence. This is done by comparing the observed transition frequency matrix to the matrix expected if successive states are independent. However, the fixed probability vector cannot be used to estimate the columns of the expected transition probability matrix. This would result in the expectation of transitions from a state to itself, which are forbidden. Rather, we must use a somewhat roundabout procedure to estimate the frequencies of transitions between independent states, subject to the constraint that states cannot succeed themselves. We begin by imagining that our sequence is actually a censored sample taken from an ordinary succession in which transitions from a state to itself can occur. The transition frequency matrix of this succession would look like the one we observe except that the diagonal elements would contain values other than zero. If we were to compute a transition probability matrix from this frequency matrix and then raise it to an appropriately high power, it would estimate the transition probability matrix of a sequence in which successive states were independent. If the diagonal elements were then discarded and the off-diagonal probabilities recalculated, the result would be the expected transition probability matrix for an embedded sequence whose states are independent.

How do we estimate the frequencies of transitions from each state to itself, when this information is not available? We do this by trial-and-error, searching for those values that, when inserted on the diagonal of the transition frequency matrix, do not change when the matrix is powered. The off-diagonal elements, however, will change until a stable configuration is reached, corresponding to the independent events model.

In practice it is not necessary to calculate the off-diagonal probabilities at all. We begin by assigning some arbitrarily large number, say 1000, to the diagonal positions of the observed transition frequency matrix. The fixed probability vector is found, by summing each row and dividing by the grand total, and then is used as an estimate of the transition probabilities along the diagonal. These probabilities are powered by squaring and multiplied by the grand total to obtain new estimates of the diagonal frequencies. These new estimates are inserted into the original transition frequency matrix and the process repeated. We can work through the first cycle of the procedure.

Step 1. Initial estimate of transition frequency matrix, with 1000 inserted in each diagonal position.

		to A	B	C	D	E	Row Totals
	A	1000	13	36	19	52	1120
	B	29	1000	5	4	0	1038
from	*C*	35	2	1000	45	12	1094
	D	29	1	44	1000	3	1077
	E	26	23	9	9	1000	1067
							5397 Grand Total

Step 2. Estimate of transition probabilities of diagonal elements, found by dividing row totals by grand total.

		to A	B	C	D	E	Row Totals
	A	0.208					0.208
	B		0.192				0.192
from	*C*			0.203			0.203
	D				0.200		0.200
	E					0.198	0.198

Step 3. Square the probabilities along the diagonal.

Step 4. Second estimate of transition frequency matrix using new diagonal elements calculated by multiplying probabilities on the diagonal by the grand total of 5397. Off-diagonal terms are the original observed frequencies. New row totals and grand total are then found

		to A	B	C	D	E	Row Totals
	A	232	13	36	19	52	352
	B	29	199	5	4	0	237
from	*C*	35	2	222	45	12	316
	D	29	1	44	215	3	292
	E	26	23	9	9	211	278
							1475 Grand Total

The process is repeated again and again, until the estimated transition frequencies along the diagonal do not change from time to time. This generally requires about 10 to 20 iterations, depending upon how closely the initial guesses were to the final, stable estimates. In this example, the estimates do not change after 10 iterations.

The final form of the transition frequency matrix with estimated diagonal frequencies is given below.

		to					
		A	*B*	*C*	*D*	*E*	Row Totals
	A	66	13	36	19	52	186
	B	29	3	5	4	0	41
from	*C*	35	2	29	45	12	123
	D	29	1	44	17	3	94
	E	26	23	9	9	12	79
Column Totals		185	42	123	94	79	523 Grand Total

This matrix could be converted into an expected transition probability matrix of the hypothetical Markov sequence by dividing each element by the corresponding row total. However, such a matrix is of little interest because it pertains to the hypothetical sequence rather than the observed embedded sequence. The marginal totals are another matter, because they are required to compute the marginal probability vector:

A	0.355
B	0.074
C	0.235
D	0.181
E	0.155

We may now calculate the expected probabilities and expected frequencies of a hypothetical sequence of independent states from the marginal probability vector. We are testing the hypothesis of independence between successive states by noting that, for example, if state A is independent of state B, then $p(A|B) = p(A)p(B)$. As $P(A)$ and $P(B)$ are given by the appropriate elements of the marginal probability vector, the estimated conditional probability that state A will follow state B is $p(A|B) = (0.355)(0.074) = 0.026$. The expected probabilities for all transitions are given below.

		to				
		A	*B*	*C*	*D*	*E*
	A	0.125	0.026	0.083	0.064	0.055
	B	0.026	0.006	0.017	0.013	0.012
from	*C*	0.083	0.017	0.055	0.043	0.036
	D	0.064	0.013	0.043	0.033	0.028
	E	0.055	0.012	0.036	0.028	0.024

The expected frequencies are found by multiplying this matrix by the grand total, 523.

		to				
		A	*B*	*C*	*D*	*E*
	A	65.5	13.6	43.5	33.5	28.8
	B	13.6	3.1	8.9	6.8	6.3
from	*C*	43.5	8.9	28.8	22.5	18.9
	D	33.5	6.8	22.5	17.3	14.7
	E	28.8	6.3	18.9	14.7	12.6

Note that the matrix is symmetrical and the diagonal elements remain unchanged, within the limits of rounding error. The off-diagonal elements are the expected frequencies of transitions within the embedded sequence, assuming independence between successive states. If the diagonal elements are stripped from the matrix, it may be compared directly to the observed transition frequency matrix because the row and column totals of the two are the same, again within rounding limits.

The comparison by χ^2 methods yields a test statistic of $\chi^2 = 172$. The test has $\nu = (m-1)^2 - m$ degrees of freedom, where m is the number of states, or in this example, $\nu = 11$. The critical value of χ^2 for 11 degrees of freedom and an $\alpha = 0.05$ level of significance is 19.68, which is far exceeded by the test statistic. Therefore, we must conclude that successive lithologies encountered in the Scottish well are not independent, but rather exhibit a strong first-order Markovian property.

If tests determine that a sequence exhibits partial dependence between successive states, the structure of this dependence may be investigated further. Simple graphs of the most significant transitions may reveal repetitive patterns in the succession. Modified χ^2 procedures are available to test the significance of individual transition pairs. Some authors have found that the eigenvalues extracted from the transition probability matrix are useful indicators of cyclicity. (It should be noted, however, that extracting the eigenvectors from an asymmetric matrix such as the transition probability matrix may not be an easy task!) These topics will not be pursued further in this book; the interested reader should refer to the texts by Kemeny (1983) and Norris (1997), as well as the book on quantitative sedimentology by Schwarzacher (1975). Chi-square tests appropriate for embedded sequences are discussed by Goodman (1968). In a geological context, the articles by Doveton (1971) and Doveton and Skipper (1974), plus the comment by Türk (1979), are recommended.

Series of Events

An interesting type of time series we will now consider is called a ***series of events.*** Geological examples of this type of data sequence include the historical record of earthquake occurrences in California, the record of volcanic eruptions in the Mediterranean area, and the incidence of landslides in the Tetons. The characteristics of these series are (a) the events are distinguishable by when they occur in time; (b) the events are essentially instantaneous; and (c) the events are so infrequent that no two occur in the same time interval. A series of events is therefore nothing more than a sequence of the intervals between occurrences. Our data may consist of the duration between successive events, or the cumulative length of time over which the events occur. One form may be directly transformed into the other.

Series-of-events models may be appropriate for certain types of spatially distributed data. We might, for example, be interested in the occurrence of a rare mineral encountered sporadically on a traverse across a thin section or in the appearance of bentonite beds in a vertical succession of sedimentary rocks. Justification for applying series-of-events models to spatial data may be tenuous, however, and depends on the assumption that the spatial sequence has been created at a constant rate. This assumption probably is reasonable in the first example, but the second requires that we assume that the sedimentation rate remained constant through the series.

The historic record of eruptions of the volcano Aso in Kyushu, Japan, has been kept since 1229 (Kuno, 1962), and is given in **Table 4–5** and file ASO.TXT. Aso is

Table 4–5. Years of eruptions of the volcano Aso for the period 1229-1962.

1229	1376	1583	1780	1927
1239	1377	1584	1804	1928
1240	1387	1587	1806	1929
1265	1388	1598	1814	1931
1269	1434	1611	1815	1932
1270	1438	1612	1826	1933
1272	1473	1613	1827	1934
1273	1485	1620	1828	1935
1274	1505	1631	1829	1938
1281	1506	1637	1830	1949
1286	1522	1649	1854	1950
1305	1533	1668	1872	1951
1324	1542	1675	1874	1953
1331	1558	1683	1884	1954
1335	1562	1691	1894	1955
1340	1563	1708	1897	1956
1346	1564	1709	1906	1957
1369	1576	1765	1916	1958
1375	1582	1772	1920	1962

a complex stratovolcano, but all historic eruptions have been explosive, ejecting ash of andesitic composition. Although the ancient monastic records contain an indication of the relative violence and duration of some eruptions, for all practical purposes we must regard the record as one of indistinguishable instantaneous explosive events. Analysis of volcanic histories may shed some light on the nature of eruptive mechanisms and can even lead to physical models of the structure of volcanoes (Wickman, 1966). Of course, we would also hope that such studies might lead to predictive tools to forecast future eruptions.

Studies of series of events may have several objectives. Usually, an investigator is interested in the ***mean rate of occurrence***, or number of events per interval of time. In addition, it may be necessary to examine the series in more detail, in order to estimate any pattern that may exist in the events. This additional information can be used to determine the precision of the estimate of the rate of occurrence, to assess the appropriateness of the sampling scheme, to detect a trend, and to detect other systematic features of the series.

Because series of events are very simple, in the sense that they consist of nominal occurrences (presence-absence), simple analytical techniques may prove to be the most effective. Cox and Lewis (1966) described a variety of graphical tools that are useful in examining series of events. These are illustrated using the data on the eruptions of Aso from **Table 4–5**.

A cumulative plot of the total number of events (n_t) to have occurred at or before time t, against time t, is given in **Figure 4–6**. This plot is especially good for showing changes in the average rate of occurrence. The slope of a straight line connecting any two points on the cumulative plot is the average number of events per unit of time for the interval between the two points.

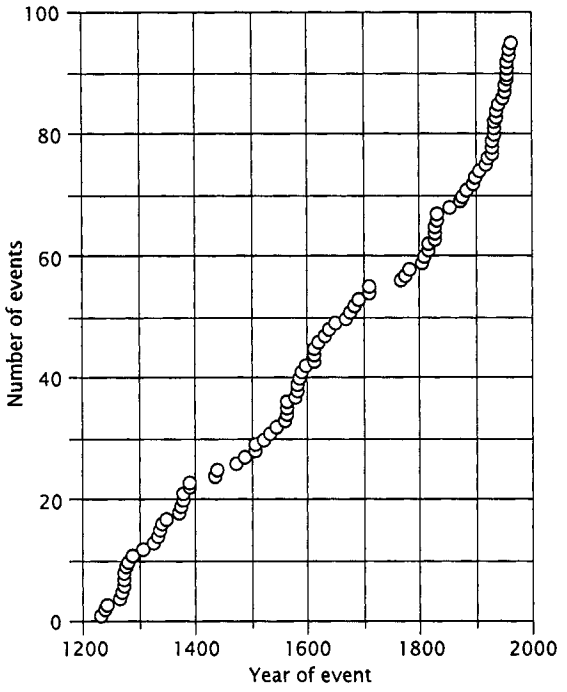


Figure 4–6. Cumulative number of eruptions of the Japanese volcano Aso plotted against years of eruptions.

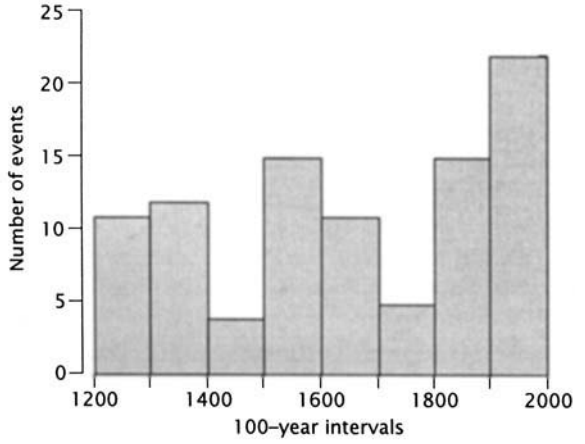


Figure 4–7. Histogram of number of eruptions of the Japanese volcano Aso occurring in successive 100-yr intervals.

A histogram of the number of events occurring in successive equal intervals of time is given in **Figure 4–7**. This histogram directly indicates local periods of fluctuation from the average rate of occurrence. The pattern shown by the histogram is sensitive to the length of the chosen intervals, so more than one histogram may be useful in examining a series.

The ***empirical survivor function*** is obtained by plotting the percent "survivors," or Y = proportion of time intervals longer than X, against X = length of time

interval. The function estimates the probability that an event has not occurred before time X. In **Figure 4–8,** the points represent the percentage of intervals between eruptions which are longer than the specified number of years. If events occur randomly in time, the survivor function will be exponential in form.

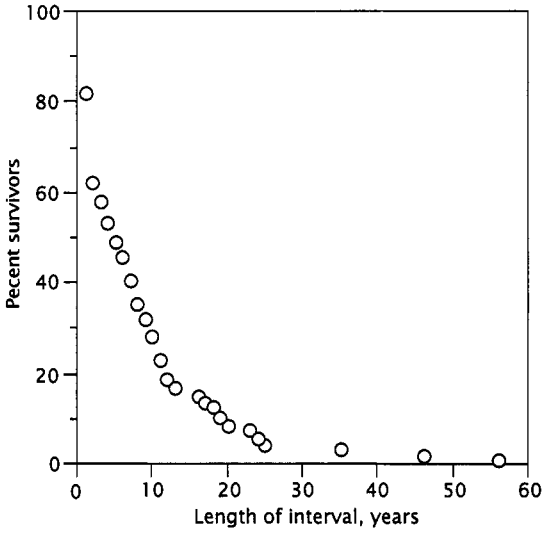


Figure 4–8. Empirical survivor function for the Japanese volcano Aso. The vertical axis gives the percent of intervals between eruptions that are longer than a specified duration, versus the duration in years along the horizontal axis.

This same function can be plotted in logarithmic form, as log Y against X. The ***log empirical survivor function*** is especially good for showing departures from randomness, which appear as deviations from the straight-line form of the plot (**Fig. 4–9**).

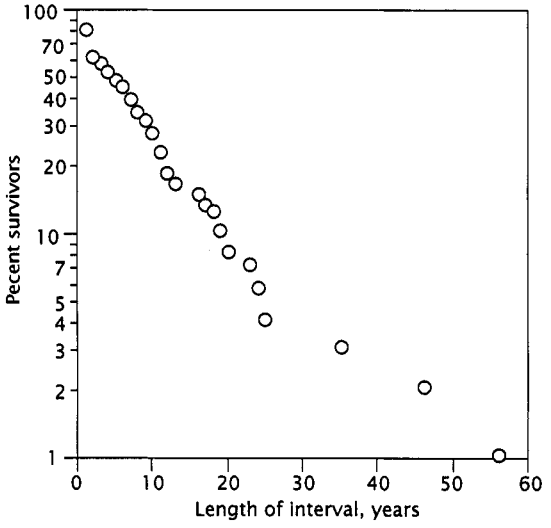


Figure 4–9. Log empirical survivor function of the Japanese volcano Aso. The vertical axis of Figure 4–8 is expressed in logarithmic form.

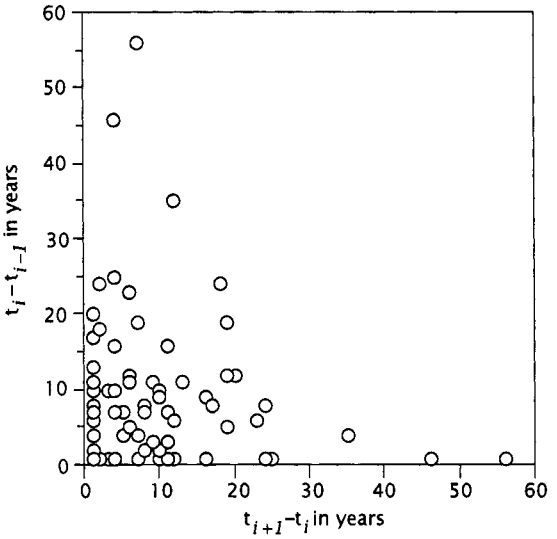


Figure 4–10. Serial correlation of durations between successive eruptions of the Japanese volcano Aso. Vertical axis is duration of quiet before the ith eruption, and horizontal axis is duration after the ith eruption.

A scatter diagram of the ***serial correlation***, or first-order autocorrelation, of successive intervals between events is shown in **Figure 4–10**. The degree of correspondence between the length of an interval and the length of the immediately preceding interval is shown by plotting $x_i = t_{i+1} - t_i$ against $y_i = t_i - t_{i-1}$ where t_i is the time of occurrence of the ith event. This plot reveals any tendency for intervals to be followed by intervals of similar length. A scatter diagram with large dispersion and relatively high concentrations of points near the axes is typical of random series of events.

In most series-of-events studies, we hope that we can describe the basic features of the series in a way that will suggest a physical mechanism for the lengths of the intervals between occurrences. First we must consider the possibility of a trend in the data. We may check for a trend in two ways. A series may be subdivided into segments of equal length, provided each segment contains several observations. The numbers of events within each segment are taken to be observations located at the midpoints of the segments. A regression can then be run with these numbers as the dependent variable, y_i, and the locations of the midpoints of the segments as values of x_i. The slope coefficient of the regression can be tested by the ANOVA given later in **Table 4–9** (p. 197) to determine if it is significantly different from zero. The process is illustrated in **Figure 4–11**. Unfortunately, this test is not particularly efficient because degrees of freedom are lost when the series is divided into segments.

There are tests specifically designed to detect a trend in the rate of occurrence of events by comparing the midpoint of the sequence to its centroid. If the sequence is relatively uniform, the two will be very similar, but if there is a trend the centroid will be displaced in the direction of increasing rate of occurrence. If t_i is the time or distance from the start of the series to the ith event and N is the total number of events, we can calculate the centroid, S, by

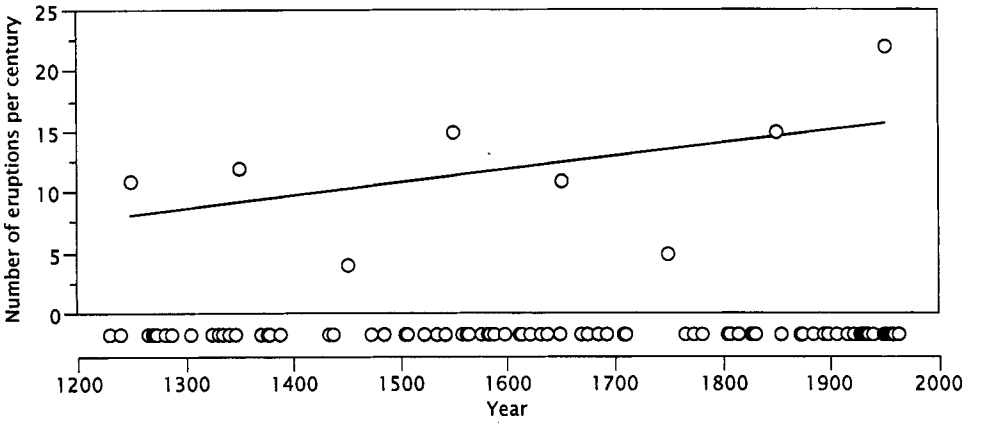


Figure 4–11. Eruptions of the Japanese volcano Aso considered as "instantaneous" happenings along a continuum of time. Cross plot shows number of eruptions per century versus midpoints of successive centuries. Fitted regression line estimates change in rate of occurrence.

$$S = \frac{\sum_{i=1}^{N} t_i}{N} \tag{4.3}$$

This statistic can in turn be used in Equation (4.4),

$$z = \frac{S - 1/2T}{T/\sqrt{12N}} \tag{4.4}$$

where T is the total length of the series, z is the standardized normal variate, and the significance of the test result can be determined by normal tables such as Appendix Table **A.1**.

The test is very sensitive to changes in the rate of occurrence of events. Specifically, if the events are considered to be the result of a process

$$Y_t = e^{\alpha+\beta t} \tag{4.5}$$

the null hypothesis states that $\beta = 0$. You will recognize that the model is exponential; if β has any value other than zero, the rate of occurrence of Y_t will change with t. It is this possibility that we are testing.

If no trends are detected in the rate of occurrence, we may conclude that the series of events is stationary. We can next check to see if successive occurrences are independent. This can be done by computing the autocorrelation of the lengths between events. That is, we regard the intervals between events as a variable, X, located at equally spaced points. If the intervals are not independent, this will be expressed as a positive autocorrelation with a tendency for large values of x_i (long intervals between events) to be succeeded by large values; similarly, there will be a tendency for small values of x_i (short intervals) to be followed by other small values. We can compute autocorrelation coefficients for successive lags and test these for significance. Usually only the first few lags will be of interest. If the autocorrelation coefficients are not significantly different from zero, as tested by methods that will

be developed later in this chapter, we can conclude that the events are occurring independently in time or space.

If we have established that the series is neither autocorrelated nor contains a trend, we may wish to test the possibility that the events are distributed according to a ***Poisson distribution.*** You will recall from Chapter 2 that the Poisson is a discrete probability distribution that can be regarded as the limiting case of the binomial when n, the number of trials, becomes very large, and p, the probability of success on any one trial, becomes very small. We can imagine that our time series is subdivided into n intervals of equal duration. If events occur randomly, the number of intervals that contain exactly 0, 1, 2,..., x events will follow the binomial distribution. As we make the lengths of the intervals progressively shorter, n becomes progressively larger and the probabilities of occurrence decline. The binomial distribution becomes difficult to compute, but the Poisson can be readily used because it does not require either n or p directly. Instead, the product $np = \lambda$ is all that is needed, which is given by the ***rate of occurrence*** of events.

The Poisson probability model assumes that (a) the events occur independently, (b) the probability that an event occurs does not change with time, (c) the probability that an event will occur in an interval is proportional to the length of the interval, and (d) the probability of more than one event occurring at the same time is vanishingly small.

The equation for the Poisson distribution in this instance is

$$p(X) = e^{-\lambda}\lambda^X / X! \tag{4.6}$$

Note that the rate of occurrence, λ, is the only parameter of the distribution. Typical Poisson frequency distributions are shown in **Figure 4–12.** The distribution is applicable to such problems as the rate that telephone calls come to a switchboard or the length of time between failures in a computer system. It seems reasonable that it also may apply to the series of geological events described at the beginning of this section. If we can determine that our series follows a Poisson distribution, we can use the characteristics of the distribution to make probabilistic forecasts of the series.

The Kolmogorov-Smirnov test provides a simple way to test the goodness of fit of a series of events to that expected from a Poisson distribution. First, the series must be converted to a cumulative form

$$y_i = \frac{t_i}{T}$$

where t_i is the time from the start of the series to the ith event, and T is the total length of the series. Three estimates can then be calculated

$$\begin{aligned} D^+ &= \sqrt{n}\max\left\{\frac{i}{n} - y_i\right\} \\ D^- &= \sqrt{n}\max\left\{y_i - \frac{i-1}{n}\right\} \\ D &= \max|D^+, D^-| \end{aligned} \tag{4.7}$$

The first test is simply the maximum positive difference between the observed series and that expected from a Poisson, the second is the maximum negative difference, and the third is the larger of the absolute values of the two. The test statistic,

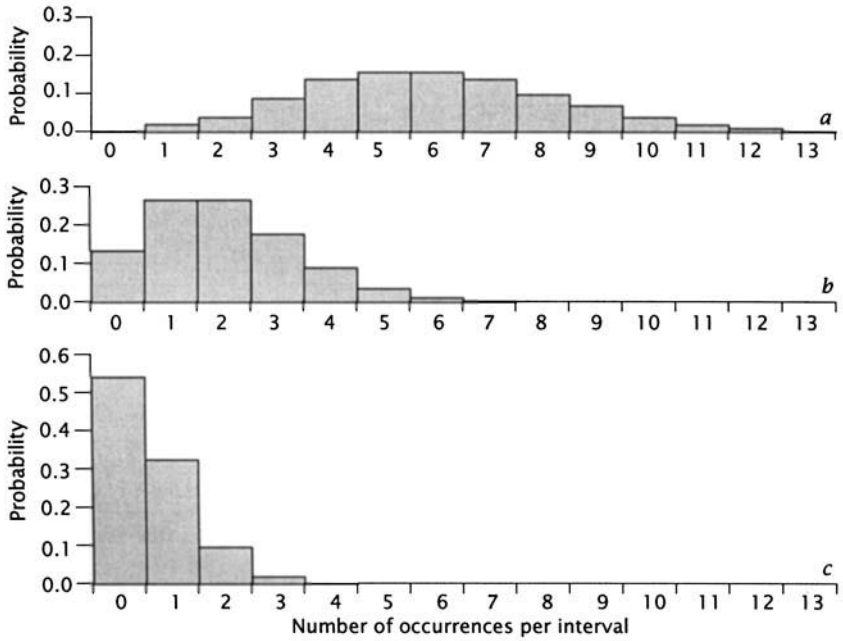


Figure 4–12. Poisson probability distributions with different rates of occurrence, λ, expressed as numbers of occurrences per interval. (*a*) $\lambda = 6.0$. (*b*) $\lambda = 2.0$. (*c*) $\lambda = 0.6$.

D, can be compared to two-tailed critical values given in Appendix Table **A.7**. If the statistic exceeds the critical value, the maximum deviation is larger than that expected in a sample collected at random from a Poisson distribution.

Runs Tests

The simplest type of sequence is a succession of observations arranged in order of occurrence, where the observations are two mutually exclusive categories or states. Consider a rock collector cracking open concretions in a search for fossils. The breaking of a concretion constitutes a trial, and each trial has two mutually exclusive outcomes: The concretion either contains a fossil or it does not. The sequence of successes and failures by the collector during the course of a day forms a special type of time series. We can experimentally create a similar succession by flipping pennies and noting the occurrence of heads or tails. The sequence generated might resemble this set of twenty trials:

H T H H T H T T T H T H T H H T T H H H

We intuitively expect, of course, that about ten heads will appear, and we can determine the probability of obtaining this (or any other) number of heads. Here we obtained 11 heads; assuming the coin is unbiased, the probability of obtaining this number in 20 trials is 0.16 or about one in six. We would expect similar trials to contain 9, 10, or 11 heads slightly more than one-third of the time. Results of this experiment follow the binomial distribution, discussed in Chapter 2.

One aspect that we have not considered, however, is the order in which the heads appear. We probably would regard a sequence such as

H H H H H H H H H H H T T T T T T T T T T

as being very strange, although the probability of obtaining this many heads in 20 trials is the same as in the preceding example. At the other extreme, the regular alternation of heads and tails

H T H T H T H T H T H T H T H T H T H T

would also appear very unusual to us, although the probability of the number of heads is unchanged. What arouses our suspicions is not the proportion of heads but the order in which they appear. We assume that heads and tails will occur at random; in the two preceding examples, it seems very unlikely that they have.

We can test these sequences for randomness of occurrence by examining the number of runs. ***Runs*** are defined as uninterrupted sequences of the same state. The first set of trials contains 13 runs, the second only 2, and the third contains 19. Runs in the first sequence shown are underlined:

(Start)

H	T	HH	T	H	TTT	H	T	H	T	HH	TT	HHH	
1	1	3	4	5	6	7	8	9	10	11	12	13	(End)

We can calculate the probability that a given sequence of runs was created by the random occurrence of two states (heads and tails, in this example). This is done by enumerating all possible ways of arranging n_1 items of state 1 and n_2 items of state 2. The total number of runs in a sequence is denoted U; tables are available which give critical values of U for specified n_1, n_2, and level of significance, α. However, if n_1 and n_2 each exceed ten, the distribution of U can be closely approximated by a normal distribution, and we can use tables of the standard normal variate z for our statistical tests. The expected mean number of runs in a randomly generated sequence of n_1 items of state 1 and n_2 items of state 2 is

$$\overline{U} = \frac{2n_1n_2}{n_1 + n_2} + 1 \tag{4.8}$$

The expected variance in the mean number of runs is

$$\sigma^2_{\overline{U}} = \frac{2n_1n_2(2n_1n_2 - n_1 - n_2)}{(n_1 + n_2)^2(n_1 + n_2 - 1)} \tag{4.9}$$

By these equations, we can determine the mean number of runs and the standard error of the mean number of runs in all possible arrangements of n_1 and n_2 items. Having calculated these, we can create a z-test by Equation (4.10), where U is the observed number of runs:

$$z = \frac{U - \overline{U}}{\sigma_{\overline{U}}} \tag{4.10}$$

You will recognize that this is simply Equation (2.37) rewritten to include the runs statistics. We can formulate a variety of statistical hypotheses which can be tested with this statistic. For example, we may wish to see if a sequence contains more

than the expected number of runs from a random arrangement; the null hypothesis and alternative are

$$H_0 : U \leq \overline{U}$$
$$H_1 : U > \overline{U}$$

and too many runs leads to rejection. The test is one-tailed. Conversely, we may wish to determine if the sequence contains an improbably low number of runs. The appropriate alternatives are

$$H_0 : U \geq \overline{U}$$
$$H_1 : U < \overline{U}$$

and too few runs will cause rejection of the null hypothesis. Again, the test is one-tailed. We may wish to reject either form of nonrandomness. A two-tailed test is appropriate, with hypotheses

$$H_0 : U = \overline{U}$$
$$H_1 : U \neq \overline{U}$$

We can work through the test procedure for the first series of coin flips and determine the likelihood of achieving this sequence by a random process. The null hypothesis states that there is no difference between the observed number of runs and the mean number of runs from random sequences of the same size. We will use a two-tailed test, and reject if there are too many or too few runs in the sequence. Therefore, the proper alternative is

$$H_1 : U \neq \overline{U}$$

Using a 5% ($\alpha = 0.05$) level of significance, our critical regions are bounded by -1.96 and $+1.96$. We first calculate the expected mean and standard deviation of runs for random sequences having n_1 heads ($n_1 = 11$) and n_2 tails ($n_2 = 9$):

$$\overline{U} = \frac{2 \cdot 11 \cdot 9}{11 + 9} + 1 = 10.9$$

$$\sigma_{\overline{U}}^2 = \frac{(2 \cdot 11 \cdot 9)(2 \cdot 11 \cdot 9 - 11 - 9)}{(9 + 11)^2(9 + 11 - 1)} = 4.6$$

The test statistic is

$$z = \frac{U - \overline{U}}{\sigma_U} \approx \frac{13 - 10.9}{2.1} = 1.0$$

The number of runs in the sequence is one standard deviation from the mean of all runs possible in such a sequence, and does not fall within the critical region. Therefore, the number of runs does not suggest that the sequence is nonrandom. The other sequences, in contrast, yield very different test results. Because n_1 and n_2 are the same for all three sequences, $\overline{U}$ and σ_U also are the same. For the second sequence, the test statistic is

$$z = \frac{2 - 10.9}{2.1} = -4.2$$

and for the third,

$$z = \frac{19 - 10.9}{2.1} = 3.9$$

Both of these values lie within the critical region, and we would reject the hypothesis that they contain the number of runs expected in random sequences.

Geologic applications of this test may not be obvious, because we ordinarily must consider more than two states in a succession. Stratigraphic sections or traverses across thin sections, for example, usually include at least three states and these cannot be ranked in a meaningful way. We will consider ways that certain sequences can be reduced to dichotomous states, but first we will examine a geologic application of the runs test to a traverse through a two-state system.

Simple pegmatites originate by crystallization of the last, volatile-laden substances squeezed off from solidifying granitic magma. Their textures result from simultaneous crystallization of quartz and feldspar at the eutectic point. If the solidifying pegmatite is undisturbed, we might suppose that quartz and feldspar begin to appear at random locations within the cooling body. This situation may persist, with grains crystallizing at random, until the entire mass is solid. However, the presence of one crystal, perhaps feldspar, might stimulate the local crystallization of additional crystals of feldspar, eventually producing a patchwork texture. Alternatively, growth of a crystal of one state might locally deplete the magma of that constituent, retarding crystallization and resulting in a highly alternating mosaic of quartz and feldspar. A large slab of polished pegmatite used as a window ledge in the washroom of a geology building provides a way for students to investigate these alternative possibilities. The polished surface allows easy discrimination of adjacent grains, so a line drawn on the ledge produces a sequence through the quartz and feldspar grains in the pegmatite. The line on the polished slab may be regarded as a random sample of possible successions through the pegmatite body from which the slab was quarried. The quartz-feldspar sequence along the line is listed in **Table 4–6.** Our problem is to determine if the alternations between quartz and feldspar form a random pattern; if there is a systematic tendency for one state to succeed itself; or whether there is a tendency for one state to immediately succeed the other. Perform a runs test on this data and evaluate the three possibilities.

Table 4–6. Sequence of 100 feldspar (F) and quartz (Q) grains encountered along traverse through pegmatite.

(Start)	F Q Q F Q Q F F Q F Q F F F F F F F Q Q F Q F F F	
	Q F F F F Q F F F Q Q F Q F Q Q Q F F F F F Q F F	
	F F F Q Q Q Q F F Q Q Q F F F F F F Q F Q F F F F	
	F Q F Q F Q F F Q F F F F F Q F F F Q Q F Q F F Q	(End)

We will now consider a related statistical procedure for examining what are called ***runs up*** and ***runs down.*** We are concerned, not with two distinct states, but whether an observation exceeds or is smaller than the preceding observation. **Figure 4–13** shows a typical sequence that can be analyzed by means of a runs test.

The segment abc is a run up, because each observation is larger than the preceding one; similarly, the segment ghi is a run down. Segment $cdef$ is a run down even though the difference between d and e is zero. This is because the interval de lies between segments cd and ef, both of which run downward; therefore, the

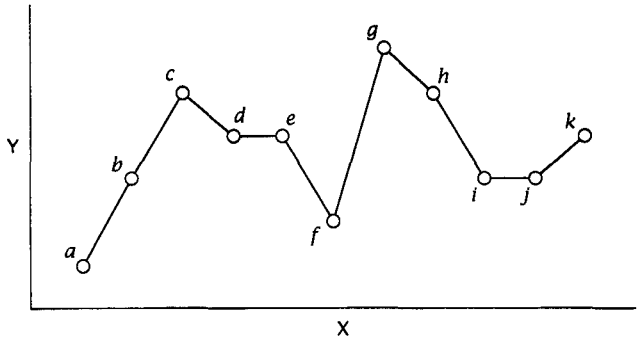


Figure 4–13. Sequence of data points to be analyzed by the method of runs up and down.

entire segment $cdef$ can be considered as a single downward run. The interval ij can be considered either as part of the run down ghi or the run up ijk, as the total number of runs remains the same in either case. In this example, we are assuming that the successive points have integer values. If the observations are expressions of magnitude, they ordinarily will contain fractional parts, and ties (two successive points with identical values) are unlikely.

By considering only differences in magnitude between successive points, we have reduced the data sequence to a string having only two states (or three, if ties occur). We can rewrite the sequence in **Figure 4–13** in the following form:

$$+ + + - 0 - + - - 0 +$$

Regarding the first zero as "−" gives a total of five runs, three of "+" and two of "−" (it makes no difference in the number of runs if we call the second zero "+" or "−"). We can now apply test procedures outlined for the case of sequences of two dissimilar items (Eqs. 4.8-4.10). We must have a large sample to utilize the normal approximation method presented here, but in most geologic problems, adequate numbers of samples will be available.

Table 4–7. Numbers of radiolarian tests per square centimeter in thin sections of siliceous shale.

(Bottom of section)																	
	1	2	3	2	3	5	7	9	9	11	10	12	7	4	3	2	3	
	2	2	1	0	2	3	2	0	3	3	4	9	10	10	8	9	12	
	10	12	14	22	17	19	14	4	2	1	0	0	8	14	16	27		(Top of section)

In the study of a silicified shale unit in the Rocky Mountains, it was noted that the rock contained unusual numbers of well-preserved radiolarian tests. Their presence in the silicified shale suggested a causal relationship, so a sequence of samples was collected at approximately equal intervals in an exposure through the unit. Thin sections were made of the samples and the number of radiolarian tests in a 10 × 10-mm area of the slides was counted. Data for 50 samples are given in **Table 4–7** and shown graphically in **Figure 4–14**. Does the abundance of

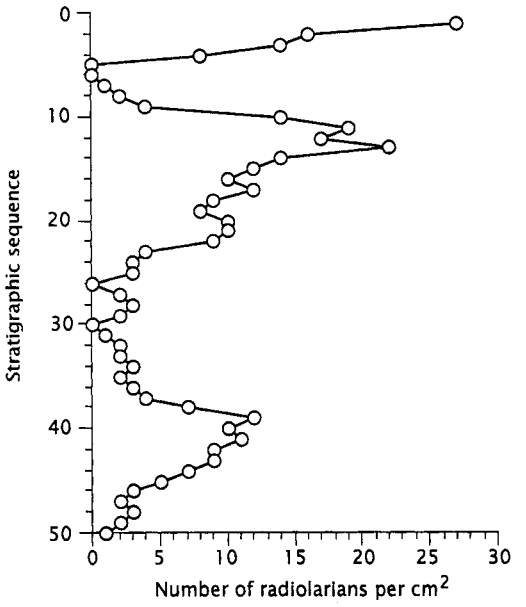


Figure 4–14. Number of radiolarian tests per square centimeter in thin sections of siliceous Mowry Shale.

radiolarians vary at random through the section? A computer program could be written that will perform the necessary calculations, but the programming effort probably exceeds the difficulty of computing the test statistic by hand.

In this procedure, observations are dichotomized by comparing their magnitudes to the preceding observations. Actually, runs tests may be applied to data dichotomized by any arbitrary scheme, provided the hypothesis being tested reflects the dichotomizing method. For example, a common test procedure is to dichotomize a series by subtracting each observation from the median of all observations, and testing the signs for randomness of runs about the median. We also can test the randomness of runs about the mean, and we will use this as a test of residuals from trends later in this chapter. Runs tests are another example of the nonparametric procedures introduced in Chapter 2.

There are a number of variants on the runs tests described here. Information about these tests may be found in texts on nonparametric statistics, such as Conover (1999, p. 122-142) and Siegel and Castellan (1988, section 4.5). Examples of the geologic application of runs tests are included in Miller and Kahn (1962, chapter 14) and Rock (1988, topic 16). Some investigators consider the length of the longest run as an indicator of nonrandomness, and others use the number of turning points, which are points in the sequence where the signs of successive observations change. In certain instances these tests may be more appropriate than the procedures described here. The runs-up-and-down test generally is regarded as the most powerful of the runs tests because it utilizes changes in magnitude of every point with respect to adjacent points. Other dichotomizing schemes reflect only changes with respect to a single value such as the median or mean.

Runs tests are appropriate when the cause of nonrandomness is the object of investigation. They test for a form of nonrandomness expressed by the presence of too few or too many runs, and do not identify overall trends. It should be

emphasized that randomness itself cannot be proven, as the condition of random occurrence is implied in the null hypothesis. Rather, at specified levels of significance, we can demonstrate that the null hypothesis is incorrect and the sequence is therefore not random. Or we can fail to reject the null hypothesis, implying that we have failed to find any indication of nonrandomness. We will next consider procedures for detecting trends, or systematic changes in average value, and will find that runs tests may be used to good advantage in conjunction with these procedures.

Least-Squares Methods and Regression Analysis

In many types of problems, we are concerned not only with changes along a sequence, but are also interested in where these changes occur. To examine these problems, we must have a collection of measurements of a variable and also must know the locations of the measurement points. Both the variable and the scale along the sequence must be expressed in units having magnitude; it is not sufficient simply to know the order of succession of points. We are interested in the general tendency of the data in most of the examples we will now consider. This tendency will be used to interpolate between data points, extrapolate beyond the data sequence, infer the presence of trends, or estimate characteristics that may be of interest to the geologist. If certain assumptions can justifiably be made about the distribution of the populations from which the samples are collected, statistical tests called ***regression analyses*** can be performed.

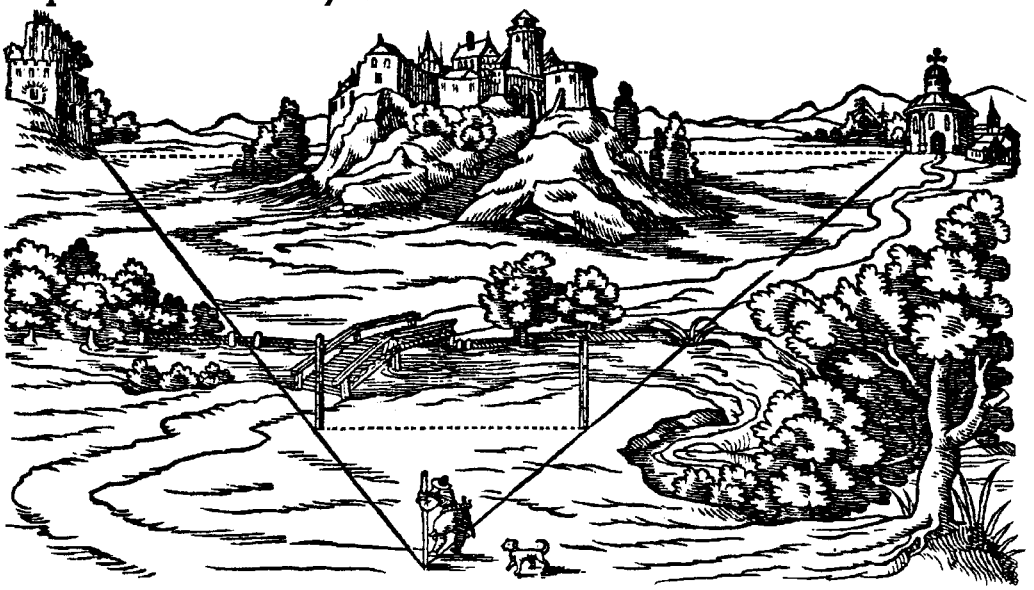
It must be emphasized that we are now using the expression "sequence" in the broadest possible sense. Regression methods are useful for much more than the analysis of observations arranged in order in time or space; they can be used to analyze *any* bivariate data set when it is useful to consider one of the variables as a function of the other. It is as though one variable forms a scale along which observations of the other variable are located, and we want to examine the nature of changes in this variable as we move up or down the scale.

Table 4–8. Moisture content of core samples of Recent mud in Louisiana estuary.

Depth, ft	Moisture (g water/100 g dried solids)
0.0	124.0
5.0	78.0
10.0	54.0
15.0	35.0
20.0	30.0
25.0	21.0
30.0	22.0
35.0	18.0

The data in **Table 4–8** are the moisture contents of samples from a core through Recent marine muds accumulating in a small inlet on the U.S. Gulf Coast in eastern Louisiana. These data are also in file LOUISMUD.TXT. The measurements were made

Chapter 5
Spatial Analysis



Although geologists study a three-dimensional world, their view of it is strongly two dimensional. This reflects in part the fact that the third dimension, depth, often is accessible to only a fraction of the extent of the other two spatial dimensions. Also, our thoughts are conditioned by the media in which we express them, and maps, photographs, and cross-sections are printed or drawn on flat sheets of paper. We may be interested in the geologic features exposed in a deep mine with successive levels, adits, and raises creating a complex three-dimensional net, yet we must reduce this network to flat projections in order to express our ideas concerning the relationships we see.

Geologic Maps, Conventional and Otherwise

Geologists are carefully trained to read, utilize, and create maps; probably no other group of scientists is as adept at expressing and envisioning dimensional relationships. Maps are compact and efficient means of expressing spatial relationships and details—they are as important to Earth scientists as the conventions for scales and notes are to the musician.

In this chapter, we will examine methods for analyzing features on what we loosely define as "maps": two-dimensional representations of areas. Usually the area is geographical (a quadrangle, mining district, country, *etc.*) and the map is a method for reducing very large-scale spatial relationships so they can be easily perceived. However, the representation may equally well be a "map" of a thin section or electron photomicrograph, where the relationships between features have been enlarged so they become visible. Maps, in this general definition, include traditional geologic and topographic maps and also aerial photographs, mine plans,

peel prints, photomicrographs, and electron micrographs. In fact, any sort of two-dimensional spatial representation is included.

Among the topics we will consider that have obvious applications to fields as diverse as geophysics and microscopy is the probability of encountering an object with a systematic search across an area. We will look at the statistics of directional data in both two and three dimensions. Many natural phenomena are expressed as complicated patterns of lines and areas that can best be described as fractals, which we will touch upon. We will also look at ways of describing and comparing more conventional shapes of individual objects, ranging in size from islands to oil fields to microfossils.

Map relationships are almost always expressed in terms of points located on the map. We are concerned with distances between points, the density of points, and the values assigned to points. Most maps are estimates of continuous functions based on observations made at discrete points. An obvious example is the topographic map; although the contour lines are an expression of a continuous and unbroken surface, the lines are calculated from measurements taken at triangulation and survey control points. An even more obvious example is a structural contour map. We do not know that the structural surface is continuous, because we can observe it only at the locations where drill holes penetrate the surface. Nevertheless, we believe that it is continuous and we estimate its form from the measurements made at the wells, recognizing that our reconstruction is inaccurate and lacking in detail because we have no data between wells.

When mapping the surface geology of a desert region, we can stand at one locality where strike and dip have been measured and extend formation boundaries on our map with great assurance because we can see the contacts across the countryside. In regions of heavy vegetation or deep weathering, however, we must make do with scattered outcrops and poor exposures; the quality of the finished map reflects to a great extent the density of control points. Geologists should be intensely interested in the effects which control-point distributions have on maps, but few studies of this influence have been published. In fact, almost all studies of point distributions have been made by geographers. In this chapter, we will examine some of these procedures and consider their application to maps and also to such problems as the distribution of mineral grains in thin sections.

Geologists exercise their artistic talents as well as their geologic skills when they create contour maps. In some instances, the addition of geologic interpretation to the raw data contained in the observation points is a valuable enhancement of the map. Sometimes, however, geologic judgment becomes biased, and the subtle effects of personal opinion detract rather than add to the utility of a map. Computer contouring is totally consistent and provides a counterbalance to overly interpretative traditional mapping. Of course, subjective judgment is necessary in choosing an algorithm to perform mapping, but methods are available that allow a choice to be made between competing algorithms, based upon specified criteria. The principal motive behind the development of automatic contouring is economic, an attempt to utilize the petroleum industry's vast investment in stratigraphic data banks. Aside from this, one of the prime benefits of computerized mapping techniques may come from the attention they focus on the contouring process and the problems they reveal about map reliability. Contour mapping is the subject of one section in this chapter.

Trend-surface analysis is a popular numerical technique in geology. However, although it is widely applied, it is frequently misused. Therefore, we will discuss

the problems of data-point distribution, lack of fit, computational "blowup," and inappropriate applications. Statistical tests are available for trend surfaces if they are to be used as multiple regressions; we will consider these tests and the assumptions prerequisite to their application.

The exchange between Earth scientists and statisticians has been mostly one way, with the notable exception of the expansion of the theory of regionalized variables. This theory, developed originally by Georges Matheron, a French mining engineer, describes the statistical behavior of spatial properties that are intermediate between purely random and completely deterministic phenomena. The most familiar application of the theory is in kriging, an estimation procedure important in mine evaluation, mapping, and other applications where values of a property must be estimated at specific geographic locations.

Two-dimensional methods are, for the most part, direct extensions of techniques discussed in Chapter 4. Trend-surface analysis is an offshoot of statistical regression; kriging is related to time-series analysis; contouring is an extension of interpolation procedures. We have simply enlarged the dimensionality of the subjects of our inquiries by considering a second (and in some cases a third) spatial variable. Of course, there are some applications and some analytical methods that are unique to map analysis. Other methods are a subset of more general multidimensional procedures. It is an indication of the importance of one- and two-dimensional problems in the Earth sciences that they have been included in individual chapters.

Systematic Patterns of Search

Most geologists devote their professional careers to the process of searching for something hidden. Usually the object of the search is an undiscovered oil field or an ore body, but for some it may be a flaw in a casting, a primate fossil in an excavation, or a thermal spring on the ocean's floor. Too often the search has been conducted haphazardly—the geologist wanders at random across the area of investigation like an old-time prospector following his burro. Increasingly, however, geologists and other Earth scientists are using systematic procedures to search, particularly when they must rely on instruments to detect their targets.

Most systematic searches are conducted along one or more sets of parallel lines. Ore bodies that are distinctively radioactive or magnetic are sought using airborne instruments carried along equally spaced parallel flight lines. Seismic surveys are laid out in regular sets of traverses. Satellite reconnaissance, by its very nature, consists of parallel orbital tracks.

The probabilities that targets will be detected by a search along a set of lines can be determined by geometrical considerations. Basically, the probability of discovery is related to the relative size of the target as compared to the spacing of the search pattern. The shape of the target and the arrangement of the lines of search also influence the probability. If the target is assumed to be elliptical and the search consists of parallel lines, the probability that a line will intersect a hidden target of specified size, regardless of where it occurs within the search area, can be calculated. These assumptions do not seem unreasonable for many exploratory surveys. Note that the probabilities relate only to intersecting a target with a line, and do not consider the problem of recognizing a target when it is hit.

McCammon (1977) gives the derivation of the geometric probabilities for circular and linear targets and parallel-line searches. His work is based mostly on the

mathematical development of Kendall and Moran (1963). An older text by Uspensky (1937) derives the more general elliptical case used here.

Assume the target being sought is an ellipse whose dimensions are given by the major semiaxis a and minor semiaxis b. (If the target is circular, then $a = b = r$, the radius of the circle.) The search pattern consists of a series of parallel traverses spaced a distance D apart (**Fig. 5–1 a**). The probability that a target (smaller than the spacing between lines) will be intersected by a line is

$$p = \frac{P}{\pi D} \tag{5.1}$$

where P is the perimeter of the elliptical target. The equation for the perimeter of an ellipse is $P = 2\pi\sqrt{(a^2 + b^2)/2}$, where a and b are the major and minor semiaxes. Substituting,

$$p = \frac{2\pi\sqrt{\frac{a^2+b^2}{2}}}{\pi D} = \frac{2\sqrt{\frac{a^2+b^2}{2}}}{D} \tag{5.2}$$

We can define a quantity Q as the numerator of Equation (5.2); that is, $Q = 2\sqrt{(a^2 + b^2)/2}$. With this simplification, the probability of intersecting an elliptical target with one line in a set of parallel search lines can be written as

$$p = \frac{Q}{D} \tag{5.3}$$

In the specific case of a circular target, a and b are both equal to the radius, so Q can be replaced by twice the radius:

$$p = \frac{2r}{D} \tag{5.4}$$

At the other extreme, one axis of the ellipse may be so short that the target becomes a randomly oriented line. This geometric relationship is known as ***Buffon's problem***, which specifies the probability that a needle of length ℓ, when dropped at random on a set of ruled lines having a spacing D, will fall across one of the lines. The probability is

$$p = \frac{2\ell}{\pi D} \tag{5.5}$$

where ℓ is the length of the target.

A similar geometric relationship, known as ***Laplace's problem***, also pertains to the probabilities in systematic searches. Laplace's problem specifies the probability that a needle of length ℓ, when dropped on a board covered with a set of rectangles, will lie entirely within a single rectangle. A variant gives the probability that a coin tossed onto a chessboard will fall entirely within one square. In exploration, the complementary probabilities are of interest, *i.e.*, that a randomly located target will be intersected one or more times by a set of lines, such as seismic traverses, arranged in a rectangular grid (**Fig. 5–1 b**).

The general equation is

$$p = \frac{Q(D_1 + D_2 - Q)}{D_1 D_2} \tag{5.6}$$

where D_1 is the spacing between one set of parallel seismic traverses and D_2 is the spacing between the perpendicular set of traverses. In the specific instance of a

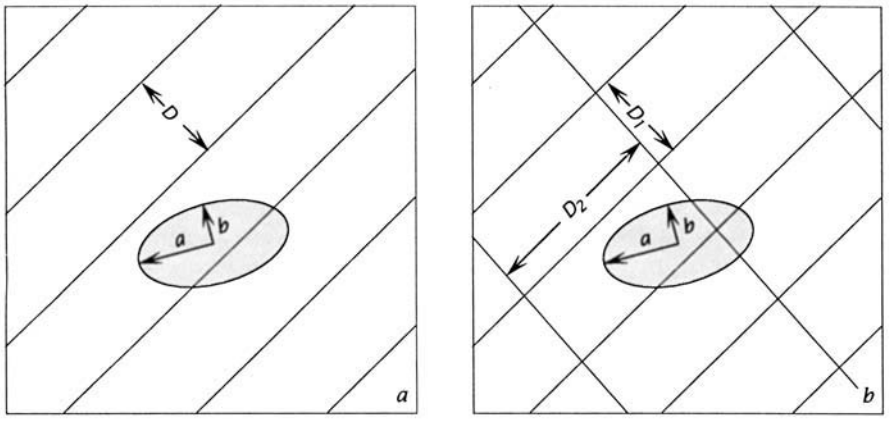


Figure 5–1. Search for an elliptical target with major semiaxis a and minor semiaxis b. (*a*) Using a parallel-line search of spacing D. (*b*) Using a grid search with spacing D_1 in one direction and D_2 in the perpendicular direction.

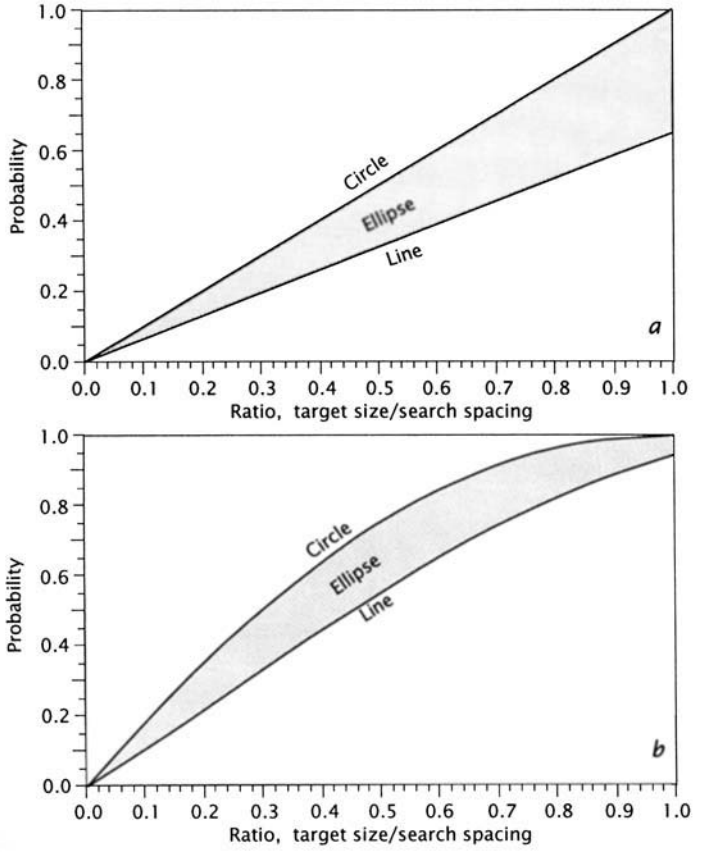


Figure 5–2. Probability of intersecting a target with a systematic pattern of search. Shape of target may range from a circle to a line; elliptical targets of various axial ratios fall in the shaded region. Horizontal axis is ratio (major dimension of target)/(spacing between search lines). (*a*) Parallel-line search pattern. (*b*) Square-grid search pattern. After McCammon (1977).

search in the pattern of a square grid, the equation simplifies to

$$p = \frac{Q}{D}\left(2 - \frac{Q}{D}\right) \tag{5.7}$$

Lambie (unpublished report, 1981) has pointed out that these equations for geometric probability are approximations of integral equations. Comparing exact probabilities found by numerical integration with those predicted by the approximation equations, he found that significant differences occur only for very elongate targets that are large with respect to spacing between search lines. Then, equations such as (5.3) and (5.6) may seriously overestimate the probabilities of detection.

The probabilities of intersecting a target, as calculated by the approximating equations, can be shown conveniently as graphs. McCammon (1977) presented such graphs in a particularly useful dimensionless form for various combinations of target shape and size relative to the spacing between the search lines. **Figure 5–2a** gives the probability of detecting an elliptical target whose shape ranges from a circle to a line, using a search pattern of parallel lines. The relative size of the target is found by dividing the target's maximum dimension by the search line

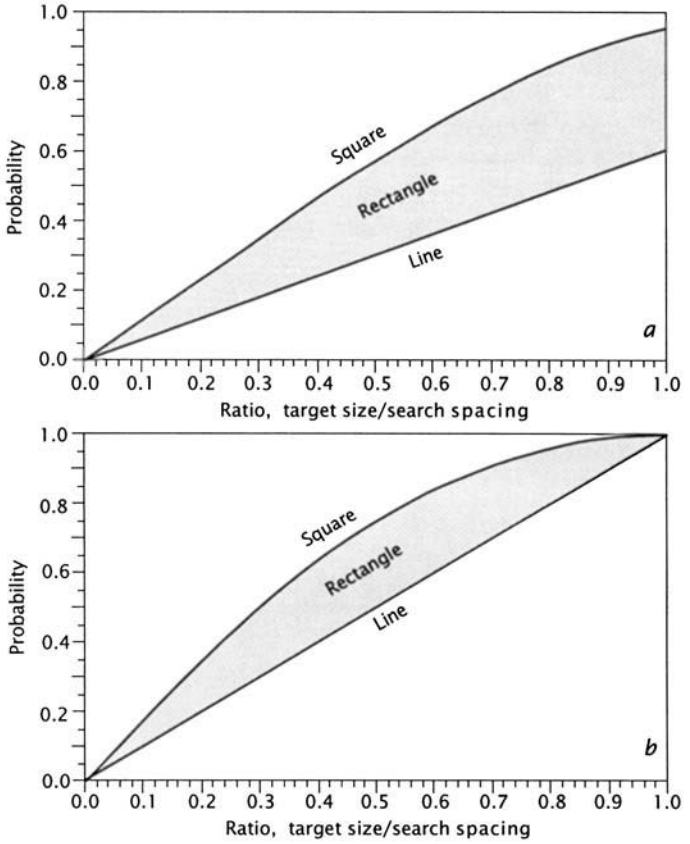


Figure 5–3. Probability of intersecting targets with regular search patterns ranging from squares to parallel lines. Rectangular search patterns with different ratios of D_1/D_2 fall in the shaded region. Horizontal axis is ratio (major dimension of target)/(minimum spacing between search lines). (*a*) Target is circular. (*b*) Target is a line. After McCammon (1977).

spacing. **Figure 5–2 b** is an equivalent graph for a search pattern consisting of a square grid of lines.

If the shape of the target is specified, the probabilities of intersection can be graphed for different patterns of search. **Figure 5–3 a**, for example, shows the probability of intersecting a circular target with search patterns ranging from a square grid, through rectangular grid patterns, to a parallel-line search. **Figure 5–3 b** is the equivalent graph for a line-shaped target. Between the two graphs, all possible shapes of elliptical targets and all possible patterns of search along two perpendicular sets of parallel lines are encompassed.

Distribution of Points

Geologists often are interested in the manner in which points are distributed on a two-dimensional surface or a map. The points may represent sample localities, oil wells, control points, or poles and projections on a stereonet. We may be concerned about the uniformity of control-point coverage, the distribution of point density, or the relation of one point to another. These are questions of intense interest to geographers as well as geologists, and the burgeoning field of locational analysis is devoted to these and similar problems. Although much of the attention of the geographer is focused on the distribution of shopping malls or public facilities, the methodologies are directly applicable to the study of natural phenomena as well.

The patterns of points on maps may be conveniently classified into three categories: regular, random, and aggregated or clustered. Examples of point distributions are shown in **Figure 5–4** and range from the most uniform possible (the face-centered hexagonal lattice in **Fig. 5–4 a**, where every point is equidistant from its six nearest neighbors) to a highly clustered pattern composed of randomly located centers around which the probability of occurrence of a point decreases exponentially with distance (**Fig. 5–4 f**). Of course most maps will have patterns intermediate between these extremes, and the problem becomes one of determining where the observed pattern lies within the spectrum of possible distributions. For example, most people would intuitively regard the distribution of points in **Figure 5–4 c** as random. However, intuition is wrong, because the map was created by dividing the map area into a 4×4 array of regular cells and then placing four points at random within each cell (except in the shortened bottom row, which received only two points per cell). The distribution therefore has both random and regular aspects and is more uniform in density than a purely random arrangement such as **Figure 5–4 d**.

The pattern of points on a map is said to be ***uniform*** if the density of points in any subarea is equal to the density of points in all other subareas of the same size and shape. The pattern is ***regular*** if the spacings between points repeat, as on a grid. That is, the distance between a point i and another point j lying in some specified direction from i is the same for all pairs of points i and j on the map. Obviously, a regular pattern also will be uniform, but the converse is not necessarily true. A ***random*** pattern can be created if any subarea is as likely to contain a point as any other subarea of the same size, regardless of the subarea's location, and the placement of a point has no influence on the placement of any other point. In an aggregated or ***clustered*** pattern, the probability of occurrence of a point varies in some inverse manner with distances to preexisting points.

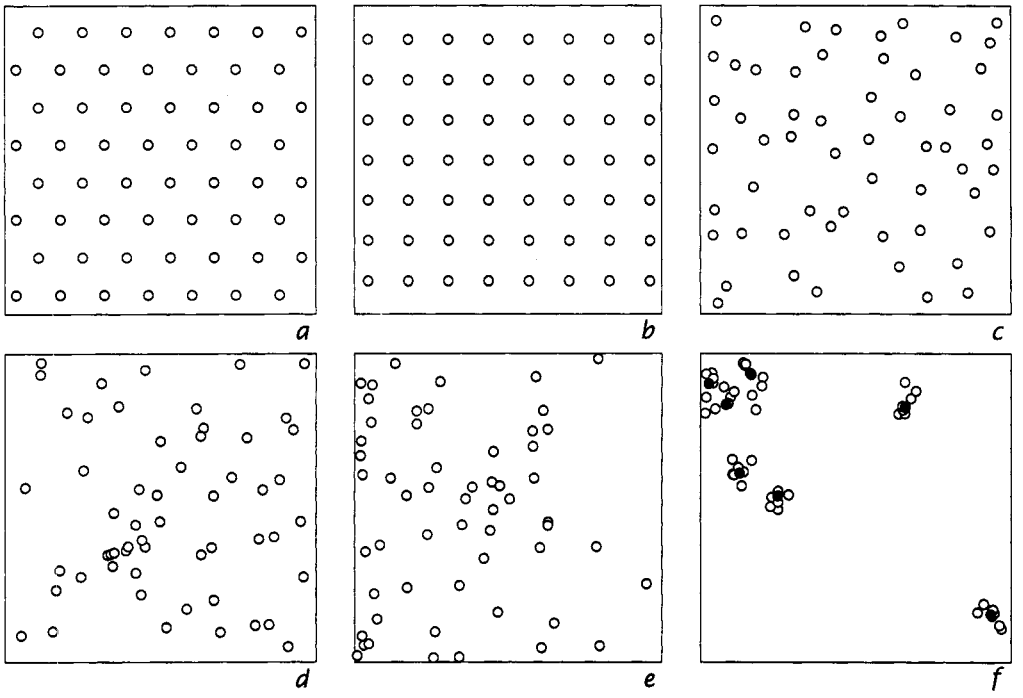


Figure 5–4. Some possible patterns of points on maps. Each map contains 56 points. (*a*) Points regularly spaced on a face-centered hexagonal grid or network. Every point is equidistant from six other points. (*b*) Points regularly arranged on a square grid. (*c*) Sets of four points placed randomly within each cell of a regular 4 × 4 grid. The bottom row contains only two points per cell. (*d*) Points located by a bivariate uniform random process. (*e*) Nonuniform pattern of points produced by logarithmic scaling of the X-axis. (*f*) Points located by randomly placing seven cluster centers (black points) and moving eight points a random direction and logarithmically scaled distance from each center.

A uniform density of data points is important in many types of analysis, including trend-surface methods which we will discuss later. The reliability of contour maps is directly dependent upon the total density of control points as well as their uniformity of distribution. However, most geologic researchers have been content with qualitative judgments of the adequacy and representativeness of the distribution of their data. Even though the desirability of a uniform density of observations is often cited, the degree of uniformity is seldom measured. The tests necessary to determine uniformity are very simple, and it is unfortunate that many geologists seem unaware of them. These tests are, however, extensively used by geographers. Haggett, Cliff, and Frey (1977); Getis and Boots (1978); Cliff and Ord (1981); and Bailey and Gatrell (1995) provide an introduction to this literature.

Uniform density

A map area may be divided into a number of equal-sized subareas (sometimes called ***quadrats***) such that each subarea contains a number of points. If the data points are distributed uniformly, we expect each subarea to contain the same number of points. This hypothesis of no difference in the number of points per subarea can be tested using a χ^2 method, and is theoretically independent of the shape or

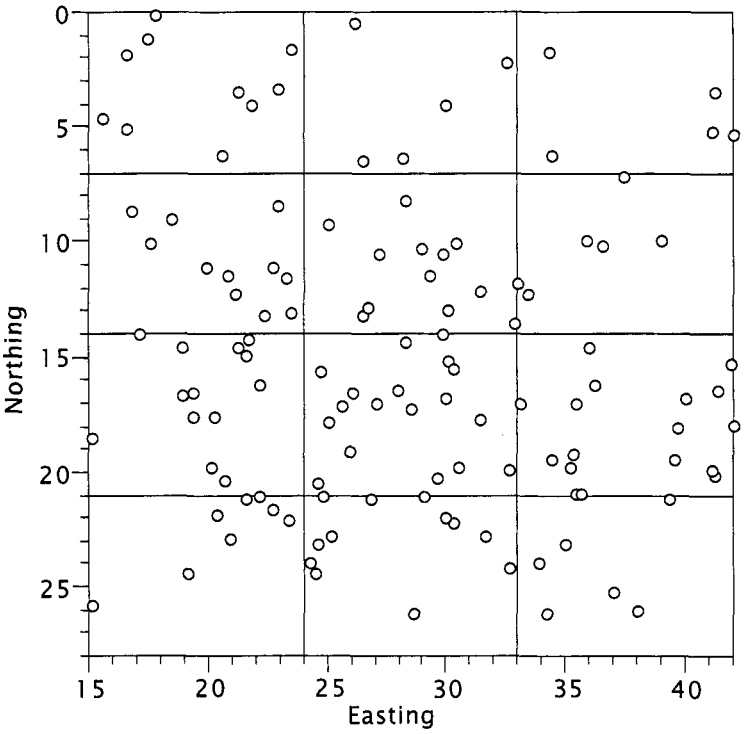


Figure 5–5. Locations of 123 exploratory holes drilled to top of Ordovician rocks (Arbuckle Group) in central Kansas. Map has been divided into 12 cells of equal size.

orientation of subareas. However, the test is most efficient if the number of subareas is a maximum (this increases the degrees of freedom), subject to the restriction that no subarea contain fewer than five points. The expected number of points in each subarea is

$$E = \frac{N}{k} \tag{5.8}$$

where N is the total number of data points and k is the number of subareas. A χ^2 test of goodness of fit of the observed distribution to the expected (uniform) distribution is

$$\chi^2 = \sum_{i=1}^{k} \frac{(O_i - E)^2}{E} \tag{5.9}$$

where O_i is the observed number of data points in subarea i and E is the expected number. The test has $\nu = k - 2$ degrees of freedom, where k is the number of subareas.

As an example of the application of this test, consider the data-point distribution shown in **Figure 5–5**. These are the locations of 123 holes drilled in the search for oil in the Ordovician Arbuckle stratigraphic succession in central Kansas. These data are listed in file ARBUCKLE.TXT. In **Figure 5–5**, the map area has been divided into 12 equal subareas, each of which we expect to contain about ten points, if the points are uniformly distributed. The observed number of points in each subarea and the computations necessary to find the test value are given in **Table 5–1**. This test has $\nu = 10$ degrees of freedom, so the critical value of χ^2 at the 5% ($\alpha = 0.05$) significance level is 18.3. The computed test value of $\chi^2 = 17.0$ does not exceed

this, so we conclude that there is no evidence suggesting that the quadrats are unevenly populated. Note that the test applies only to the uniformity of point densities between areas of a specified size and shape. It is possible that we could select quadrats of different sizes or shapes that might not be uniformly populated, especially if they were smaller than those used in this test.

Table 5–1. Number of wells in 12 subareas of central Kansas.

Observed Number of Points	$\frac{(O-E)^2}{E}$
10	0.006
5	2.689
5	2.689
11	0.055
13	0.738
5	2.689
12	0.299
16	3.226
16	3.226
9	0.152
13	0.738
8	0.494
TOTAL = 123	$\chi^2 = 16.995^a$

[a]Test value is not significant at the $\alpha = 0.05$ level.

Random patterns

Establishing that a pattern is uniform does not specify the nature of the uniformity, for both regular and random patterns are expected to be homogeneous. For many purposes, verifying uniformity is sufficient; but, if we desire more information about the pattern, we must turn to other tests. If points are distributed at random across a map area, even though the coverage is uniform, we do not expect exactly the same number of points to lie within each subarea. Rather, there will be some preferred number of points that occur in most subareas and there will be progressively fewer subareas that contain either more points or fewer. This is apparent in the example we just worked; although our hypothesis of uniformity specified that we expect about ten observations in each subarea, we actually found some areas that contained more than ten and some that contained fewer.

You will recall that the Poisson probability distribution is the limiting case of the binomial distribution when p, the probability of a success, is very small and $(1 - p)$ approaches 1.0. The Poisson distribution can be used to model the occurrence of rare, random occurrences in time, as it was used in Chapter 4, or it can be used to model the random placement of points in space. Although the Poisson distribution, like the binomial, uses the numbers of successes, failures, and trials in the calculation of probabilities, it can be rewritten so that neither the number of failures nor the total number of trials is required. Rather, it uses the number of points per quadrat and the density of points in the entire area to predict how many quadrats should contain specified numbers of points. These predicted

or expected numbers of quadrats can be used in a χ^2 procedure to test whether the points are distributed at random within the area.

As an application, we can determine if oil discoveries in a basin occur at random or are distributed in some other fashion. It is not intuitively obvious that the Poisson distribution can be expressed in a form appropriate for this problem, so we will work through its development.

Assume a basin has an area, a, in which m discovery wells are randomly located. The ***density*** of discovery wells in the basin is designated λ, and is simply

$$\lambda = \frac{m}{a} \tag{5.10}$$

The basin may be divided into small lease tracts, each of area A (here the term "tract" is equivalent to "quadrat"). In turn, each tract may be divided into n extremely small, equal-sized subareas which we might regard as potential drilling sites. The probability that any one of these extremely small subareas contains a discovery well tends toward zero as n becomes infinitely large.

The area of each drilling site is A/n. The probability that a site contains a discovery well is

$$p = \lambda \frac{A}{n}$$

and the probability that it does not contain a discovery well is

$$1 - p = \left(1 - \lambda \frac{A}{n}\right)$$

We wish to investigate the probability that r of the n drilling sites within a tract contain discovery wells, and $n - r$ drilling sites do not. The probability of a specific combination of discovery and nondiscovery well sites within a tract is

$$P = \left(\lambda \frac{A}{n}\right)^r \left(1 - \lambda \frac{A}{n}\right)^{n-r}$$

However, within a tract, there are $\binom{n}{r}$ combinations of the n drilling sites, of which r contain discovery wells and all are equally probable. The probability that a tract will contain exactly r discovery wells is therefore

$$P(r) = \binom{n}{r} \left(\lambda \frac{A}{n}\right)^r \left(1 - \lambda \frac{A}{n}\right)^{n-r}$$

Note that this is simply the binomial probability of r discovery wells on n drilling sites.

The combinations can be expanded into factorials,

$$P(r) = \frac{n(n-1)(n-2)\cdots(n-r+1)}{r!} \frac{(\lambda A)^r}{n^r} \left(1 - \frac{\lambda A}{n}\right)^n \left(1 - \frac{\lambda A}{n}\right)^{-r}$$

Rearranging and canceling terms yields

$$P(r) = \left(1 - \frac{1}{n}\right)\left(1 - \frac{2}{n}\right) \cdots \left(1 - \frac{r-1}{n}\right) \left(1 - \frac{\lambda A}{n}\right)^{-r} \left[\left(1 - \frac{\lambda A}{n}\right)^n \frac{(\lambda A)^r}{r!}\right] \tag{5.11}$$

As n becomes infinitely large, all of the fractions that contain n in their denominator become infinitesimally small and vanish, so all terms inside parentheses simply become equal to 1. The terms inside the brackets simplify to

$$P(r) = e^{(-\lambda A)} \frac{(\lambda A)^r}{r!} \tag{5.12}$$

Note that n, the number of drilling sites, has vanished from the equation leaving only the discovery-well density, λ, the number of discovery wells, r, and the area, A, of the tracts. This is an expression of the Poisson distribution, as applied to the probability of rare, random events (discovery wells) occurring within geographic areas. Also note that λA is simply the mean number of wells per tract, because it is the product of the density of discovery wells times the area of a tract. In practice, we estimate λA from the total number of discovery wells, m, and the total number of tracts, T

$$\lambda A = \frac{m}{T} \tag{5.13}$$

We can now perform a χ^2 test to see if the number of wells per tract matches that expected if the wells are randomly located according to the Poisson model. The number of tracts that contain exactly r discovery wells can be found by

$$\begin{aligned} n_r &= mP(r) \\ &= me^{(-\lambda A)} \frac{(\lambda A)^r}{r!} \end{aligned} \tag{5.14}$$

If λA is estimated by m/T, the equation becomes

$$n^r = me^{(-m/T)} \frac{(m/T)^r}{r!} \tag{5.15}$$

Figure 5–6 shows the locations of discovery wells in part of the Eastern Shelf area of the Permian Basin in Fisher and Noland counties of Texas. The area has been divided into a 10×16 grid of 160 tracts, or quadrats, each containing approximately 10 mi^2. Since there are 168 discovery wells in the area, the mean number of wells per tract is

$$\frac{m}{T} = \frac{168}{160} = 1.05$$

We can count the number of tracts in the map that contain no discovery wells, exactly one discovery, two discoveries, and so forth. Using Equation (5.15), we can also calculate the expected number of tracts that contain these same numbers of wells. The expected and observed numbers of tracts for the Permian Basin area are given in **Table 5–2**. This table contains all of the figures necessary to calculate a χ^2 test of goodness of fit, which is essentially a comparison of the two histograms shown in **Figure 5–7**. The last three categories must be combined so that the observed number of tracts is equal to or greater than five

$$\chi^2 = \frac{(70 - 56.0)^2}{56.0} + \frac{(42 - 58.8)^2}{58.8} + \frac{(26 - 30.9)^2}{30.9} + \frac{(17 - 10.8)^2}{10.8} + \frac{(5 - 3.5)^2}{3.5} = 13.28$$

The test statistic has $c - 2$ degrees of freedom, where c is the number of categories (one degree of freedom is lost because the expected frequencies are constrained

to sum to 160, and a second degree of freedom is required for estimation of the parameter λ). For $c = 5$ categories, there are three degrees of freedom.

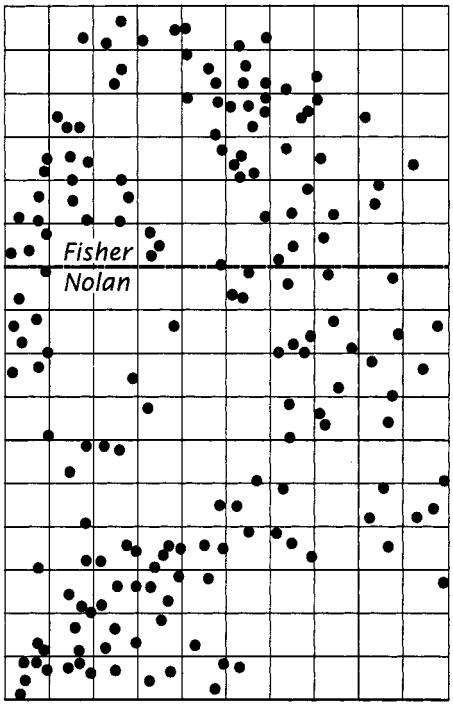


Figure 5–6. Locations of oil-field discovery wells in part of the Eastern Shelf area of the Permian Basin, Fisher and Noland counties, Texas. Quadrats are approximately 10 mi^2 in size.

Table 5–2. Calculation of expected numbers of tracts containing r discoveries in eastern part of Permian Basin, Texas, assuming a Poisson distribution.

Number of Discoveries Per Tract (r)	Poisson Equation	Probability Tract Contains r Discoveries	Number of Tracts	
			Expected	Observed
0	$P_{(0)} = e^{(-1.05)}\frac{1.05^0}{0!}$	0.3499	56.0	70
1	$P_{(1)} = e^{(-1.05)}\frac{1.05^1}{1!}$	0.3674	58.8	42
2	$P_{(2)} = e^{(-1.05)}\frac{1.05^2}{2!}$	0.1929	30.9	26
3	$P_{(3)} = e^{(-1.05)}\frac{1.05^3}{3!}$	0.0675	10.8	17
4	$P_{(4)} = e^{(-1.05)}\frac{1.05^4}{4!}$	0.0177	2.8	3
5	$P_{(5)} = e^{(-1.05)}\frac{1.05^5}{5!}$	0.0037	0.6	1
6	$P_{(6)} = e^{(-1.05)}\frac{1.05^6}{6!}$	0.0007	0.1	1
TOTALS		0.9998	160.0	160

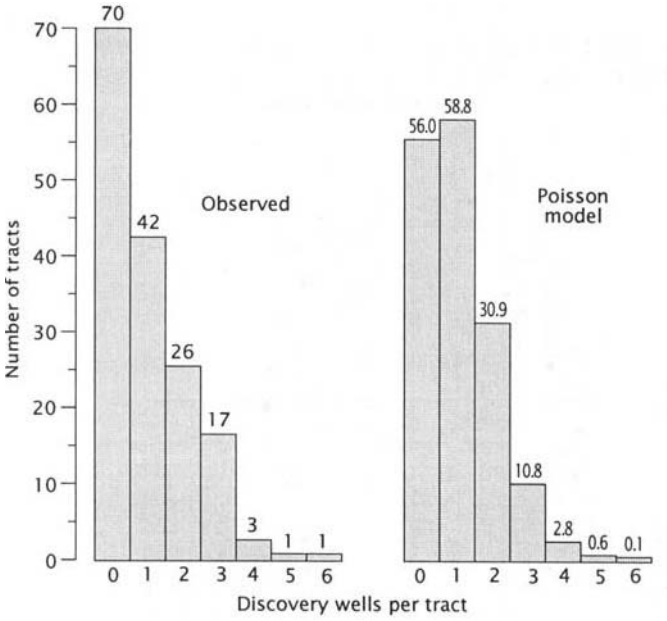


Figure 5–7. Histograms showing observed numbers of discovery wells per tract in an area of the Permian Basin, and the number expected if fields are distributed randomly according to a Poisson model.

The critical value of χ^2 for $\nu = 3$ and $\alpha = 0.05$ is 7.81. The test statistic far exceeds this value, so we must reject the hypothesis of equality between the observed and expected distributions and conclude that the Poisson model is not appropriate. Oil discoveries have not been made randomly within this area of the Permian Basin.

In the process of fitting the Poisson model to this data, we have generated some information that may provide additional insight into the nature of the spatial distribution. The mean number of discoveries per tract is estimated by Equation (5.13). The variance in number of discoveries per tract is

$$s^2 = \frac{\sum_{i=1}^{T} (r_i - m/T)^2}{T - 1} \tag{5.16}$$

where r_i is the number of discoveries in the ith tract. The summation extends over all T tracts. The alternative results of comparing the estimated mean and variance are

$m/T > s^2$	Pattern more uniform than random
$m/T = s^2$	Pattern random
$m/T < s^2$	Pattern more clustered than random

Of course, some difference between m/T and s^2 may arise due to random variation in the particular set of tracts chosen. The statistical significance of the observed difference may be tested by a t-test based on the standard error of the mean, which is the variance that would be expected in values of m/T if a basin were repeatedly sampled by different sets of tracts of the same size. The standard error in the mean number of discoveries per tract is

$$s_e = \sqrt{2/(T-1)} \tag{5.17}$$

The t-test compares the ratio between m/T and s^2, which should be equal to 1.0 if the two statistics are the same

$$t = \frac{\left(\frac{m/T}{s^2}\right) - 1.0}{s_e} \tag{5.18}$$

The test has $T - 1$ degrees of freedom.

For the eastern Permian Basin area, the variance in number of wells per tract is

$$s^2 = \frac{231.6}{159} = 1.46$$

The standard error of the mean number of wells per tract can be estimated as

$$s_e = \sqrt{\frac{2}{159}} = 0.112$$

The t-statistic for the test of equivalence of the mean and variance is

$$t = \frac{(1.05/1.46) - 1.0}{0.112} = -8.86$$

At a significance level of $\alpha = 0.05$ and 159 degrees of freedom, the critical value of t for a two-tailed test is 1.96; the computed statistic far exceeds this and so we may conclude as we did in the χ^2 test that the spatial distribution is not random. Since the variance is significantly greater than the mean, we must also conclude that discovery wells are areally clustered.

Clustered patterns

Many naturally occurring spatial distributions show a pronounced tendency toward clustering. This is especially true of certain biological variables, such as presence of specific organisms or occurrences of an infectious disease. The descendants of a sedentary parent, perhaps a coral or a tree, tend to grow nearby, leading to development of densely populated areas surrounded by areas that are relatively barren. Clustered patterns of points can be modeled by many theoretical distributions, most of which can be regarded as combinations of two or more simpler distributions. One of the distributions describes the locations of the centers of clusters, while the other describes the pattern of individual points around the centers of the clusters.

The negative binomial distribution can be used to model the occurrence of clustered points in space in a manner equivalent to the use of the Poisson to model randomly arranged points. An extensive discussion with citations to studies in many fields is given by Ripley (1981). Griffiths (1962, 1966) advocated the use of the negative binomial as an appropriate model for the occurrence of oil fields and ore bodies.

One derivation of the negative binomial is as a compound Poisson and logarithmic distribution with clusters of points randomly located within a region; individual points within a cluster follow a logarithmic distribution. In the formulation appropriate for describing spatial patterns, the negative binomial is

$$P(r) = \binom{k+r-1}{r} \left(\frac{p}{1+p}\right)^r \left(\frac{1}{1+p}\right)^k \tag{5.19}$$

In terms of the oil-field distribution problem we have just considered, r is the number of discovery wells in a tract, p is the probability that a given drilling site contains a discovery well, and k is a measure of the degree of clustering of the discoveries. If k is large, clustering is less pronounced and the spatial distribution approaches the Poisson, or randomness. As k approaches zero, the pattern of clustering becomes more pronounced. The density, λ, is equal to

$$\lambda = kp \tag{5.20}$$

If k is not an integer (and in general it will not be), this combinatorial equation cannot be solved. Then, the following approximation must be used:

$$\begin{aligned} P(0) &= \frac{1}{(1+p)^k} \\ P(r) &= \frac{(k+r-1)(p/1+p)}{r} P(r-1) \end{aligned} \tag{5.21}$$

As with the Poisson distribution, λ is estimated by the average density of discoveries per tract, m/T. The clustering parameter, k, is estimated by

$$k = \frac{(m/T)^2}{s^2 - (m/T)} \tag{5.22}$$

where s^2 is the variance in number of discovery wells per tract. Then, the probability p can be estimated as

$$p = \frac{\lambda}{k} = \frac{(m/T)}{k} \tag{5.23}$$

We can apply the negative binomial model to the data on discovery wells in the eastern part of the Permian Basin (**Fig. 5–6**) to see if this distribution can adequately describe their spatial distribution. The mean and variance of the number of discovery wells per tract have already been found: $m/T = 1.05$ and $s^2 = 1.46$. The clustering effect can be estimated using Equation (5.22)

$$k = \frac{1.05^2}{1.46 - 1.05} = 2.69$$

In turn, the probability of a discovery well occurring in a tract is

$$p = \frac{1.05}{2.69} = 0.390$$

Using the approximation equations, the probability that a given tract will contain no discovery wells is

$$P(0) = \frac{1}{(1+0.390)^{2.69}} = 0.4124$$

The probability that a tract will contain exactly one discovery well is

$$P(1) = \frac{(2.69+1-1)(0.390/1.390)}{1} \times 0.4124 = 0.3112$$

Table 5–3. Expected numbers of tracts containing r discoveries in eastern part of Permian Basin, Texas, assuming a negative binomial distribution.

Number of Discoveries Per Tract (r)	Probability Tract Contains r Discoveries	Number of Tracts	
		Expected	Observed
0	0.4124	66.0	70
1	0.3112	49.8	42
2	0.1611	25.8	26
3	0.0706	11.3	17
4	0.0281	4.5	3
5	0.0106	1.7	1
6	0.0038	0.6	1
TOTALS	0.9988	159.7	160

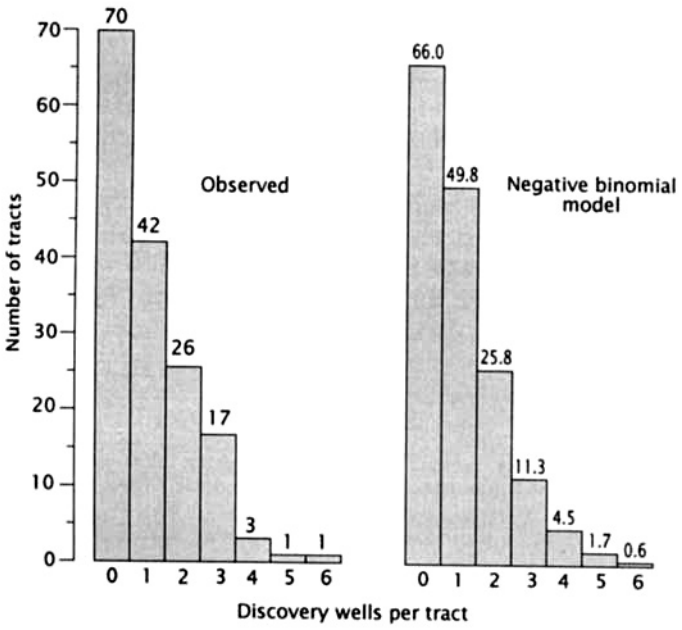


Figure 5–8. Histograms showing observed numbers of discovery wells per tract in an area of the Permian Basin, and the number expected in a clustered (negative binomial) model.

The probabilities that a tract will contain exactly two, three, or other number of discovery wells can be calculated in a similar fashion. Then, the expected number of tracts containing r discoveries can be determined simply by multiplying these probabilities by 160, the total number of tracts. **Table 5–3** gives the expected numbers of tracts for up to six discoveries per tract.

The numbers of tracts containing exactly r discoveries as predicted by the negative binomial model are compared to the corresponding observed numbers of tracts in **Figure 5–8**. The goodness of fit of the negative binomial can be tested by

a χ^2 test exactly like that used to check the fit of the Poisson model. Again, it is necessary to combine the final three categories so a frequency of five or more is obtained. The test statistic is $\chi^2 = 4.82$, with $(5 - 2 = 3)$ degrees of freedom. This is less than the critical value of χ^2 for $\alpha = 0.05$ and $\nu = 3$, so we cannot reject the negative binomial as a model of the spatial distribution of discovery wells in the eastern part of the Permian Basin. Keep in mind that this is not equivalent to proof that the wells do follow a negative binomial model, because it is possible that some other clustered model might provide an even better fit. However, the negative binomial does generate a spatial distribution that is statistically indistinguishable from the one observed.

Nearest-neighbor analysis

An alternative to quadrat analysis is ***nearest-neighbor analysis.*** The data used are not the numbers of points within subareas, but the distances between closest pairs of points. Since it is not necessary to select a quadrat size, nearest-neighbor procedures avoid the possibility of finding that a pattern is random at one scale but not at another. Also, since there are usually many more pairs of nearest neighbors than quadrats, the analysis is more sensitive. A good introduction to nearest-neighbor techniques is given by Getis and Boots (1978). Ripley (1981) provides a review of theory and applications in several fields, as do Cliff and Ord (1981). Shaw and Wheeler (1994) and Bailey and Gatrell (1995) discuss computational aspects of nearest-neighbor analyses.

Nearest-neighbor analysis compares characteristics of the observed set of distances between pairs of nearest points with those that would be expected if the points were randomly placed. The characteristics of a theoretical random pattern can be derived from the Poisson distribution. If we ignore the effect of the edges of our map, the expected mean distance between nearest neighbors is

$$\overline{\delta} = \frac{1}{2}\sqrt{A/n} \tag{5.24}$$

where A is the area of the map and n is the number of points. You will recall that A/n is the point density, λ. The sampling variance of $\overline{\delta}$ is given by

$$\sigma^2_{\overline{\delta}} = \frac{(4 - \pi)\,A}{4\pi n^2} \tag{5.25}$$

If we work out the constants,

$$\sigma^2_{\overline{\delta}} = \frac{0.06831\,A}{n^2} \tag{5.26}$$

The standard error of the mean distance between nearest neighbors is the square root of $\sigma^2_{\overline{\delta}}$

$$s_e = \frac{0.26136}{\sqrt{A/n^2}} \tag{5.27}$$

The distribution of $\overline{\delta}$ is normal provided n is greater than 6, so we can use the simple z-test given in Chapter 2 to test the hypothesis that the observed mean

distance between nearest neighbors, $\bar{d}$, is equal to the value of $\bar{\delta}$ from a random pattern of points of the same density. The test is

$$z = \frac{\bar{d} - \bar{\delta}}{s_e} \tag{5.28}$$

This is the form of the nearest-neighbor test that is commonly presented, but unfortunately it has a serious defect for most practical purposes. The expected value $\bar{\delta}$ assumes that edge effects are not present, which means that the observed pattern of points must extend to infinity in all directions if $\bar{d}$ and $\bar{\delta}$ are to be validly compared. Since the map does not extend indefinitely, the nearest neighbors of points near the edges must lie within the body of the map, and so $\bar{d}$ is biased toward a greater value (Upton and Fingleton, 1985). There are several corrections for this problem. If data are available beyond the limits of the area being analyzed, the map can be surrounded by a ***guard region***. Then, nearest-neighbor distances between points inside the map and points in the guard region can be included in the calculation of $\bar{d}$. Alternatively, we can consider our map to be drawn not on a flat plane but on a torus. In this case, in the right map edge would be adjacent to the left edge and the top adjacent to the bottom. The nearest neighbor of a point along the right edge of the map might lie just inside the left edge (this concept should be familiar to anyone who has contoured point densities on stereonets). Another way of regarding this particular correction is to imagine that the pattern of points repeats in all directions, like floor tiles. Any point lying adjacent to an edge of the map has the opportunity to find a point across the edge that may be a closer neighbor than the nearest point within the map.

A third correction involves adjusting $\bar{d}$ so that the boundary effects are included in its expected value. Using numerical simulation, Donnelly (1978) found these alternative expressions for the theoretical mean nearest-neighbor distance and its sampling variance:

$$\bar{\delta} \approx \frac{1}{2}\sqrt{\frac{A}{n}} + \left(0.514 + \frac{0.412}{\sqrt{n}}\right)\frac{p}{n} \tag{5.29}$$

and

$$s_{\bar{\delta}}^2 \approx 0.070\frac{A}{n^2} + 0.035p\frac{\sqrt{A}}{n^{5/2}} \tag{5.30}$$

In these approximations, p is the perimeter of the rectangular map. Note that if the map has no edges, as when it is considered to be drawn on a torus, p is zero and these equations are identical to equations (5.24) and (5.26).

The expected and observed mean nearest-neighbor distances can be used to construct an index to the spatial pattern. The ratio

$$R = \frac{\bar{d}}{\bar{\delta}} \tag{5.31}$$

is the ***nearest-neighbor statistic*** and ranges from 0.0 for a distribution where all points coincide and are separated by distances of zero, to 1.0 for a random distribution of points, to a maximum value of 2.15. The latter value characterizes a distribution in which the mean distance to the nearest neighbor is maximized. The distribution has the form of a regular hexagonal pattern where every point

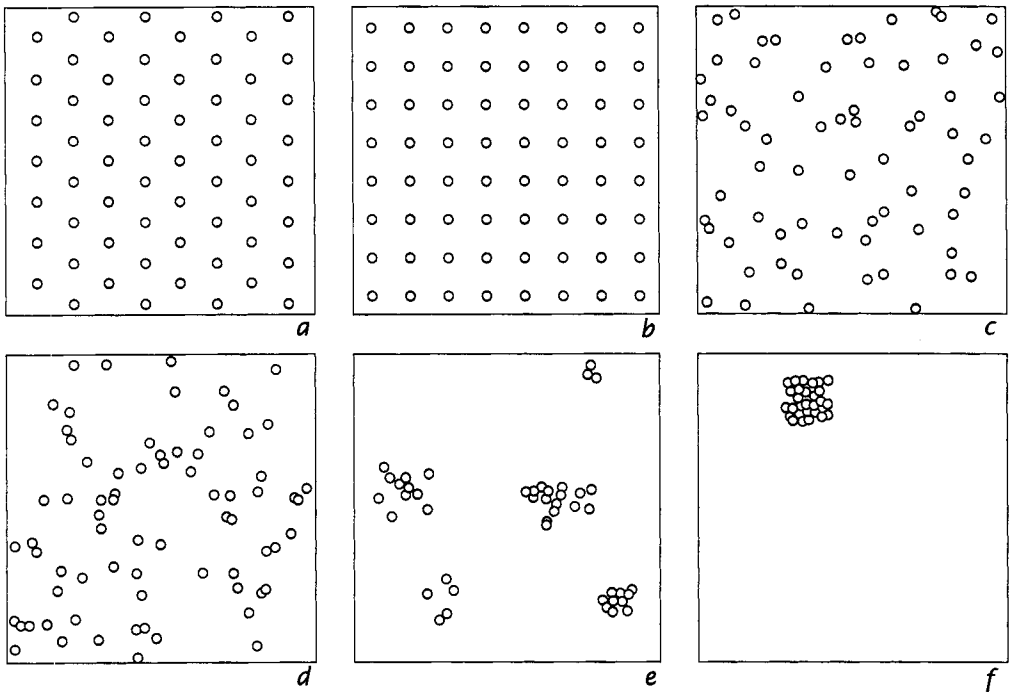


Figure 5–9. Nearest-neighbor statistics, R, for patterns of points on maps. (*a*) Points in a regular hexagonal network, $R = 2.15$. (*b*) Points in a regular square network, $R = 2.00$. (*c*) Points placed randomly within regular hexagonal cells, $R = 1.26$. (*d*) Points placed at random locations, $R = 0.91$. (*e*) Points placed randomly within five random clusters, $R = 0.34$. (*f*) Points placed randomly within a single cluster, $R = 0.13$. Point density, λ, is the same for all patterns. From Olea (1982).

is equidistant from six other points. **Figure 5–9** shows a series of patterns with different values of the nearest-neighbor statistic, all having the same point density.

We will illustrate the application of the nearest-neighbor method using the map shown in **Figure 5–10**. The "map" actually represents a polished facing stone on the front of a bank in a university town. It provides an interesting subject of study for an igneous petrology class. The stone is black anorthosite and contains small, scattered, euhedral crystals of magnetite. The instructor uses the slab to demonstrate a variety of topics, including examples of numerical techniques in petrography. For pedagogical purposes, it has been decreed that the slab is mounted in its original orientation. That is, it represents a vertical surface; "down" is toward the bottom of the slab. The map shows the location of all visible magnetite grains on the surface. Coordinates of each grain, in centimeters from the lower left corner of the slab, are listed in file BANK.TXT. Are magnetite grains uniformly distributed across the surface, or do they tend to be clustered? Is the density of crystals greater near the bottom of the slab than near the top? These and similar questions are of great importance in determining the petrogenesis of an igneous rock, and can be effectively investigated using the techniques we have discussed. Test the hypothesis of uniform, random distribution of crystals by both quadrat and nearest-neighbor analysis. This problem may be done by hand by measuring distances directly on **Figure 5–10**, or the distances may be computed using the

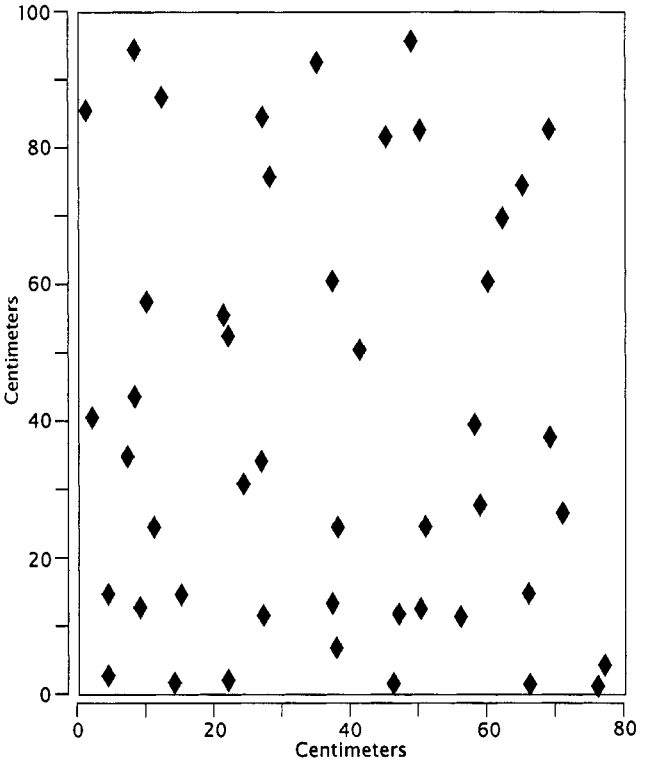


Figure 5–10. Representation of a polished slab of anorthosite facing stone showing locations of magnetite crystals listed in file BANK.TXT.

coordinates in file BANK.TXT. Ripley (1981, p. 175–181) gives an exhaustive analysis of these data, using a variety of techniques.

Distribution of Lines

Some naturally occurring patterns are composed of lines, such as lineaments seen on satellite images, the tracery of joints exposed on a weathered granite surface, or the microfractures seen in a thin section of a deformed rock. Just as a set of points can form a pattern that ranges from uniform to tightly clustered, so can sets of lines. Of course, lines are more complex than points because they possess length and orientation, as well as location. Their analysis is correspondingly more difficult, and statistical methods suitable for the study of patterns of lines seem less well developed than those applied to patterns of points. Few studies have examined the distribution of lengths of lines, except for some work on the lognormal distribution (Aitchison and Brown, 1969). A small number of workers have investigated the spacing between lines in a pattern, a problem analogous to nearest-neighbor analysis of points (Miles, 1964; Dacey, 1967). A much larger body of literature exists on the orientation of lines, a topic we will consider in the next section.

We can define a random pattern of lines as one in which any line is equally likely to cross any location, and any orientation of the crossing line is also equally likely. Such random patterns can be generated in many ways; one procedure consists of

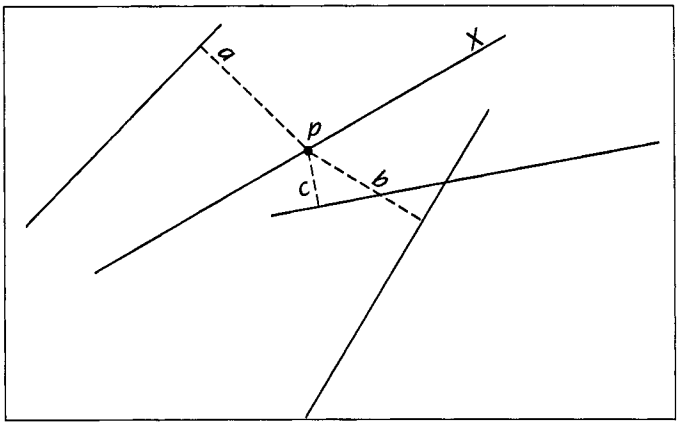


Figure 5–11. Calculation of nearest-neighbor distances between lines. Point p is chosen at random on a line X. Dashed lines a, b, and c are perpendiculars drawn from point p to nearby lines. The shortest of these, perpendicular line c, is the distance to the nearest neighbor of line X. The process is repeated to find the nearest-neighbor distances for all lines.

choosing two pairs of coordinates from a random number table, then drawing a line through them. Another consists of drawing a radius at a randomly chosen angle, measuring out along the radius a random distance from the center, then constructing a perpendicular to the radial line. Repeating either procedure will result in patterns of lines that are statistically indistinguishable.

We can define a measure of line density that is analogous to λ, the point density:

$$\lambda = L/A \tag{5.32}$$

The quantity L is simply the total length of lines on the map, which has an area A. λ is the parameter that determines the form of the Poisson distribution; as we would expect, the Poisson model describes the distribution of many properties of a pattern formed by random lines.

The distribution of distances between pairs of lines can be examined by calculating a nearest-neighbor measure. We must first randomly pick a point on each of the lines in the map. From each point, the distance is measured to the nearest line, in a direction perpendicular to that line. The mean nearest-neighbor distance $\overline{d}$ is the average of these measurements. The procedure is illustrated in **Figure 5–11**.

Dacey (1967) has determined that the expected nearest-neighbor distance $\overline{\delta}$ for a pattern of random lines is

$$\overline{\delta} = \frac{0.31831}{\lambda} \tag{5.33}$$

and that the expected variance is

$$\sigma_{\overline{\delta}}^2 = \frac{0.10132}{\lambda^2} \tag{5.34}$$

From the expected variance and the number of lines in the pattern, we can find the standard error of our estimate of the mean nearest-neighbor distance. The standard error is

$$s_e = \sqrt{\frac{\sigma_{\overline{\delta}}^2}{n}} \tag{5.35}$$

This allows us to calculate a simple z-statistic for testing the significance of the difference between the expected and observed mean nearest-neighbor distance:

$$z = \frac{\bar{d} - \bar{\delta}}{s_e} \tag{5.36}$$

The test is two-tailed; if the value of z is not significant, we conclude that the observed pattern of lines cannot be distinguished from a pattern generated by a random (Poisson) process. We can also create a nearest-neighbor index identical to that used for point patterns by taking the ratio of the observed and expected mean nearest-neighbor distances, or $\bar{d}/\bar{\delta}$. The index is interpreted exactly as is the index for point patterns.

This test will work for sets of lines that are straight or curved, provided the lines do not reverse direction frequently. Also, the lines should be at least one and one-half times longer than the average distance between the lines. If the number of lines on the map is small, the estimated density should be adjusted by the factor $(n-1)/n$, where n is the number of lines in the pattern. The estimate of the line density is, therefore

$$\lambda = \frac{(n-1)L}{nA} \tag{5.37}$$

A simple alternative way of investigating the nature of a set of lines on a map involves converting the two-dimensional pattern into a one-dimensional sequence. We can do this by drawing a ***sampling line*** at random across the map and noting where the line intersects the lines in the pattern. The distribution of intervals between the points of intersection along the sampling line will provide information about the spatial pattern. We can test this one-dimensional sequence using methods presented in Chapter 4. If a single sampling line does not provide enough intersections for a valid test, we can draw a randomly oriented continuation of the sampling line from the point where the sampling line intersects the last line on the map, and a second randomly oriented continuation from the last line on the map intersected by this continuation, and so on (**Fig. 5–12**). The zigzag path of the sampling line is a ***random walk***, and the succession of intersections can be

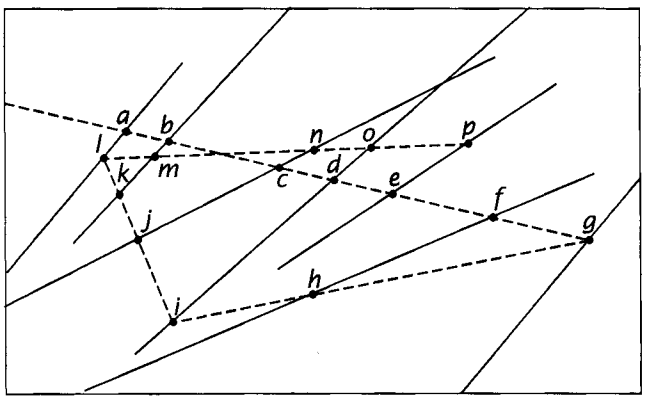


Figure 5–12. Random-walk sampling line (dashed) drawn across pattern of lines on a map. Intersections along sampling line form a sequence of intervals, $a-b$, $b-c$, ..., $o-p$, that can be tested for randomness.

treated as though they occurred along a single, straight sampling line. This and other methods for investigating the density of patterns of lines are reviewed by Getis and Boots (1978). A computer program for computing nearest-neighbor distances, orientation, and other statistical measures of patterns of lines is given by Clark and Wilson (1994).

Analysis of Directional Data

Directional data are an important category of geologic information. Bedding planes, fault surfaces, and joints are all characterized by their attitudes, expressed as strikes and dips. Glacial striations, sole marks, fossil shells, and water-laid pebbles may have preferred orientations. Aerial and satellite photographs may show oriented linear patterns. These features can be measured and treated quantitatively like measurements of other geologic properties, but it is necessary to use special statistics that reflect the circular (or spherical) nature of directional data.

Following the practice of geographers, we can distinguish between ***directional*** and ***oriented*** features. Suppose a car is traveling north along a highway; the car's motion has direction, while the highway itself has only a north-south orientation. Strikes of outcrops and the traces of faults are examples of geologic observations that are oriented, while drumlins and certain fossils such as high-spired gastropods have clear directional characteristics.

We may also distinguish observations that are distributed on a circle, such as paleocurrent measurements, and those that are distributed spherically, such as measurements of metamorphic fabric. The former data are conventionally shown as ***rose diagrams***, a form of circular histogram, while the latter are plotted as points on a projection of a hemisphere. Although geologists have plotted directional measurements in these forms for many years, they have not used formal statistical techniques extensively to test the veracity of the conclusions they have drawn from their diagrams. This is doubly unfortunate; not only are these statistical tests useful, but the development of many of the procedures was originally inspired by problems in the Earth sciences.

Figure 5–13 is a map of glacial striations measured in a small area of southern Finland; the measurements are listed in **Table 5–4** and contained in file FINLAND.TXT. The directions indicated by the striations can be expressed by plotting them as unit vectors or on a circle of unit radius as in **Figure 5–14 a**. If the circle is subdivided into segments and the number of vectors within each segment counted, the results can be expressed as the rose diagram, or circular histogram, shown as **Figure 5–14 b**.

Nemec (1988) pointed out that many of the rose diagrams published by geologists violate the basic principal on which histograms are based and, as a consequence, the diagrams are visually misleading. Recall that areas of columns in a histogram are proportional to the number (or percentage) of observations occurring in the corresponding intervals. For a rose diagram to correctly represent a circular distribution, it must be constructed so that the areas of the wedges (or "petals") of the diagram are proportional to class frequencies. Unfortunately, most rose diagrams are drawn so that the radii of the wedges are proportional to frequency. The resulting distortion may suggest the presence of a strong directional trend where none exists (**Fig. 5–15**).

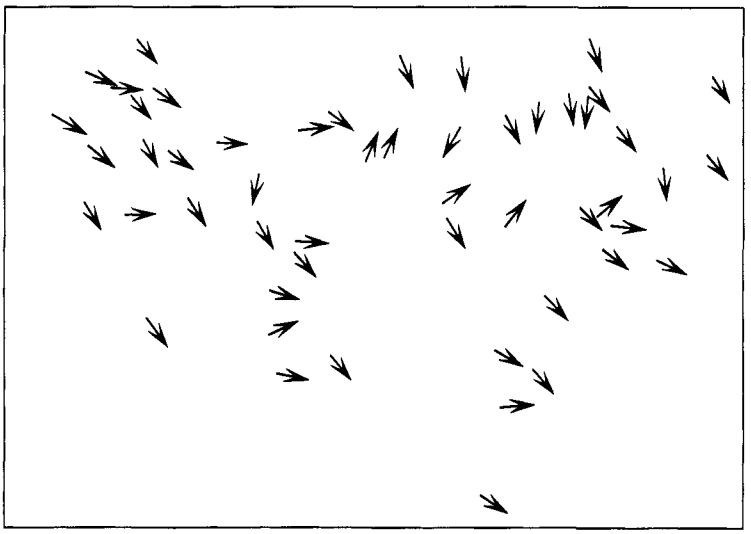


Figure 5–13. Map showing location and direction of 51 measurements of glacial striations in a 35-km^2 area of southern Finland.

Table 5–4. *Vector directions of glacial striations measured in an area of southern Finland; measurements given in degrees clockwise from north.*

23	105	127	144	171
27	113	127	145	172
53	113	128	145	179
58	114	128	146	181
64	117	129	153	186
83	121	132	155	190
85	123	132	155	212
88	125	132	155	
93	126	134	157	
99	126	135	163	
100	126	137	165	

If we define a radius for a sector of a rose diagram that represents either one observation, or 1%, we can easily calculate the appropriate radii that represent any number of observations or relative frequencies,

$$r_f = r_u\sqrt{f} \tag{5.38}$$

where r_u is the unit radius representing one observation or 1%, f is the frequency (in counts or percent) of observations within a class, and r_f is the radius of the class sector. In other words, the radius should be proportional to the square root of the frequency rather than to the frequency itself.

Rose diagrams, even if properly scaled, suffer from the same problems as ordinary histograms; their appearance is extremely sensitive to the choice of class widths and starting point and they exhibit variations similar to the histogram

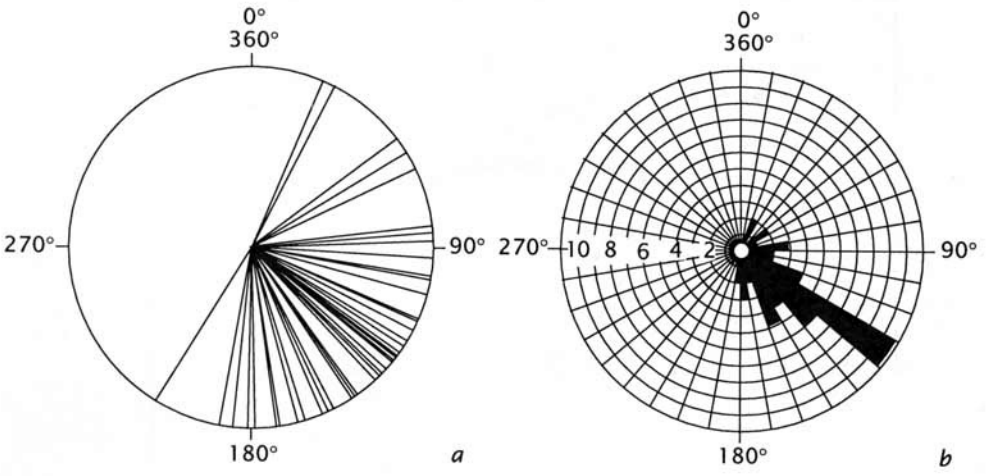


Figure 5–14. Directions of glacial striations shown on Figure 5–13. (*a*) Directions plotted as unit vectors. (*b*) Directions plotted as a rose diagram showing numbers of vectors within successive 10° segments.

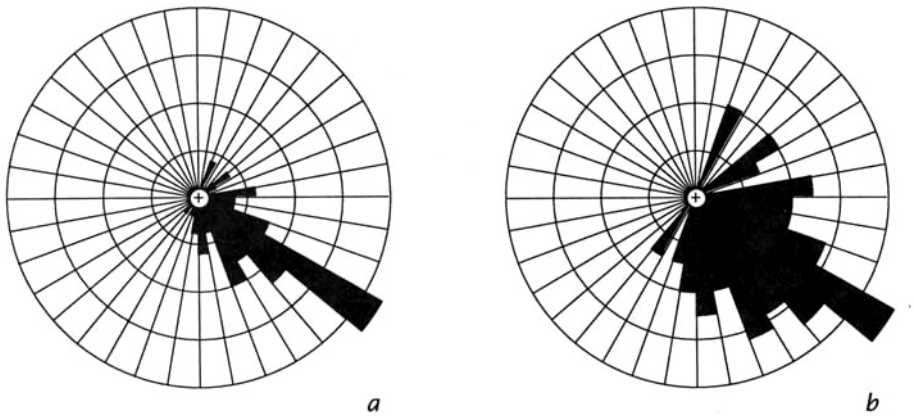


Figure 5–15. Rose diagram of glacial striations shown on Figure 5–13 plotted in 10° segments. (*a*) Length of petals proportional to frequency. (*b*) Area of petals proportional to frequency.

examples shown in **Figure 2–11** on p. 30. Wells (1999) provides a computer program that quickly constructs rose diagrams with different conventions and also includes an assortment of graphical alternatives that may be superior to conventional rose diagrams for some uses (**Fig. 5–16**).

To compute statistics that describe characteristics of an entire set of vectors, we must work directly with the individual directional measurements rather than with a graphical summary such as a rose diagram. (Note that the following discussion uses geological and geographic conventions in which angles are measured clockwise from north, or from the positive end of the Y-axis. Many papers on directional statistics follow a mathematical convention in which angles are measured counterclockwise from east, or from the positive end of the X-axis.)

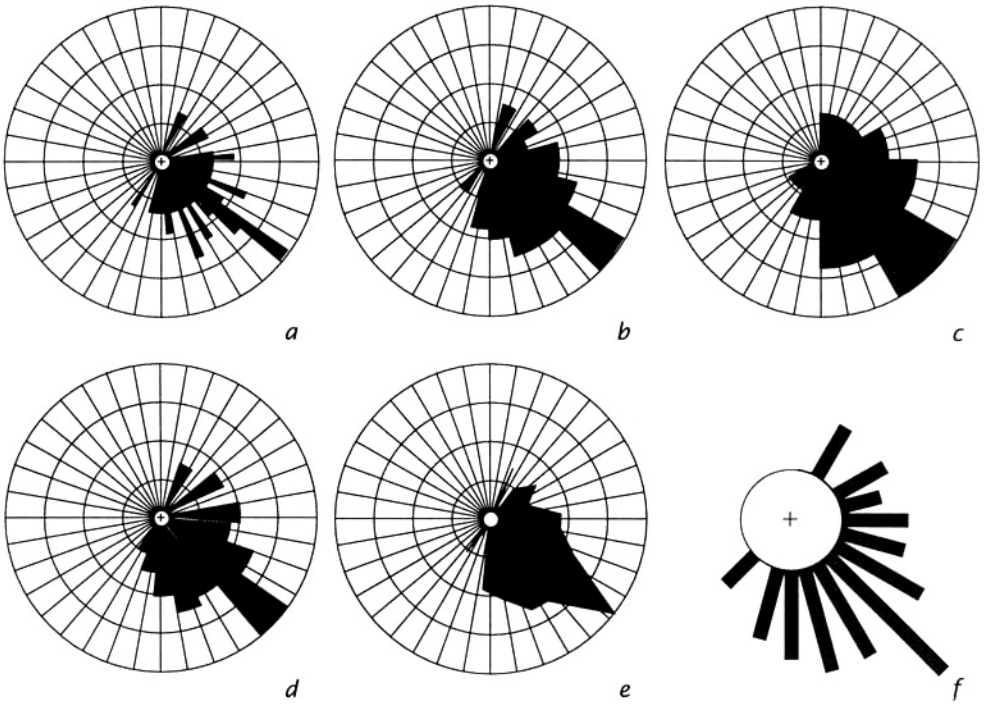


Figure 5–16. Effect of choice of segment size and origin on appearance of rose diagrams. Data are directions of glacial striations from file FINLAND.TXT: (*a*) 5° segments, 0° origin, outer ring 20%; (*b*) 15° segments, 0° origin, outer ring 30%; (*c*) 30° segments, 0° origin, outer ring 40%; (*d*) 15° segments, 10° origin—compare to (*b*). Alternative graphical forms include (*e*) kite diagram, 15° segments, 0° origin—sometimes used in statistical presentations; (*f*) circular histogram, 15° segments, 0° origin—widely used to plot wind directions.

The dominant direction in a set of vectors can be found by computing the ***vector resultant***. The X- and Y-coordinates of the end point of a unit vector whose direction is given by the angle θ are

$$\begin{aligned} X_i &= \cos\theta_i \\ Y_i &= \sin\theta_i \end{aligned} \qquad \textbf{(5.39)}$$

Three such vectors are shown plotted in **Figure 5–17**. Also shown is the vector resultant, R, obtained by summing the sines and cosines of the individual vectors:

$$\begin{aligned} X_r &= \textstyle\sum_{i=1}^{n} \cos\theta_i \\ Y_r &= \textstyle\sum_{i=1}^{n} \sin\theta_i \end{aligned} \qquad \textbf{(5.40)}$$

From the resultant, we can obtain the ***mean direction***, $\overline{\theta}$, which is the angular average of all of the vectors in a sample. It is directly analogous to the mean value of a set of scalar measurements

$$\overline{\theta} = \tan^{-1}(Y_r/X_r) = \tan^{-1}\left(\textstyle\sum_{i=1}^{n} \sin\theta_i \Big/ \sum_{i=1}^{n} \cos\theta_i\right) \qquad \textbf{(5.41)}$$

Obviously, the magnitude or length of the resultant depends in part on the amount of dispersion in the sample of vectors, but it also depends upon the number of

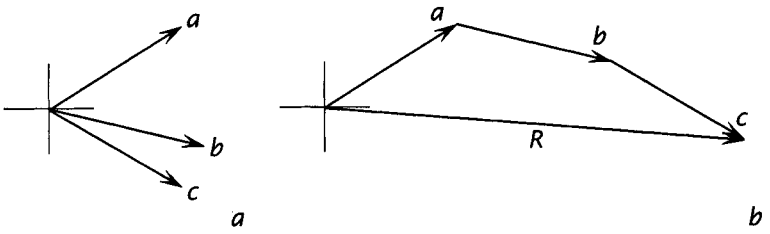


Figure 5–17. Determination of mean direction of a set of unit vectors. (*a*) Three vectors taken from Figure 5–16. (*b*) Vector resultant, R, obtained by combining the three unit vectors. Order of combination is immaterial.

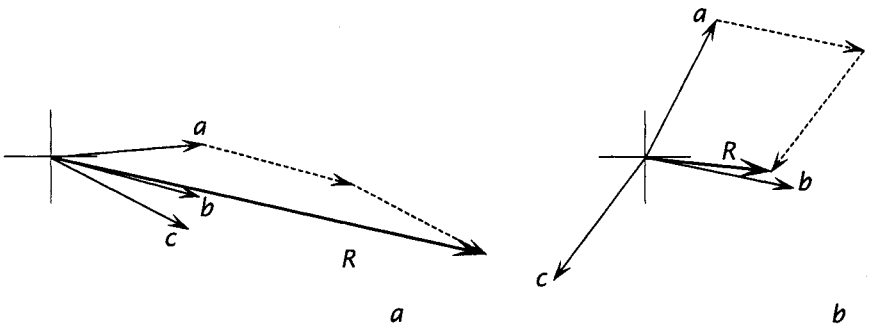


Figure 5–18. Use of length of resultant to express dispersion in a collection of unit vectors. (*a*) Three vectors tightly clustered around a common direction. Resultant R is relatively long, approaching the value of n. (*b*) Three widely dispersed vectors; resultant length is less than 1.0.

vectors. In order to compare resultants from samples of different sizes, they must be converted into a standardized form. This is done simply by dividing the coordinates of the resultant by the number of observations, n

$$\begin{aligned} \overline{C} &= X_r/n = \tfrac{1}{n}\textstyle\sum_{i=1}^{n} \cos\theta_i \\ \overline{S} &= Y_r/n = \tfrac{1}{n}\textstyle\sum_{i=1}^{n} \sin\theta_i \end{aligned} \qquad \textbf{(5.42)}$$

Note that these coordinates also define the centroid of the end points of the individual unit vectors.

The resultant provides information not only about the average direction of a set of vectors, but also on the spread of the vectors about this average. **Figure 5–18 a** shows three vectors that deviate only slightly from the mean direction. The resultant is almost equal in length to the sum of the lengths of the three vectors. In contrast, three vectors in **Figure 5–18 b** are widely dispersed; their resultant is very short. The length of the resultant, R, is given by the Pythagorean theorem:

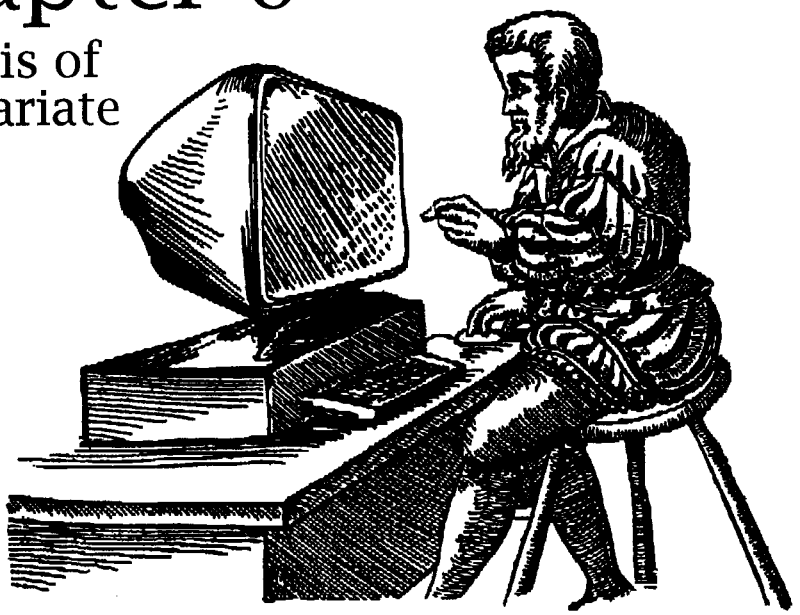
$$R = \sqrt{X_r^2 + Y_r^2} = \sqrt{\left(\textstyle\sum_{i=1}^{n} \cos\theta_i\right)^2 + \left(\textstyle\sum_{i=1}^{n} \sin\theta_i\right)^2} \qquad \textbf{(5.43)}$$

The length of the resultant can be standardized by dividing by the number of observations. The standardized resultant length can also be found from the standardized end points

$$\overline{R} = \frac{R}{n} = \sqrt{\overline{C}^2 + \overline{S}^2} \qquad \textbf{(5.44)}$$

Chapter 6

Analysis of Multivariate Data



In previous chapters we have considered the analysis of data consisting of only a single variable measured on each specimen or observational unit. In Chapters 4 and 5 we also considered the influence of the temporal or geographic coordinates of the sample points. We will now examine techniques for the analysis of multivariate data, in which each observational unit is characterized by several variables. Multivariate methods allow us to consider changes in several properties simultaneously. Examples of data appropriate for multivariate analysis abound in geology. They include chemical analyses, where the variables may be percentage compositions or parts per million of trace elements; measures on streams, such as discharge, suspended sediment load, depth, dissolved solids, pH, and oxygen content; and paleontologic variables, perhaps a large number of measurements made on specimens of an organism. Dozens of other examples quickly spring to mind. Some are simple extensions of problems we have considered previously; others are entirely new classes of problems.

Multivariate methods are extremely powerful, for they allow the researcher to manipulate more variables than can otherwise be assimilated. They are complicated, however, both in their theoretical structure and in their operational methodology. For some of the procedures, statistical theory and tests have been worked out only for the most restrictive set of assumptions. The nature and behavior of the tests under more relaxed, general assumptions (such as those necessary for most real-world problems) are inadequately known. In fact, some of the procedures we will consider have no theoretical statistical basis at all, and tests of significance have yet to be devised. Nevertheless, these methods seem to hold the most promise for fruitful returns in geological investigations. Most of the problems in geology involve complex and interacting forces which are impossible to isolate and study individually. Often a meaningful decision as to the relative worth of one of a number of possible variables cannot be made. The best course of action frequently is

to examine as many facets of a problem as possible, and sort out, *a posteriori*, the major factors. The methods discussed in this chapter can be a significant help.

Multiple Regression

The first topic we will consider in our final chapter is actually a familiar subject under a new and more general guise. This is multiple regression, which includes polynomial curve fitting (discussed in Chapter 4) and trend-surface analysis (discussed in Chapter 5). However, we will now remove the restrictions that limited us to considerations of change as a function of temporal or spatial coordinates. Any observed variable can be considered to be a function of any other variable measured on the same samples. In Chapter 4 we considered changes in moisture content that occurred with changes in depth in the sediment. We could equally well have measured the montmorillonite content of the sediment in the core and examined the changes in water content that may accompany changes in montmorillonite percentage. In fact we could have measured several variables, perhaps organic content, mean grain size, and bulk density, and we could have examined the differences in water content associated with changes in each or all of these variables. In a sense, variables may be considered as dimensions, and their values as coordinates, so we can envision changes occurring "along" a dimension defined by a variable such as mineral content. Casting variables as dimensions is nothing new; we perform this every time we plot two variables against one another, because we are substituting spatial scales in the plot for the original scales on which the variables were measured. Such interchangeability is explicit in the references to "p-dimensional space" which abound in the literature of multivariate analysis. Just as trend surfaces are a generalization of curve-fitting procedures to two-dimensional space, multiple regression is a further generalization to "many-dimensional" space.

We will not consider multiple regression in great detail because the theoretical and computational essentials have been presented in earlier chapters. You will recall from Chapter 4 that polynomial regressions (having one independent variable) can be represented in a model equation of the general form

$$y_i = \beta_0 + \beta_1 x_{1i} + \beta_2 x_{1i}^2 \cdots + \beta_m x_{1i}^m + \varepsilon_i \qquad \textbf{(6.1)}$$

The model states that the value of a dependent variable, y_i, at a location i is equal to a constant term plus the sum of a series of powers of an independent variable, x_{1i}, also observed at location i, plus a random error that is unique for location i. A least-squares solution to a linear equation of this type can be found by solving a set of normal equations for the β coefficients. These can be expressed in matrix form as

$$\mathbf{S_{xy}} = \mathbf{S_{xx}}\,\mathbf{b} \qquad \textbf{(6.2)}$$

with a solution

$$\mathbf{b} = \mathbf{S_{xx}^{-1}}\,\mathbf{S_{xy}} \qquad \textbf{(6.3)}$$

where $\mathbf{S_{xy}}$ is a column matrix of the sums of cross products of y, with $x_1, x_1^2, \ldots, x_1^m$; $\mathbf{S_{xx}}$ is a matrix of sums of squares and cross products of the $x_1, x_1^2, \ldots, x_1^m$ powers; and $\mathbf{b}$ estimates $\boldsymbol{\beta}$, the column matrix of unknown regression coefficients. In Chapter 4, we found the entries in the various matrices by labeling rows and columns and cross multiplying.

Although we regarded this problem as involving only one independent variable (or two, in the case of trend-surface analysis as discussed in Chapter 5), it can be regarded as containing m independent variables. This can readily be seen if we rewrite the model equation as

$$y_i = \beta_0 + \beta_1 x_{1i} + \beta_2 x_{2i} + \cdots + \beta_m x_{mi} + \varepsilon_i \tag{6.4}$$

and define the variables as $x_1 = x_1$, $x_2 = x_1^2$, $x_3 = x_1^3$, and so forth. Thus, the regression procedures we have considered up to this point have simply involved the definition of the independent variables in a specific manner.

A regression of any m independent variables upon a dependent variable can be expressed as in Equation (6.4). The normal equations that will yield a least-squares solution can be found by appropriate labeling of the rows and columns of the matrix equation and cross multiplying to find the entries in the body of the matrix. For three independent variables, we obtain

$$\begin{array}{c} \\ X_0 \\ X_1 \\ X_2 \\ X_3 \end{array} \begin{array}{c} \begin{array}{cccc} X_0 & X_1 & X_2 & X_3 \end{array} \\ \begin{bmatrix} & & & \\ & & & \\ & & & \\ & & & \end{bmatrix} \end{array} \begin{bmatrix} b_0 \\ b_1 \\ b_2 \\ b_3 \end{bmatrix} = \begin{array}{c} Y \\ \begin{bmatrix} \\ \\ \\ \end{bmatrix} \end{array}$$

where, again, x_0 is a dummy variable equal to 1 for every observation. The matrix equation, after cross multiplication, is

$$\begin{bmatrix} n & \sum x_1 & \sum x_2 & \sum x_3 \\ \sum x_1 & \sum x_1^2 & \sum x_1 x_2 & \sum x_1 x_3 \\ \sum x_2 & \sum x_1 x_2 & \sum x_2^2 & \sum x_2 x_3 \\ \sum x_3 & \sum x_1 x_3 & \sum x_2 x_3 & \sum x_3^2 \end{bmatrix} \begin{bmatrix} b_0 \\ b_1 \\ b_2 \\ b_3 \end{bmatrix} = \begin{bmatrix} \sum y \\ \sum x_1 y \\ \sum x_2 y \\ \sum x_3 y \end{bmatrix} \tag{6.5}$$

The β's in the regression model are estimated by the b's, the sample ***partial regression coefficients***. They are called partial regression coefficients because each gives the rate of change (or slope) in the dependent variable for a unit change in that particular independent variable, *provided* all other independent variables are held constant. Some statistics books emphasize this point by using the notation

$$y_i = b_0 + b_{1.23} x_{1i} + b_{2.13} x_{2i} + b_{3.12} x_{3i} + \varepsilon_i$$

The coefficient $b_{1.23}$, for example, is read "the regression coefficient of variable x_1 on y as variables x_2 and x_3 remain constant." In general, these coefficients will differ from the ***total regression coefficients***, which are the simple regressions of each individual x variable on the dependent y variable. We ordinarily expect multiple regression coefficients to account for more of the total variation in y than will any of the total regression coefficients. This is because multiple regression considers all possible interactions within combinations of variables as well as the variables themselves.

We will consider a problem in geomorphology to illustrate a typical application of multiple regression. For this study, a well-dissected area of relatively homogeneous geology was selected in eastern Kentucky. The study region contains many drainage basins of differing sizes; from these, all third-order basins were chosen,

and several variables were measured on each. The order of a drainage basin is defined by the number of successive levels of junctions on its stream from the stream's sources to the point where it joins another stream of equal or higher order. Thus, a third-order basin has two levels of junctions within its boundaries. Basin size, however, may be defined by many alternative methods. One of these is basin magnitude, which essentially is a count of the number of sources in the basin. A collection of basins of specified order may contain many different magnitudes. The relationship between magnitude and order of streams in drainage basins is shown in **Figure 6–1**. Seven variables were measured on the collection of third-order basins:

Y — Basin magnitude, defined by the number of sources.
X_1 — Elevation of the basin outlet, in feet.
X_2 — Relief of the basin, in feet.
X_3 — Basin area, in square miles.
X_4 — Total length of the stream in the basin, in miles.
X_5 — Drainage density, defined as total length of stream in basin/basin area.
X_6 — Basin shape, measured as the ratio of inscribed to circumscribed circles.

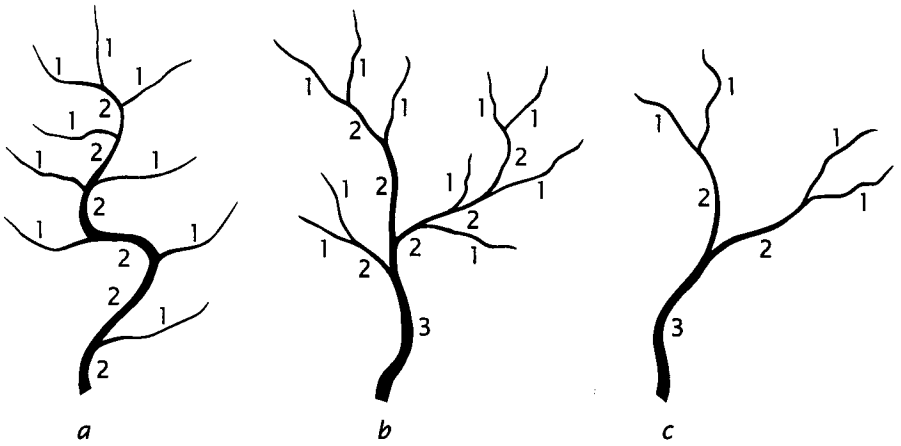


Figure 6–1. Contrast between stream magnitude and stream order. (*a*) Tenth-magnitude stream of second order. (*b*) Tenth-magnitude stream of third order. (*c*) Fourth-magnitude stream of third order. Magnitude is based on number of joining streams; order is based on succession of joining.

Our problem is to determine the influence of the six independent X variables on variable Y. Multiple regression, using basin magnitude as the dependent variable, is an appropriate technique. From the regression, the influence that all the variables have on basin magnitude can be assessed. File KENTUCKY.TXT contains measurements on these variables for 50 third-order basins in eastern Kentucky, taken from Krumbein and Shreve (1970). The significance of the linear relationship can be tested by analysis-of-variance methods presented in Chapter 4. **Table 4–9** (p. 197), for example, outlines the ANOVA for simple linear regression which may be expanded to multiple regression by changing the various degrees of freedom to account for additional variables. The modified ANOVA is shown in **Table 6–1**. The

Table 6–1. ANOVA for multiple regression with m independent variables.

Source of Variation	Sum of Squares	Degrees of Freedom	Mean Squares	F-Test
Linear Regression	SS_R	m	MS_R	MS_R / MS_D
Deviation	SS_D	$n - m - 1$	MS_D	
Total Variation	SS_T	$n - 1$		

Table 6–2. Completed ANOVA for the significance of regression of six geomorphic variables on basin magnitude.[1]

Source of Variation	Sum of Squares	Degrees of Freedom	Mean Squares	F-Test
Linear Regression	1800.70	6	300.12	11.38**
Deviation	1134.12	43	26.38	
Total Variation	2934.82	49		

[1] Regression equation: $y_i = -2.24 + 0.01\ X_{1i} + 0.02\ X_{2i} - 23.28\ X_{3i} + 6.26\ X_{4i} - 0.20\ X_{5i} - 11.66\ X_{6i}$. R = 0.78.

** $p < 0.0001$ (highly significant).

completed ANOVA for multiple regression on basin magnitude is shown in **Table 6–2**. The regression coefficients are also shown.

In multiple-regression problems, we usually are interested in the relative effectiveness of the independent variables as predictors of the dependent variable. We cannot determine this from a direct examination of the regression coefficients, however, because their magnitudes are dependent upon the magnitudes of the variables themselves, which in part reflect the units of measurement. This is apparent in trend-surface analysis, where coefficients of higher orders almost invariably decrease in absolute size, even though higher orders may make greater contributions to the trend than lower orders. This results from the fact that a geographic coordinate, raised to a power as it is in high orders, is much larger in magnitude than the original coordinate. The higher order regression coefficients become correspondingly smaller.

Fortunately, it is easy to standardize the partial regression coefficients by converting them to units of standard deviation. The standard partial regression coefficients, B_k, are found by

$$B_k = b_k \frac{s_k}{s_y} \tag{6.6}$$

where s_k is the standard deviation of variable x_k and s_y is the standard deviation of y. Because the standard partial regression coefficients are all expressed in units

of standard deviation, they may be compared directly with each other to determine the most effective variables.

To compute the matrix of sums of squares and products necessary in the normal equation set, we found the diagonal entries, $\sum x_k^2$. It is a simple matter to convert these sums of squares to corrected sums of squares, SS_k, and then to the standard deviations necessary to compute the partial correlation coefficients. However, it is possible to solve the normal equations in a manner that will yield the standardized partial regression coefficients directly, and gain an important computational advantage in the process.

The major sources of error in multiple regression occur in the creation of the entries in the $\mathbf{S_{XX}}$ matrix and during the inversion process. The sums of squares of the variables may become so large that significant digits are lost by truncation. If the entries in the $\mathbf{S_{XX}}$ matrix differ greatly in their magnitudes, an additional loss of digits may occur during inversion, especially if high correlations exist among the variables. Some computer programs may be capable of retaining only one or two significant digits in the coefficients, and with certain data sets retention may even be worse. Studies have shown that calculations using double-precision arithmetic may not be sufficient to overcome this problem. However, a few simple modifications in our computational procedure will gain us two to six significant digits during computation and greatly increase the accuracy of the computed regression (Longley, 1967, p. 821-827).

The most obvious step that can be taken is to convert all observations to deviations from the mean. This reduces the absolute magnitude of variables and centers them about a common mean of zero. As an inevitable consequence, the coefficient b_0 will become zero, so the matrix equation can be reduced by one row and one column. This simple step may gain several significant digits. However, we also may reduce the size of entries in the matrix still further by converting them all to correlations. This is equivalent to expressing the original variables in the standard normal form of zero mean and unit standard deviation. The matrix equation for regression then has the form

$$\mathbf{R_{XX}\,B = R_{XY}} \tag{6.7}$$

which can be solved by the operation

$$\mathbf{B = R_{XX}^{-1}\,R_{XY}} \tag{6.8}$$

where $\mathbf{R_{XY}}$ represents the column vector of correlations between y and the x_k independent variables. The $m \times m$ matrix of correlations between the x_k variables is represented by $\mathbf{R_{XX}}$. For example, the normal equation for three independent variables has the form

$$\begin{bmatrix} 1 & r_{12} & r_{13} \\ r_{21} & 1 & r_{23} \\ r_{31} & r_{32} & 1 \end{bmatrix} \begin{bmatrix} B_1 \\ B_2 \\ B_3 \end{bmatrix} = \begin{bmatrix} r_{x_1y} \\ r_{x_2y} \\ r_{x_3y} \end{bmatrix} \tag{6.9}$$

Note that the equation has one less row and column than the equivalent equation using the original variables (Eq. 6.5).

Computing the regression equation in standardized form has the disadvantage that the correlation matrix must be created first, increasing the computational effort. In order to preserve accuracy, the correlations must be calculated using the

definitional equation for the sums of products (Eq. 2.23; p. 40) rather than with the computational form for correlation given in Equation (2.28). This is because Equation (2.28) involves squaring the quantities $\sum x_j^2$ and $\sum x_k^2$. If these sums are large, the squares may be inaccurate because of truncation. This problem is avoided if the means are subtracted from each observation prior to calculation of the sums of squares. The sums of squares are then found by Equations (2.19) and (2.23). This process requires that the data be handled twice—first to calculate the means, and then to subtract out this quantity during calculations. Although this involves a significant increase in labor if computations are performed by hand, the additional effort is trivial on a digital computer. Also, the resulting coefficients must be "unstandardized" if they are to be used in a predictive equation with raw data. However, these disadvantages are more than offset by the increased stability and accuracy of the matrix solution, and the standardized coefficients provide a way of assessing the importance of individual variables in the regression. Partial regression coefficients can be derived from the standardized partial regression coefficients by the transformation

$$b_k = B_k \frac{s_y}{s_k} \tag{6.10}$$

The constant term, b_0, can be found by

$$b_0 = \overline{Y} - b_1\overline{X}_1 - b_2\overline{X}_2 - \ldots - b_m\overline{X}_m \tag{6.11}$$

Although the various sums of squares change if the data are standardized (*i.e.*, the correlation form of the matrix equation is used), the ratios of the sums of squares remain the same. Therefore, tests of significance based on standardized regression are identical to those based on an unstandardized regression. Quantities such as the coefficient of multiple correlation (R) and percentage of goodness of fit (100% R^2) also remain unchanged.

We can compare the partial regression coefficients between basin magnitude and the other six basin properties in both raw and standardized form:

$$\mathbf{b}' = \begin{bmatrix} -2.244 & 0.005 & 0.226 & -0.233 & 0.063 & -0.002 & -0.117 \end{bmatrix}$$

$$\mathbf{B}' = \begin{bmatrix} 0.000 & 0.049 & 0.284 & -0.458 & 0.975 & -0.120 & -0.163 \end{bmatrix}$$

Although the standardized partial regression coefficients suggest that the basin properties having the most pronounced relationship with basin magnitude are x_2 (relief), x_3 (area), and x_4 (stream length), these values do not take into account the uncertainty associated with each estimated parameter. The easiest way to consider this aspect is by expanding the analysis of variance to test the significance of each independent variable.

The sum of squares attributable to a single variable, x_j, can be determined by calculating $SS_{R(m)}$ for the regression with all m variables, calculating $SS_{R(m-1)}$, which is the sum of squares for regression using all variables except the jth variable, then finding the difference. This process can be repeated for each independent variable in turn, in order to assess the contribution that each makes to the total regression. Fortunately, there is an easier way to calculate the individual regression sums of squares, which simply requires dividing the square of each partial regression coefficient by the diagonal elements of $\mathbf{S}_{\mathbf{XX}}^{-1}$ that correspond to each of the variables. If we designate $\mathbf{C}_{\mathbf{XX}} = \mathbf{S}_{\mathbf{XX}}^{-1}$, then

$$SS_{R(x_j)} = b_j^2 / c_{jj} \tag{6.12}$$

Once the regression sums of squares of the individual variables have been calculated, they can be entered into an expanded ANOVA table such as that shown in **Table 6–3** and tested for significance. The F-test ratios are formed from the mean squares due to partial regression with each of the individual variables in the numerators, and the mean square due to deviation from the regression model as the denominator. Each F-test has 1 and $(n - m - 1)$ associated degrees of freedom. The F-tests will not change if the calculations are based on standardized partial regression coefficients.

Table 6–3. ANOVA for testing the significance of partial regression of individual variables.

Source of Variation	Sum of Squares	Degrees of Freedom	Mean Squares	F-Test
Regression	SS_R	m	MS_R	MS_R/MS_D
Addition due to x_1	SS_{R1}	1	MS_{R1}	MS_{R1}/MS_D
...	...	...	...	...
Addition due to x_m	SS_{Rm}	1	MS_{Rm}	MS_{Rm}/MS_D
Deviation from regression	SS_D	$n - m - 1$	MS_D	
Total Variation	SS_T	$n - 1$		

A complete ANOVA for testing the significance of the partial regression of each geomorphic variable on basin magnitude is given in **Table 6–4.** Although basin relief, basin area, and stream length all have the largest standardized partial regression coefficients, the contribution to the total regression made by basin area is not statistically significant. This is because the partial regression coefficient for basin area has an associated high standard error.

Although the standardized partial regression coefficients provide a guide to the most effective variables in the regression, they are not an infallible index to the "best possible" regression equation. Suppose you examine the regression equation and decide two variables are contributing a negligible amount to the regression and can be discarded. When one of the variables is omitted and the regression is recalculated, the goodness of fit and the regression equation, of course, change. Now suppose you decide to discard the second variable; again the regression changes. But the change might be quite different from the change that would occur if the first discarded variable were still in the regression. This occurs because the interaction effects of the two discarded variables with other variables cannot be assessed without recomputing the regression. If we want to search through a large set of variables and "weed out" those which are not helpful in the problem, we must do more than simply examine the partial regression coefficients.

Table 6–4. Completed ANOVA for testing the significance of regression of individual geomorphic variables on basin magnitude.

Source of Variation	Sum of Squares	Degrees of Freedom	Mean Squares	F-Test
Regression	1800.70	6	300.12	11.38[a]
Outlet Elevation	5.69	1	5.69	0.22[b]
Basin Relief	201.43	1	201.43	7.64[c]
Basin Area	46.17	1	46.17	1.75[d]
Stream Length	243.95	1	243.95	9.25[e]
Drainage Density	22.91	1	22.91	0.87[f]
Basin Circularity	67.99	1	67.99	2.58[g]
Deviation	1134.12	43	26.38	
Total Variation	2934.82	49		

[a] $p<0.0001$ (highly significant).
[b] $p=0.645$ (not significant).
[c] $p=0.008$ (highly significant).
[d] $p=0.193$ (not significant).
[e] $p=0.004$ (highly significant).
[f] $p=0.357$ (not significant).
[g] $p=0.116$ (not significant).

Increasing the number of independent variables in the regression equation will always increase the SS_R (except in the situation where a new variable is perfectly correlated with a previous variable). However, the increase may not be significant. The loss of degrees of freedom for deviations may offset the reduction in SS_D, and actually increase the mean squares due to deviation. If this happens, the F-ratio for the significance of the regression will decrease, and the addition of another variable has actually detracted from the regression. To determine the very best possible regression (in the sense of having the most significant F-ratio), all possible combinations of the variables would have to be examined. This is possible if we are dealing with few variables, but the number of possible variable combinations is equal to $2^m - 1$, and the computational effort is formidable if m is large. Other procedures are available which yield a nearly optimal regression with much less effort. These include schemes such as the backward elimination procedure, the forward selection procedure, stepwise regression, and stagewise regression. These methods may not find identical regression equations in a large selection of possible variables, but all will produce approximately equivalent results. A consideration of each is beyond the scope of this book; we will be content with a brief description

of one of the techniques. These methods are well described in some of the texts listed in the Selected Readings at the end of the chapter, especially in Marascuilo and Levin (1983) and in Draper and Smith (1998).

The backward elimination procedure consists of computing a regression including all possible variables and selecting the least significant variable. The selection proceeds by examining the standardized partial regression coefficients for the smallest value and then recomputing the regression, omitting that variable. The significance of the deleted variable is tested by the analysis of variance shown in **Table 6–3.** If the variable is not making a significant contribution to the regression, it is permanently discarded. The reduced regression model is then fitted to the data, a new set of standardized partial regression coefficients for the reduced equation is calculated, and the process is repeated. At each step, the regression equation is reduced by one variable, until all remaining variables are significant.

It is instructive to examine the collection of six independent variables measured on river basins (file KENTUCKY.TXT) and see if any can be discarded without significantly affecting the multiple regression on basin magnitude. We can find a minimal set of regressions by examining the standardized partial regression coefficients, deleting the smallest of these, and recomputing the regression. Repeatedly running a multiple-regression program obviously is less efficient than using a stepwise computer program, but it has the advantage that every step in the process can be examined closely. When you are confident that you understand the elimination process and the changes that occur in the regression coefficients, you may turn to a more automated procedure.

Although multiple regression is "multivariate" in the sense that more than one variable is measured on each observational unit, it really is a univariate technique because we are concerned only with the variance of one variable, y. Behavior of the independent variables, the x's, is not subject to analysis.

The next topic we will consider is discriminant function analysis, which involves identification or the placing of objects into predefined groups. The discrimination between two alternative groups is a process that is computationally intermediate between univariate procedures and true multivariate methods in which many variables are considered simultaneously. Two groups, each characterized by a set of multiple variables, can be discriminated by solving a set of simultaneous equations almost identical to those involved in multiple regression. The right-hand vector of the matrix equation, however, does not contain cross products between independent variables and a single dependent variable, but rather differences between the multivariate means of the two groups that are to be discriminated.

Tests of discriminant functions involve multivariate extensions of simple univariate statistical tests of equality. These will be considered next, followed by a discussion of multivariate classification, or the sorting of objects into homogeneous groups. We will then consider eigenvector techniques, including principal component and factor analysis. The final topics will include multivariate extensions of discriminant analysis and multiple regression.

This list of topics is certainly not all-inclusive. However, the subjects have been chosen because they have found special utility in the Earth sciences. They include a wide variety of computational techniques and encompass many fundamental concepts. An understanding of the theory and operational procedures involved in these methods should provide you with a sufficient background to evaluate other multivariate techniques as well.

Discriminant Functions

One of the most widely used multivariate procedures in Earth science is the discriminant function. We will consider it at length for two reasons: discrimination is a powerful statistical tool and it can be regarded as either a way to treat univariate problems related to multiple regression, or multivariate problems related to the statistical tests we will discuss later. Discriminant functions therefore provide an additional link between univariate and multivariate statistics.

First, however, we must define the process of ***discrimination***, and carefully distinguish it from the related process of classification. Suppose we have assembled two collections of shale samples of known freshwater and saltwater origin. We may have determined their origin from an examination of their fossil content. A number of geochemical variables have been measured on each specimen, including the content of vanadium, boron, iron, and so forth. The problem is to find the linear combination of these variables that produces the maximum difference between the two previously defined groups. If we find a function that produces a significant difference, we can use it to allocate new specimens of shale of unknown origin to one of the two original groups. In other words, new shale samples, not containing diagnostic fossils, can then be categorized as marine or freshwater on the basis of the linear discriminant function of their geochemical components. [This problem was considered by Potter, Shimp, and Witters (1963).]

Classification can be illustrated with a similar example. Suppose we have obtained a large, heterogeneous collection of shale specimens, each of which has been geochemically analyzed. On the basis of the measured variables, can the shales be separated into groups (or ***clusters***, as they are commonly called) that are both relatively homogeneous and distinct from other groups? The process by which this can be done has been highly developed by numerical taxonomists, and will be considered in a later section. There are several obvious differences between these procedures and those of discriminant function analysis. A classification is internally based; that is, it does not depend on *a priori* knowledge about relations between observations as does a discriminant function. The number of groups in a discriminant function is set prior to the analysis, while in contrast the number of clusters that will emerge from a classification scheme cannot ordinarily be predetermined. Similarly, each original observation is defined as belonging to a specific group in a discriminant analysis. In most classification procedures, an observation is free to enter any cluster that emerges. Other differences will become apparent as we examine these two procedures. The result of a cluster analysis of shales would be a classification of the observations into several groups. It would then be up to us to interpret the geological meaning (if any) of the groups so found.

A simple linear discriminant function transforms an original set of measurements on a specimen into a single ***discriminant score***. That score, or transformed variable, represents the specimen's position along a line defined by the linear discriminant function. We can therefore think of the discriminant function as a way of collapsing a multivariate problem down into a problem which involves only one variable.

Discriminant function analysis consists of finding a transform which gives the maximum ratio of the difference between two group multivariate means to the multivariate variance within the two groups. If we regard our two groups as forming clusters of points in multivariate space, we must search for the one orientation along which the two clusters have the greatest separation while each cluster

simultaneously has the least inflation. This can be graphically shown for two-dimensional cases, as in **Figure 6–2,** which is a scatter plot of the two groups of data listed in file SANDS.TXT. One group contains grain-size statistics of modern beach sands collected along the Gulf Coast in Texas; the second group contains grain-size statistics for sands collected offshore in the Gulf of Mexico. Both data sets consist of two variables, the median grain size and the grain-size sorting coefficient. Although the two clusters of points overlap, it is apparent that a line of division could be placed between the two clusters such that most of the beach sands would be on one side and most offshore sands would be on the other. An adequate separation between the sands of the two groups cannot be made using either median grain size or sorting coefficient alone. However, it is possible to find the orientation of an axis along which the two sets of sands are separated the most and inflated the least. The coordinates of this axis are the coefficients of the linear discriminant function.

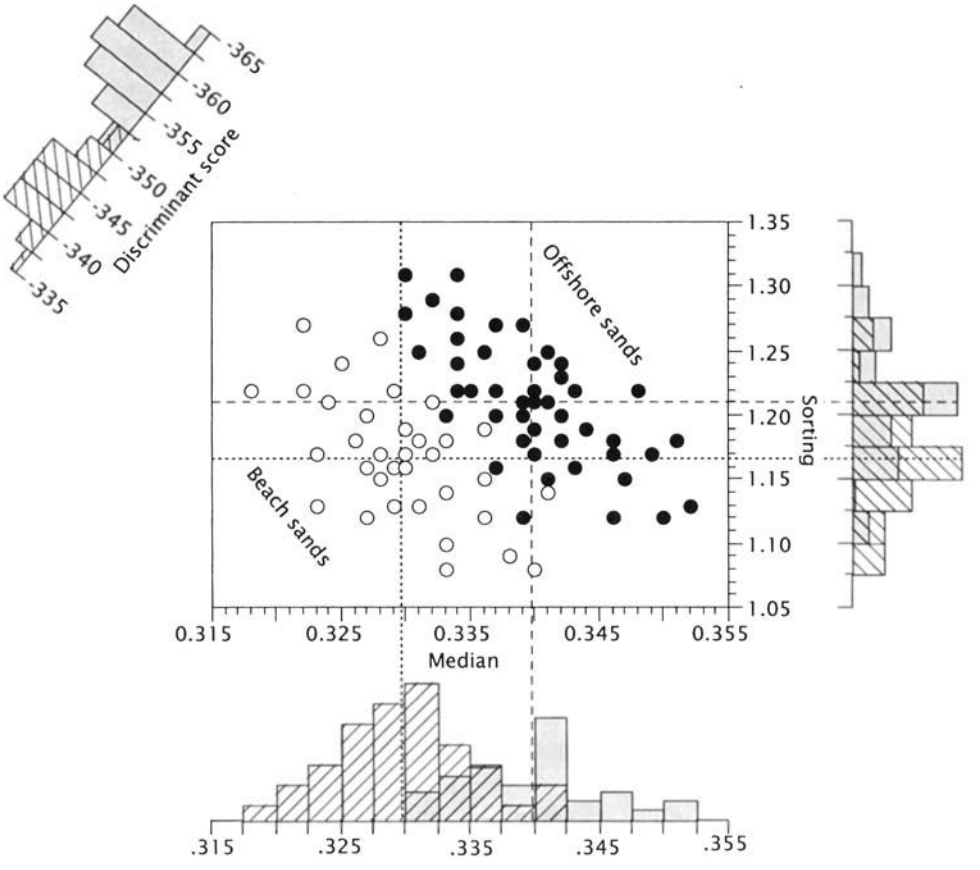


Figure 6–2. Plot of distributions of median grain size and sorting coefficient for samples of modern sands, with scatter plot of both variables. Samples indicated by open circles are beach sands, those indicated by solid dots are offshore sands. Dashed lines indicate bivariate means of the two groups. Distribution of discriminant scores also is shown along line parallel to discriminant axis.

One method that can be used to find the discriminant function is regression; however, the dependent variable consists of the differences between the

multivariate means of the two groups. In matrix notation, we must solve an equation of the form

$$\mathbf{S}\boldsymbol{\lambda} = \mathbf{D} \tag{6.13}$$

where **S** is an $m \times m$ matrix of pooled variances and covariances of the m variables. The coefficients of the discriminant equation are represented by a column vector of the unknown lambdas. Lowercase lambdas (λ) are used by convention to represent the coefficients of the discriminant function. These are exactly the same as the betas (β) used (also by convention) in regression equations. They should not be confused with lambdas used to represent eigenvalues in principal component or factor analyses.

The right-hand side of the equation consists of the column vector of m differences between the means of the two groups, which we will refer to as **A** and **B**. You will recall from Chapter 3 that such an equation can be solved by inversion and multiplication, as

$$\boldsymbol{\lambda} = \mathbf{S}^{-1}\mathbf{D} \tag{6.14}$$

where $\mathbf{S}^{-1}$ is the inverse of the variance-covariance matrix formed by pooling the matrices of the sums of squares and cross products of the two groups, A and B. To compute the discriminant function, we must determine the various entries in the matrix equation. The mean differences are found simply by

$$d_j = \overline{A}_j - \overline{B}_j = \frac{\sum_{i=1}^{n_a} a_{ij}}{n_a} - \frac{\sum_{i=1}^{n_b} b_{ij}}{n_b} \tag{6.15}$$

In this notation, a_{ij} is the ith observation on variable j in group A and $\overline{A}_j$ is the mean of variable j in group A, which is the arithmetic average of the n_a observations of variable j in group A. The same conventions apply to group B. The multivariate means of groups A and B can be regarded as forming two vectors. The difference between these multivariate means therefore also forms a vector

$$\mathbf{D} = \overline{\mathbf{A}} - \overline{\mathbf{B}}$$

or, in expanded form,

$$\begin{bmatrix} d_1 \\ d_2 \\ \vdots \\ d_m \end{bmatrix} = \begin{bmatrix} \overline{A}_1 \\ \overline{A}_2 \\ \vdots \\ \overline{A}_m \end{bmatrix} - \begin{bmatrix} \overline{B}_1 \\ \overline{B}_2 \\ \vdots \\ \overline{B}_m \end{bmatrix}$$

To construct the matrix of pooled variances and covariances, we must compute a matrix of sums of squares and cross products of all variables in group A and a similar matrix for group B. For example, considering only group A,

$$SP_{Ajk} = \sum_{i=1}^{n_a} a_{ij}a_{ik} - \frac{\sum_{i=1}^{n_a} a_{ij} \sum_{i=1}^{n_a} a_{ik}}{n_a}$$

Here, a_{ij} denotes the ith observation of variable j in group A as before, and a_{ik} denotes the ith observation of variable k in the same group. Of course, this quantity will be the sum of squares of variable k whenever $j = k$. Similarly, a matrix of sums of squares and cross products can be found for group B:

Table 6–5. Matrices necessary to compute discriminant function between beach sands and offshore sands listed in file SANDS.TXT.

Vector mean of beach sands:	$\begin{bmatrix} 0.3297 & 1.1674 \end{bmatrix}$
Vector mean of offshore sands:	$\begin{bmatrix} 0.3399 & 1.2100 \end{bmatrix}$
Vector of mean differences:	$\begin{bmatrix} -0.0101 & -0.0426 \end{bmatrix}$
Corrected sums of squares for beach sands:	$\begin{bmatrix} 0.000925 & -0.004886 \\ -0.004886 & 0.075662 \end{bmatrix}$
Corrected sums of squares for offshore sands:	$\begin{bmatrix} 0.001384 & -0.008440 \\ -0.008440 & 0.107000 \end{bmatrix}$
Pooled variance-covariance matrix:	$\begin{bmatrix} 0.000029 & -0.000687 \\ -0.000687 & 0.002312 \end{bmatrix}$
Inverse of pooled variance-covariance matrix:	$\begin{bmatrix} 59{,}098.3047 & 4311.6403 \\ 4311.6403 & 747.0581 \end{bmatrix}$

$$SP_{Bjk} = \sum_{i=1}^{n_b} b_{ij} b_{ik} - \frac{\sum_{i=1}^{n_b} b_{ij} \sum_{i=1}^{n_b} b_{ik}}{n_b}$$

We will denote the sums of products matrix from group A as $\mathbf{S}_A$ and that from group B as $\mathbf{S}_B$. The matrix of pooled variance can now be found as

$$\mathbf{S} = \frac{\mathbf{S}_A + \mathbf{S}_B}{n_a + n_b - 2} \tag{6.16}$$

Remember this equation for the pooled variance; we will use it later in a T^2 test of the equality of the multivariate means of the two groups. Although the amount of mathematical manipulation that must be performed to calculate the coefficients of a discriminant function appears large, it actually is less formidable than it seems at first glance. To demonstrate, we can calculate a discriminant function between the two groups of observations in file SANDS.TXT. Group A consists of the beach sands and Group B consists of the offshore sands.

Table 6–5 contains the calculations necessary to find the two vectors of multivariate means and the two matrices of sums of squares and products. From these, the matrix of pooled variances is calculated. We now have all of the entries

necessary to estimate the discriminant function coefficients:

$$\begin{matrix} \mathbf{S} & & \mathbf{D} & & \boldsymbol{\lambda} \end{matrix}$$

$$\begin{bmatrix} 59,098.305 & 4311.640 \\ 4311.640 & 747.058 \end{bmatrix} \cdot \begin{bmatrix} -0.010 \\ -0.043 \end{bmatrix} = \begin{bmatrix} -783.442 \\ -75.602 \end{bmatrix}$$

The set of λ coefficients we have found are entries in the discriminant function equation which has the form

$$\begin{aligned} R_i &= \lambda_1 x_{1i} + \lambda_2 x_{2i} \\ &= -783.442 x_{1i} - 75.602 x_{2i} \end{aligned} \tag{6.17}$$

Equation (6.17) is a linear function; that is, all the terms are added together to yield a single number, the discriminant score, R_i. In a two-dimensional example, we can plot the discriminant function as a line on the scatter diagram of the two original variables. It is a line through the plot whose slope, α, is

$$\alpha = \lambda_2 / \lambda_1 \tag{6.18}$$

Substitution of the midpoint between the two group means into the discriminant function equation yields the discriminant index, R_0. That is, for each value of x_{ji} in Equation (6.17), we insert the terms

$$x_{j\cdot} = \frac{\overline{A}_j + \overline{B}_j}{2} \tag{6.19}$$

In our example,

$$\begin{aligned} R_0 &= (-783.442 \cdot 0.335) + (-75.602 \cdot 1.189) \\ &= -352.146 \end{aligned}$$

The discriminant index, R_0, is the point along the discriminant function line that is exactly halfway between the center of group A and the center of group B. Next, we may substitute the multivariate mean of group A into the equation (that is, we set $x_j = \overline{A}_j$) to obtain R_A and substitute the multivariate mean of group B (setting $x_j = \overline{B}_j$) to obtain R_B. The centers of the two original groups projected onto the axis defined by the discriminant function are R_A and R_B.

For group A,

$$\begin{aligned} R_A &= (-783.442 \cdot 0.330) + (-75.602 \cdot 1.167) \\ &= -346.560 \end{aligned}$$

and for group B,

$$\begin{aligned} R_B &= (-783.442 \cdot 0.340) + (-75.602 \cdot 1.210) \\ &= -357.732 \end{aligned}$$

The three points may be plotted as in **Figure 6–3**. In fact, every observation in the analysis can be entered into the equation and its position along the discriminant function located. These values are the ***raw discriminant scores***. This has been done on **Figure 6–3**; note that a few members of group A are located on the

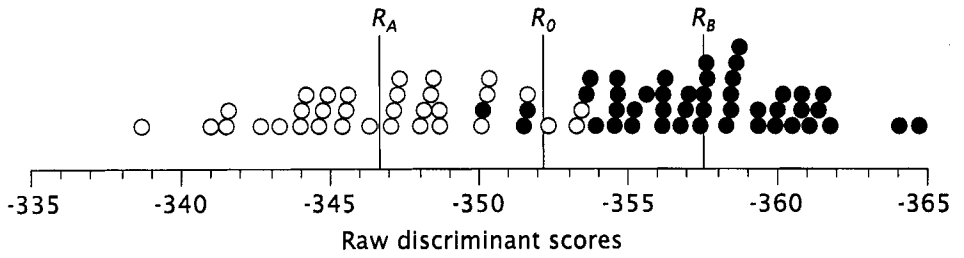


Figure 6–3. Projection of beach and offshore sands onto discriminant function line shown in Figure 6–2. R_A is projection of bivariate mean of beach sands, R_B is projection of bivariate mean of offshore sands, and R_0 is discriminant index.

group B side of R_0 and a few members of group B are located on the group A side. These are observations that have been misclassified by the discriminant function. The ***misclassification ratio***, or percent of observations that the discriminant function places into the wrong group, is sometimes taken as an indication of the function's discriminatory power. However, the misclassification ratio is biased and can be misleading because it is calculated by reusing the observations that were used to estimate the coefficients of the discriminant function in the first place. It seems likely that the function may be less successful in correctly classifying new observations. Reyment and Savazzi (1999) discuss alternative ways of evaluating the goodness of a discriminant function.

We have calculated the ***raw discriminant function*** which yields raw scores whose units are products of the units of measurement attached to the original variables. There actually are an infinity of discriminant functions that will maximize the difference between the two groups, but all of these alternatives are proportional to the classical, or raw, solution. If $\boldsymbol{\lambda}$ is the vector of coefficients determined by Equation (6.14), then all sets $c\boldsymbol{\lambda}$ (where c is an arbitrary constant), will serve equally well. Although different computer programs may yield sets of coefficients that seem to be different, all of them are proportional to each other. Alternative choices include:

1. The raw coefficients are divided by the pooled mean squares within groups, or

$$c = MS_W^{-1}$$

where

$$MS_W = \boldsymbol{\lambda}' \mathbf{S} \boldsymbol{\lambda}$$

This standardizes the coefficients to dimensionless z-scores.

2. The raw coefficients are first divided by MS_W, then rescaled by dividing every coefficient by the first coefficient, which becomes equal to 1.
3. Each raw coefficient is divided by the square root of the sum of the squared raw coefficients, or

$$c = \left(\sum_{j=1}^{m} \lambda_j^2 \right)^{-1/2}$$

The sum of the squares of the transformed coefficients will then be equal to 1.

Tests of significance

If we are willing to make some assumptions about the nature of the data used in the discriminant function, we can test the significance of the separation between the two groups. Five basic assumptions about the data are necessary: (a) the observations in each group are randomly chosen, (b) the probability of an unknown observation belonging to either group is equal, (c) variables are normally distributed within each group, (d) the variance-covariance matrices of the groups are equal in size, and (e) none of the observations used to calculate the function were misclassified. Of these, the most difficult to justify are (b), (c), and (d). Fortunately, the discriminant function is not seriously affected by limited departures from normality or by limited inequality of variances. Justification of (b) must depend upon *a priori* assessment of the relative abundance of the groups under examination. If the assumption of equal abundance seems unjustified, a different assumption may be made, which will shift the position of R_0. [See Anderson (1984, chapter 6) for an extensive discussion of alternative decision rules for discrimination.]

The first step in a test of the significance of a discriminant function is to measure the separation or distinctness of the two groups. This can be done by computing the distance between the centroids, or multivariate means, of the groups. The measure of distance is derived directly from univariate statistics. We can obtain a measure of the difference between the means of two univariate samples, $\overline{X}_1$ and $\overline{X}_2$, by simply subtracting one from the other. However, this difference is expressed in the same units as the original observations. If the difference is divided by the pooled standard deviation, we obtain a ***standardized difference*** in which the difference between the means of the two groups is expressed in dimensionless units of standard deviation, or z-scores:

$$d = \frac{\overline{X}_1 - \overline{X}_2}{s_p} \tag{6.20}$$

When both sides of Equation (6.20) are squared, the denominator is the pooled variance of the two samples, s_p^2:

$$d^2 = \frac{\left(\overline{X}_1 - \overline{X}_2\right)^2}{s_p^2} \tag{6.21}$$

Suppose that instead of a single variable, two variables are measured on each observation in the two groups. The difference between the bivariate means of the two groups can be expressed as the ordinary Euclidean, or straight-line, distance between them. Again denoting the two groups as A and B,

$$\text{Euclidean distance} = \sqrt{\left(\overline{A}_1 - \overline{B}_1\right)^2 + \left(\overline{A}_2 - \overline{B}_2\right)^2} \tag{6.22}$$

In general, if m variables are measured on each observation, the straight-line distance between the multivariate means of the two groups is

$$\text{Euclidean distance} = \sqrt{\sum_{j=1}^{m} \left(\overline{A}_j - \overline{B}_j\right)^2} \tag{6.23}$$

The square of the Euclidean distance is $\sum_{j=1}^{m} \left(\overline{A}_j - \overline{B}_j\right)^2$; you can verify that this is the same as the matrix product,

$$\text{Euclidean distance}^2 = \mathbf{D}'\mathbf{D} \tag{6.24}$$

The Euclidean distance and its square, unfortunately, are expressed as hodgepodges of the original units of measurement. To be interpretable, they must be standardized. Comparison with Equation (6.20) suggests that standardization must involve division by the multivariate equivalent of the variance, which is the variance-covariance matrix **S**. Of course, division is not a defined operation in matrix algebra, but we can accomplish the same end by multiplying by the inverse. Multiplying Equation (6.24) by the inverse of the variance-covariance matrix yields the standardized squared distance,

$$D^2 = \mathbf{D}' \mathbf{S}^{-1} \mathbf{D} \tag{6.25}$$

This standardized measure of difference between the means of two multivariate groups is called ***Mahalanobis' distance.*** Substituting quantities from **Table 6–5** into Equation (6.25), we obtain

$$\begin{aligned} D^2 &= \begin{bmatrix} -0.010 & -0.043 \end{bmatrix} \begin{bmatrix} 59,098.305 & 4311.640 \\ 4311.640 & 747.058 \end{bmatrix} \begin{bmatrix} -0.010 \\ -0.043 \end{bmatrix} \\ &= 11.172 \end{aligned}$$

Interestingly, we can obtain exactly the same distance measure by substituting the vector of mean differences into the discriminant function equation itself:

$$\begin{aligned} D^2 &= \begin{bmatrix} -0.010 & -0.043 \end{bmatrix} \begin{bmatrix} -783.442 \\ -75.602 \end{bmatrix} \\ &= 11.172 \end{aligned}$$

Mahalanobis' distance can be visualized on **Figure 6–3**, where it is equal to the distance between R_A and R_B.

The significance of Mahalanobis' distance can be tested using a multivariate equivalent of the t-test of the equality of two means, called Hotelling's T^2 test. We will discuss this test more extensively in the next section. Here, we simply note that it has the form

$$T^2 = \frac{n_a n_b}{n_a + n_b} D^2 \tag{6.26}$$

and can be transformed to an F-test. The test of multivariate equality, using this more familiar statistic, is

$$F = \left(\frac{n_a + n_b - m - 1}{(n_a + n_b - 2)\, m} \right) \left(\frac{n_a n_b}{n_a + n_b} \right) D^2 \tag{6.27}$$

with m and $(n_a + n_b - m - 1)$ degrees of freedom. The null hypothesis tested by this statistic is that the two multivariate means are equal, or that the distance between them is zero. That is,

$$H_0 : \quad D = 0$$

against

$$H_1 : \quad D > 0$$

The appropriateness of this as a test of a discriminant function should be apparent. If the means of the two groups are very close together, it will be difficult to tell them apart, especially if both groups have large variances. In contrast, if the two means are well separated and scatter about the means is small, discrimination will

be relatively easy. As an exercise, it may be instructive to calculate the significance of the discriminant function for the example we have just worked.

Not all of the variables we have included in the discriminant function will be equally useful in distinguishing one group from another. We may wish to isolate those variables that are not especially helpful and eliminate them from future analyses. Selecting the most effective set of discriminators for discriminant function analysis would seem to be analogous to selecting the most efficient predictors in multiple regression. The problem, however, is more complicated because the "dependent" or predicted variable in a discriminant function is composed of differences between two sets of the same variables that are used as "independent" predictors of the discrimination. Unlike regression, where the sums of squares of y do not change as different variables x_j are added to the equation, the sums of squares of the differences between groups A and B do change as variables are added or deleted.

Some idea of the effectiveness of the variables as discriminators can be gained by computing the ***standardized differences***,

$$D_j = \frac{\overline{A}_j - \overline{B}_j}{s_{pj}} \tag{6.28}$$

This is simply the difference between the means of the two groups A and B for variable j, divided by the pooled standard deviation of variable j. Since the measure does not consider interactions between variables, it is useful only as a general guide to discriminating power. Stepwise discriminant analysis programs may use standardized differences in choosing the order in which variables are added to the discriminant function. Marascuilo and Levin (1983) discuss "after-the-fact" contrast procedures that can be used to select the most important variables. However, the significance of different combinations of variables can be tested only by computing the various functions and determining the relative amounts of separation the different equations produce between the two groups. To avoid bias, such tests should be run on independent random samples.

Discriminant function analysis provides a natural transition between two major classes of multivariate statistical techniques. On one hand, it is closely related to multiple regression and trend-surface analysis. On the other, it can be expressed as an eigenvalue problem, related to principal component analysis, factor analysis, and similar multivariate methods. There are advantages to the use of eigenvectors in calculating the discriminant function, because they allow us to simultaneously discriminate between more than two groups. However, we will delay a consideration of this topic until we examine the basic elements of eigenvector analysis and some of the simpler eigenvector techniques.

Multivariate Extensions of Elementary Statistics

In Chapter 2, we considered some simple geologic problems that could be examined by elementary statistical methods. We will begin our consideration of multivariate methods in geology with some direct extensions of these simple tests. You will recall that the variation measured in most naturally occurring phenomena could be described by the normal distribution. This is a reflection of the central limit theorem, which states that observations which are the sums of many independently operating processes tend to be normally distributed as the number of effects becomes

large. It is this tendency that allows us to use the normal probability distribution as a basis for statistical tests and provides the starting point for the development of the t-, F-, and χ^2 distributions and others. The concept of the normal distribution can be extended to include situations in which observational units consist of many variables.

Suppose we collect rocks from an area and measure a set of properties on each specimen. The measurements may include determinations of chemical or mineralogical constituents, specific gravity, magnetic susceptibility, radioactivity, or any of an almost endless list of possible variables. We can regard the set of measurements made on an individual rock as defining a vector $\mathbf{X}_i = [\, x_{1i} \quad x_{2i} \quad \cdots \quad x_{mi} \,]$, where there are m measured characteristics or variables. If a sample of observations, each represented by vectors X_i, is randomly selected from a population that is the result of many independently acting processes, the observed vectors will tend to be multivariate normally distributed. Considered individually, each variate is normally distributed and characterized by a mean, μ_j, and a variance, σ_j^2. The ***joint probability distribution*** is a p-dimensional equivalent of the normal distribution, having a vector mean $\mu = [\, \mu_1 \quad \mu_2 \quad \cdots \quad \mu_m \,]$ and a variance generalized into the form of a diagonal matrix:

$$\mathbf{\Sigma} = \begin{bmatrix} \sigma_1^2 & 0 & \cdots & 0 \\ 0 & \sigma_2^2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \sigma_m^2 \end{bmatrix}$$

In addition to these obvious extensions of the normal distribution to the multivariate case, the multivariate normal distribution has an important additional characteristic. This is the covariance, cov_{jk}, which occupies all of the off-diagonal positions of the matrix $\mathbf{\Sigma}$. Thus, in the multivariate normal distribution, the mean is generalized into a vector and the variance into a matrix of variances and covariances. In the simple case of $m = 2$, the probability distribution forms a three-dimensional bell curve such as that in **Figure 2–19**, shown as a contour map in **Figure 6–4**. Although the distributions of variables x_1 and x_2 are shown along their respective axes, the essential characteristics of the joint probability distribution are better shown by the major and minor axes of the probability density ellipsoid. Many of the multivariate procedures we will discuss are concerned with the relative orientations of these major and minor axes.

One of the simplest tests we considered in Chapter 2 was a t-test of the probability that a random sample of n observations had been drawn from a normal population with a specified mean, μ, and an unknown variance, σ^2. The test, given in Equation (2.45) on p. 70, can be rewritten in the form

$$t = \frac{(\overline{X} - \mu)\sqrt{n}}{\sqrt{s^2}} \tag{6.29}$$

An obvious generalization of this test to the multivariate case is the substitution of a vector of sample means for $\overline{X}$, a vector of population means for μ, and a variance-covariance matrix for s^2. We have defined the vector of population means as $\boldsymbol{\mu}$, so a vector of sample means can be designated $\overline{\mathbf{x}}$. Similarly, $\mathbf{\Sigma}$ is the matrix of population variances and covariances, so $\mathbf{S}$ represents the matrix of sample variances and covariances. Both $\overline{\mathbf{x}}$ and $\boldsymbol{\mu}$ are taken to be column vectors, although equivalent equations may be written in which they are assumed to be row vectors. A column vector of differences between the sample means and the population means

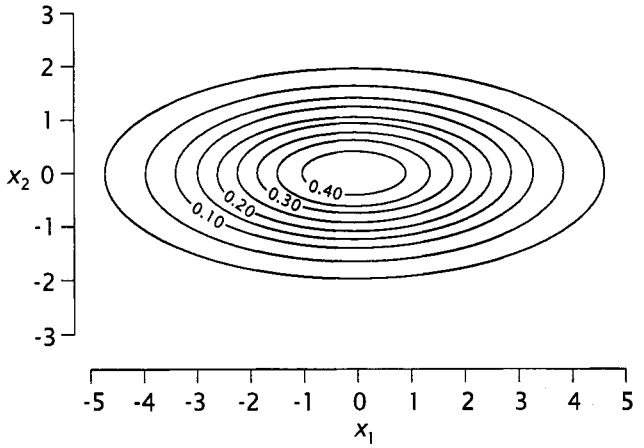


Figure 6–4. Contour map of bivariate normal probability distribution. See Figure 2.19 on p. 40 for perspective diagram of same distribution.

is obtained by subtracting these two vectors. Substituting these quantities directly into Equation (6.29) gives

$$t = \frac{(\bar{\mathbf{x}} - \boldsymbol{\mu})\sqrt{n}}{\sqrt{\mathbf{S}}}$$

Unfortunately, there is no equally obvious way of solving this equation so that it yields a single value of t. We must reduce the vectors and the matrix to single numbers if we wish to apply this test. If we were to multiply the column vector $(\bar{\mathbf{x}} - \boldsymbol{\mu})$ by a row vector having the same number of elements, the result would be a single number. We will therefore define an arbitrary row vector, **A**, whose transpose is a column vector, $\mathbf{A}'$. Multiplication of the column vector of differences $(\bar{\mathbf{x}} - \boldsymbol{\mu})$ by the row vector **A** gives a single number, and premultiplication of **S** by **A** and postmultiplication by $\mathbf{A}'$ also yields a single number. That is, our test has become

$$t = \frac{\mathbf{A}(\bar{\mathbf{x}} - \boldsymbol{\mu})\sqrt{n}}{\mathbf{A}\sqrt{\mathbf{S}}\mathbf{A}'}$$

However, we have also changed what we are testing, from a null hypothesis of

$$H_0 : \boldsymbol{\mu}_1 = \boldsymbol{\mu}_0$$

to

$$H_0^* : \mathbf{A}\boldsymbol{\mu}_1 = \mathbf{A}\boldsymbol{\mu}_0$$

The original hypothesis, H_0, is true only if the new hypothesis, H_0^*, holds for all possible values of **A**. It is sufficient, however, to test only the maximum possible value of the test statistic, because if H_0^* is rejected for any value of **A**, the hypothesis H_0 is also rejected. With a bit of mathematical manipulation, we can determine the conditions under which a maximum test statistic will result for any arbitrary vector **A**. This involves introducing the constraint $\mathbf{ASA}' = 1$ and expressing the equation in a form that incorporates a determinant. In the process, we can eliminate the troublesome square roots by squaring the equation. This also squares the test value, which is referred to as ***Hotelling's*** T^2, in honor of Harold Hotelling, the

American statistician who formulated this generalization of Student's t. When all operations are complete, we find that the test statistic can be expressed as

$$T^2 = n\,(\bar{\mathbf{x}} - \boldsymbol{\mu})'\,\mathbf{S}^{-1}\,(\bar{x} - \boldsymbol{\mu}) \tag{6.30}$$

That is, the arbitrary vector A is equal to the vector of differences between the means, $(\bar{\mathbf{x}} - \boldsymbol{\mu})$. We must find the inverse of the variance-covariance matrix, premultiply this inverse by a row vector of differences, $(\bar{\mathbf{x}} - \boldsymbol{\mu})'$, and then postmultiply by a column vector of these same differences. The test statistic is a multivariate extension of the t-statistic, Hotelling's T^2. Critical values of T^2 can be determined by the relation

$$F = \frac{n - m}{m(n-1)}T^2 \tag{6.31}$$

where n is the number of observations and m is the number of variables, allowing us to use conventional F-tables rather than special tables of the T^2 distribution. More complete discussions of this and related tests are given in texts on multivariate statistics such as Overall and Klett (1983), Harris (1985), Krzanowski (1988), and Morrison (1990).

Although the expression of this test in a form such as Equation (6.30) is easy, computation of a test value for an actual data set may be very laborious. For example, suppose we have measured the content of four elements in seven lunar samples. We wish to test the hypothesis that these samples have been drawn from a population having the same mean as terrestrial basalts. Assume we take our values for the populations' means from the *Handbook of Physical Constants* (Clark, 1966, p. 4). Hotelling's T^2 seems appropriate to test the hypothesis that the vector of lunar sample means is no different than the vector of basalt means given in this reference.

We must first compute the vector of four sample means and the 4×4 matrix of variances and covariances. The vector of differences between sample and population means, $(\bar{\mathbf{x}} - \boldsymbol{\mu})$, must also be computed. Next, we must find the inverse of the variance-covariance matrix, or $\mathbf{S}^{-1}$. We then must perform two matrix multiplications, $(\bar{\mathbf{x}} - \boldsymbol{\mu})'\mathbf{S}^{-1}(\bar{\mathbf{x}} - \boldsymbol{\mu})$, and multiply by n to produce T^2. From this description, you can appreciate that the computational effort becomes increasingly greater as the number of variables grows larger.

The data for the seven lunar samples are listed in **Table 6–6**, with the "population" means from Clark. Intermediate values in the computation of T^2 are also given, with the final test value of T^2 and the equivalent F-statistic, which has m and $(n - m)$ degrees of freedom. The test statistic of $F = 73.11$ far exceeds the critical value of $F_{4,3,0.01} = 28.71$, so we conclude that the mean composition of the sample of lunar basalts is significantly different than the mean composition of the population of terrestrial basalts.

We have dwelled on the T^2 test against a known mean not because this specific test has greater utility in geology than other multivariate tests, but to illustrate the close relationship between conventional statistics and multivariate statistics. Multivariate equivalents can be formulated directly from most univariate tests with the proper expansion of the basic assumptions. However, the transition from ordinary algebra to matrix algebra often obscures the underlying similarity between the two applications. Although we usually regard multivariate methods as an extension of univariate statistics, univariate, or ordinary, statistical analysis should be considered as a special subset of the general area of multivariate analysis.

Table 6–6. Abundances of four elements in seven lunar samples and mean abundances of same elements in terrestrial basalts (after Wanke and others, 1970).

Lunar Samples	Si	Al	Fe	Mg
1	19.4	5.9	14.7	5.0
2	21.5	4.0	15.7	3.7
3	19.2	4.0	15.4	4.3
4	18.4	5.4	15.2	3.4
5	20.6	6.2	13.2	5.5
6	19.8	5.7	14.8	2.8
7	18.7	6.0	13.8	4.6
MEANS	19.66	5.31	14.69	4.19
"Population" Means	22.10	7.40	10.10	4.00
Differences	−2.44	−2.09	4.59	0.19

Variance-covariance matrix:

$$\begin{bmatrix} 1.179524 & -0.307619 & 0.059286 & 0.079286 \\ -0.307619 & 0.868095 & -0.683095 & 0.301905 \\ 0.059286 & -0.683095 & 0.801429 & -0.546905 \\ 0.079286 & 0.301905 & -0.546905 & 0.891429 \end{bmatrix}$$

Inverse of variance-covariance matrix:

$$\begin{bmatrix} 1.061478 & 0.994883 & 0.817269 & 0.070054 \\ 0.994883 & 5.209577 & 5.336676 & 1.421289 \\ 0.817269 & 5.336676 & 7.660054 & 2.819468 \\ 0.070054 & 1.421289 & 2.819468 & 2.363995 \end{bmatrix}$$

$T^2 = 584.78$
$F = 73.10$

In the remaining discussion in this section, we will consider multivariate tests that are the m-dimensional equivalent of some of the tests we considered in Chapter 2. However, we will not point out the details of the extrapolation from the univariate to the general case as we have done with the T^2 test. These derivations can be found in many texts on multivariate statistics, some of which are listed in the Selected Readings at the end of this chapter.

Equality of two vector means

The test we have just considered is a one-sample test against a specified population mean vector. Suppose instead we have collected two independent random samples and we wish to test the equivalency of their mean vectors. We assume that the two samples are drawn from multivariate normal populations, both having the same unknown variance-covariance matrix $\boldsymbol{\Sigma}$. We wish to test the null hypothesis

$$H_0 : \boldsymbol{\mu}_1 = \boldsymbol{\mu}_0$$

against

$$H_1 : \boldsymbol{\mu}_1 \neq \boldsymbol{\mu}_0$$

The null hypothesis states that the mean vector of the parent population of the first sample is the same as the mean vector of the parent population from which the second sample was drawn.

The test we must use is a multivariate equivalent of Equation (2.48) on p. 73. In that two-sample t-test, we used a pooled estimate of the population variance based on both samples. Accordingly, we must compute a pooled estimate, $\mathbf{S}_p$, of the common variance-covariance matrix from our two multivariate samples. This is done by calculating a matrix of sums of squares and products for each sample. We can use the terminology of discriminant functions and denote the matrix of sums of squares and cross products of sample A as $\mathbf{S}_A$; similarly, the matrix from sample B is $\mathbf{S}_B$. The pooled estimate of the variance-covariance matrix is

$$\mathbf{S}_p = (n_A + n_B - 2)^{-1} (\mathbf{S}_A + \mathbf{S}_B) \tag{6.32}$$

We must next find the difference between the two mean vectors, $\mathbf{D} = \bar{\mathbf{x}}_A - \bar{\mathbf{x}}_B$. Our T^2 test has the form

$$T^2 = \frac{n_A n_B}{n_A + n_B} \mathbf{D}' \mathbf{S}_p^{-1} \mathbf{D} \tag{6.33}$$

The significance of the T^2 test statistic can be determined by the F-transformation:

$$F = \frac{n_A + n_B - m - 1}{(n_A + n_B - 2)m} T^2 \tag{6.34}$$

which has m and $(n_A + n_B - m - 1)$ degrees of freedom (Morrison, 1990).

Equality of variance–covariance matrices

An underlying assumption in the two preceding tests is that the samples are drawn from populations having the same variance-covariance matrix. This is the multivariate equivalent of the assumption of equal population variances necessary to perform t-tests of means. In practice, an assumption of equality may be unwarranted, because samples which exhibit a high mean often will also have a large variance. You will recall from Chapter 4 that such behavior is characteristic of many geologic variables such as mine-assay values and trace-element concentrations. Equality of variance-covariance matrices may be checked by the following "test of generalized variances" which is a multivariate equivalent of the F-test (Morrison, 1990).

Suppose we have k samples of observations, and have measured m variables on each observation. For each sample a variance-covariance matrix, $\mathbf{S}_k$, may be computed. We wish to test the null hypothesis

$$H_0 : \boldsymbol{\Sigma}_1 = \boldsymbol{\Sigma}_2 = \cdots = \boldsymbol{\Sigma}_k$$

against the alternative

$$H_1 : \boldsymbol{\Sigma}_i \neq \boldsymbol{\Sigma}_j$$

The null hypothesis states that all k population variance-covariance matrices are the same. The alternative is that at least two of the matrices are different. Each variance-covariance matrix $\mathbf{S}_i$ is an estimate of a population matrix $\boldsymbol{\Sigma}_i$. If the parent populations of the k samples are identical, the sample estimates may be

combined to form a pooled estimate of the population variance-covariance matrix. The pooled estimate is created by

$$\mathbf{S}_p = \left(\left(\sum_{i=1}^{k} n_i\right) - k\right)^{-1} \sum_{i=1}^{k} (n_i - 1)\, \mathbf{S}_i \tag{6.35}$$

where n_i is the number of observations in the ith group and the summation over n_i gives the total number of all observations in all k samples. This equation is algebraically equivalent to Equation (6.32) when $k = 2$.

From the pooled estimate of the population variance-covariance matrix, a test statistic, M, can be computed:

$$M = \left\{\left(\sum_{i=1}^{k} n_i\right) - k\right\} \ln \left|s_p^2\right| - \sum_{i=1}^{k} \left\{(n_i - 1) \ln \left|s_i^2\right|\right\} \tag{6.36}$$

The test is based on the difference between the logarithm of the determinant of the pooled variance-covariance matrix and the average of the logarithms of the determinants of the sample variance-covariance matrices. If all the sample matrices are the same, this difference will be very small. As the variances and covariances of the samples deviate more and more from one another, the test statistic will increase. Tables of critical values of M are not widely available, so the transformation

$$C^{-1} = 1 - \frac{2m^2 + 3m - 1}{6\,(m + 1)\,(k - 1)} \left(\sum_{i-1}^{k} \frac{1}{n_i - 1} - \frac{1}{\left(\sum_{i=1}^{k} n_i - k\right)}\right) \tag{6.37}$$

can be used to convert M to an approximate χ^2 statistic:

$$\chi^2 \approx MC^{-1} \tag{6.38}$$

The approximate χ^2 value has degrees of freedom equal to $\nu = (1/2)(k - 1)$. If all the samples contain the same number of observations, n, Equation (6.37) can be simplified to

$$C^{-1} = 1 - \frac{(2m^2 + 3m - 1)(k + 1)}{6(m + 1)k(n - 1)} \tag{6.39}$$

The χ^2 approximation is good if the number of k samples and m variables do not exceed about 5 and each variance-covariance estimate is based on at least 20 observations.

To illustrate the process of hypothesis testing using multivariate statistics, we will work through the following problem. Note that the number of observations is just sufficient for some of the approximations to be strictly valid; we will consider them to be adequate for the purposes of this demonstration.

In a local area in eastern Kansas, all potable water is obtained from wells. Some of these wells draw from the alluvial fill in stream valleys, while others tap a limestone aquifer that also is the source of numerous springs in the region. Residents prefer to obtain water from the alluvium, as they feel it is of better quality. However, the water resources of the alluvium are limited, and it would be desirable for some users to obtain their supplies from the limestone aquifer.

In an attempt to demonstrate that the two sources are equivalent in quality, a state agency sampled wells that tapped each source. The water samples were analyzed for chemical compounds that affect the quality of water. Some of the data

Table 6–7. Multivariate statistics for cation composition of water samples collected from wells in an area of eastern Kansas: x_1 = silica, x_2 = iron, x_3 = magnesium, x_4 = sodium + potassium, x_5 = calcium. Data given in file WELLWATR.TXT.

Vector mean of water from wells in limestone

$$\bar{\mathbf{x}}_L = [\,9.760 \quad 13.955 \quad 30.935 \quad 25.930 \quad 33.270\,]$$

Vector mean of water from wells in alluvium

$$\bar{\mathbf{x}}_A = [\,12.055 \quad 16.080 \quad 34.465 \quad 29.910 \quad 25.055\,]$$

Variance-covariance matrix of water from wells in limestone, $|\mathbf{S}_L| = 1.8838 \cdot 10^8$

$$\mathbf{S}_L = \begin{bmatrix} 5.1615 & 0.5134 & 7.3683 & -1.4103 & -3.4402 \\ 0.5134 & 21.0247 & 10.6948 & -4.0896 & -25.3972 \\ 7.3683 & 10.6948 & 102.8045 & -38.5269 & -58.1689 \\ -1.4103 & -4.0896 & -38.5269 & 98.8654 & 7.2520 \\ -3.4402 & -25.3972 & -58.1689 & 7.2520 & 290.8706 \end{bmatrix}$$

Variance-covariance matrix of water from wells in alluvium, $|\mathbf{S}_A| = 2.1777 \cdot 10^8$

$$\mathbf{S}_A = \begin{bmatrix} 5.6394 & 0.7333 & 8.6868 & -2.9822 & -4.7095 \\ 0.7333 & 23.1733 & 12.7656 & -4.5593 & -26.9878 \\ 8.6868 & 12.7656 & 103.3982 & -42.3949 & -58.1232 \\ -2.9822 & -4.5593 & -42.3949 & 106.9525 & 9.2199 \\ -4.7095 & -26.9878 & -58.1232 & 9.2199 & 275.1616 \end{bmatrix}$$

Pooled variance-covariance matrix, $|\mathbf{S}_p| = 2.0351 \cdot 10^8$

$$\mathbf{S}_p = \begin{bmatrix} 5.4005 & 0.6233 & 8.0275 & -2.1962 & -4.0749 \\ 0.6233 & 22.0990 & 11.7302 & -4.3244 & -26.1925 \\ 8.0275 & 11.7302 & 103.1013 & -40.4609 & -58.1461 \\ -2.1962 & -4.3244 & -40.4609 & 102.9089 & 8.2360 \\ -4.0749 & -26.1925 & -58.1461 & 8.2360 & 283.0661 \end{bmatrix}$$

Inverse of pooled variance-covariance matrix

$$\mathbf{S}_p^{-1} = \begin{bmatrix} 0.2101 & 0.0027 & -0.0178 & -0.0024 & -3.0820 \cdot 10^{-4} \\ 0.0027 & 0.0521 & -0.0036 & 4.9006 \cdot 10^{-4} & 0.0041 \\ -0.0178 & -0.0036 & 0.0148 & 0.0051 & 0.0023 \\ -0.0024 & 4.9006 \cdot 10^{-4} & 0.0051 & 0.0116 & 7.2056 \cdot 10^{-4} \\ -3.0820 \cdot 10^{-4} & 0.0041 & 0.0023 & 7.2056 \cdot 10^{-4} & 0.0044 \end{bmatrix}$$

from these analyses are given in the file WELLWATR.TXT. The variance-covariance matrices, inverses, and determinants for the two data sets and for the pooled data are given in **Table 6–7**. From these we can test the equivalence of the two vector means. We will assume that the samples have been drawn randomly from multivariate normal populations.

We must first test the assumption that the variance-covariance matrices for the two samples are equivalent using the test statistic M given in Equation (6.36):

$$\begin{aligned} M &= (20 + 20 - 2)\ln 2.0351 \cdot 10^8 - (19 \ln 1.8838 \cdot 10^8 + 19 \ln 2.1777 \cdot 10^8) \\ &= 0.1804 \end{aligned}$$

The transformation factor, C^{-1}, must also be calculated to allow use of the χ^2 approximation:

$$C^{-1} = 1 - \frac{2 \cdot 5^2 + 3 \cdot 5 - 1}{6(5+1)(2-1)} \left(\frac{1}{19} + \frac{1}{19} - \frac{1}{40-2} \right)$$
$$= 0.8637$$

The χ^2 statistic is approximately $0.1804 \cdot 0.8637 = 0.1558$, with degrees of freedom equal to $\nu = 1/2(2-1)(5)(5+1) = 15$.

The critical value of χ^2 for $\nu = 15$ with a 5% level of significance is 25.00. The computed statistic is less than this value and does not fall into the critical region, so we may conclude that there is nothing in our samples which suggests that the variance-covariance structures of the parent populations are different. We may pool the two sample variance-covariance matrices and test the equality of the multivariate means using the T^2 test of Equation (6.33):

$$T^2 = \frac{20 \cdot 20}{20+20} 1.4847 = 14.847$$

The value 1.4847 is the product of the matrix multiplications $\mathbf{D}'\mathbf{S}_p^{-1}\mathbf{D}$ specified in Equation (6.33). The T^2 statistic may be converted to an F-statistic by Equation (6.34):

$$F = \frac{(20+20-5-1)}{(20+20-2)5} 14.847 = 2.657$$

Degrees of freedom are $\nu_1 = 5$ and $\nu_2 = (20 + 20 - 5 - 1) = 34$. The critical value for F with 5 and 34 degrees of freedom at the 5% ($\alpha = 0.05$) level of significance is 2.49. Our computed test statistic just exceeds this critical value, so we conclude that our samples do, indeed, indicate a difference in the means of the two populations. In other words, there is a statistically significant difference in composition of water from the two aquifers. This simple test will not pinpoint the chemical variables responsible for this difference, but it does substantiate the natives' contention that they can tell a difference in the water!

Multivariate techniques equivalent to the analysis-of-variance procedures discussed in Chapter 2 are available. In general, these involve a comparison of two $m \times m$ matrices that are the multivariate equivalents of the among-group and within-group sums of squares tested in ordinary analysis of variance. The test statistic consists of the largest eigenvalue of the matrix resulting from the comparison. We will not consider these tests here because their formulation is complicated and their applications to geologic problems have been, so far, minimal. This is not a reflection on their potential utility, however. Interested readers are referred to chapter 5 of Griffith and Amrhein (1997), which presents worked examples of MANOVA's applied to problems in geography. Koch and Link (1980) include a brief illustration of the application of multivariate analysis of variance to geochemical data. Statistical details are discussed by Morrison (1990).

Cluster Analysis

Cluster analysis is the name given to a bewildering assortment of techniques designed to perform classification by assigning observations to groups so each group is more or less homogeneous and distinct from other groups. This is the special forte of taxonomists, who attempt to deduce the lineage of living creatures from

their characteristics and similarities. Taxonomy is highly subjective and dependent upon the individual taxonomist's skills, developed through years of experience. In this respect, the field is analogous in many ways to geology. As in geology, researchers dissatisfied with the subjectivity and capriciousness of traditional methods have sought new techniques of classification which incorporate the massive data-handling capabilities of the computer. These workers, responsible for many of the advances made in numerical classification, call themselves numerical taxonomists.

Numerical taxonomy has been a center of controversy in biology, much like the suspicion that swirled around factor analysis in the 1930's and 1940's and provoked acrimonious debates among psychologists. As in that dispute, the techniques of numerical taxonomy were overzealously promoted by some practitioners. In addition, it was claimed that a numerically derived taxonomy better represented the phylogeny of a group of organisms than could any other type of classification. Although this has yet to be demonstrated, rapid progress in genotyping suggests that an objective phylogeny may someday be possible. The conceptual underpinnings of taxonomic methods such as cluster analysis are incomplete; the various clustering methods lie outside the body of multivariate statistical theory, and only limited tests of significance are available (Hartigan, 1975; Milligan and Cooper, 1986; Bock, 1996). Although cluster analysis has become an accepted tool for researchers and there are an increasing number of books on the subject, a more complete statistical basis for classification has yet to be fashioned. In spite of this, many of the methods of numerical taxonomy are important in geologic research, especially in the classification of fossil invertebrates and the study of paleoenvironments.

The purpose of cluster analysis is to assemble observations into relatively homogeneous groups or "clusters," the members of which are at once alike and at the same time unlike members of other groups. There is no analytical solution to this problem, which is common to all areas of classification, not just numerical taxonomy. Although there are alternative classifications of classification procedures (Sneath and Sokal, 1973; Gordon, 1999), most may be grouped into four general types.

1. ***Partitioning methods*** operate on the multivariate observations themselves, or on projections of these observations onto planes of lower dimension. Basically, these methods cluster by finding regions in the space defined by the m variables that are poorly populated with observations, and that separate densely populated regions. Mathematical "partitions" are placed in the sparse regions, subdividing the variable space into discrete classes. Although the analysis is done in the m-dimensional space defined by the variables rather than the n-dimensional space defined by the observations, it proceeds iteratively and may be extremely time-consuming (Aldenderfer and Blashfield, 1984; Gordon, 1999).
2. ***Arbitrary origin methods*** operate on the similarity between the observations and a set of arbitrary starting points. If n observations are to be classified into k groups, it is necessary to compute an asymmetric $n \times k$ matrix of similarities between the n samples and the k arbitrary points that serve as initial group centroids. The observation closest or most similar to a starting point is combined with it to form a cluster. Observations are iteratively added to the nearest cluster, whose centroid is then recalculated for the expanded cluster.

3. ***Mutual similarity procedures*** group together observations that have a common similarity to other observations. First an $n \times n$ matrix of similarities between all pairs of observations is calculated. Then the similarity between columns of this matrix is iteratively recomputed. Columns representing members of a single cluster will tend to have intercorrelations near +1, while having much lower correlations with nonmembers.
4. ***Hierarchical clustering*** joins the most similar observations, then successively connects the next most similar observations to these. First an $n \times n$ matrix of similarities between all pairs of observations is calculated. Those pairs having the highest similarities are then merged, and the matrix is recomputed. This is done by averaging the similarities that the combined observations have with other observations. The process iterates until the similarity matrix is reduced to 2×2. The progression of levels of similarity at which observations merge is displayed as a dendrogram.

Hierarchical clustering techniques are most widely applied in the Earth sciences, probably because their development has been closely linked with the numerical taxonomy of fossil organisms. Because of the widespread use of heirarchical techniques, we will consider them in some detail.

Suppose we have a collection of objects we wish to arrange into a hierarchical classification. In biology, these objects are referred to as "operational taxonomic units" or OTU's (Sneath and Sokal, 1973). We can make a series of measurements on each object which constitutes our data set. If we have n objects and measure m characteristics, the observations form an $n \times m$ data matrix, **X**. Next, some measure of resemblance or similarity must be computed between every pair of objects; that is, between the rows of the data matrix. Several coefficients of resemblance have been used, including a variation of the correlation coefficient $\hat{r}_{ij}$ in which the roles of objects and variables are interchanged. This can be done by transposing **X** so rows become columns and *vice versa*, then calculating $\hat{r}_{ij}$ in the conventional manner (Eq. 2.28; p. 43), following the matrix algorithm given in Chapter 3. Although called "correlation," this measure is not really a correlation coefficient in the conventional sense because it involves "means" and "variances" calculated across all the variables measured on two objects, rather than the means and variances of two variables.

Another commonly used measure of similarity between objects is a standardized m-space Euclidean distance, d_{ij}. The distance coefficient is computed by

$$d_{ij} = \sqrt{\frac{\sum_{k=1}^{m} (x_{ik} - x_{jk})^2}{m}} \tag{6.40}$$

where x_{ik} denotes the kth variable measured on object i and x_{jk} is the kth variable measured on object j. In all, m variables are measured on each object, and d_{ij} is the distance between object i and object j. As you would expect, a small distance indicates the two objects are similar or "close together," whereas a large distance indicates dissimilarity. Commonly, each element in the $n \times m$ raw data matrix **X** is standardized by subtracting the column means and dividing by the column standard deviations prior to computing distance measurements. This ensures that each variable is weighted equally. Otherwise, the distance will be influenced most strongly by the variable which has the greatest magnitude. In some instances this may be desirable, but unwanted effects can creep in through injudicious choice of

measurement units. As an extreme example, we might measure three perpendicular axes on a collection of pebbles. If we measure two of the axes in centimeters and the third in millimeters, the third axis will have proportionally ten times more influence on the distance coefficient than either of the other two variables.

Other measures of similarity that are less commonly used in the Earth sciences include a wide variety of ***association coefficients*** which are based on binary (presence-absence) variables or a combination of binary and continuous variables. The most popular of these are the ***simple matching coefficient, Jaccard's coefficient***, and ***Gower's coefficient***—all ratios of the presence-absence of properties. They differ primarily in the way that mutual absences (called "negative matches") are considered. Sneath and Sokal (1973) discuss the relative merits of these and other coefficients of association. ***Probabilistic similarity coefficients*** are used with binary data and consider the gain or loss of information when objects are combined into clusters. Again, Sneath and Sokal (1973) provide a comprehensive summary.

Computation of a similarity measurement between all possible pairs of objects will result in an $n \times n$ symmetrical matrix, **C**. Any coefficient c_{ij} in the matrix gives the resemblance between objects i and j. The next step is to arrange the objects into a hierarchy so objects with the highest mutual similarity are placed together. Then groups or clusters of objects are associated with other groups which they most closely resemble, and so on until all of the objects have been placed into a complete classification scheme. Many variants of clustering have been developed; a consideration of all of the possible alternative procedures and their relative merits is beyond the scope of this book. Rather, we will discuss one simple clustering technique called the ***weighted pair-group method*** with ***arithmetic averaging***, and then point out some useful modifications to this scheme.

Extensive discussions of hierarchical and other classification techniques are contained in books by Jardine and Sibson (1971), Sneath and Sokal (1973), Hartigan (1975), Aldenderfer and Blashfield (1984), Romesburg (1984), Kaufman and Rousseeuw (1990), Backer (1995), and Gordon (1999). Diskettes containing clustering programs are included in some of the these books or are available separately at modest cost. In addition, most personal computer programs for statistical analysis contain modules for hierarchical clustering.

Table 6–8 contains measurements made on six greywacke thin sections, identified as A, B, ... , F. The values represent the average of the apparent maximum diameters of ten randomly chosen grains of quartz, rock fragment, and feldspar and the average of the apparent maximum diameters of ten intergranular pores in each thin section. The table also gives a symmetric matrix of similarities, in the form of "correlation" coefficients calculated between the six thin sections.

The first step in clustering by a pair-group method is to find the mutually highest correlations in the matrix to form the centers of clusters. The highest correlation (disregarding the diagonal element) in each column of the matrix in **Table 6–8** is shown in boldface type. Specimens A and B form mutually high pairs, because A most closely resembles B, and B most closely resembles A. C and D also form mutually high pairs. E most closely resembles D, but these two do not form a mutually high pair because D resembles C more than it does E. To qualify as a mutually high pair, coefficients c_{ij} and c_{ji} must be the highest coefficients in their respective columns.

We can indicate the resemblance between our mutually high pairs in a diagram such as **Figure 6–5 a**. Object C is connected to D at a level of $\hat{r} = 0.99$, indicating

Table 6–8. Average apparent grain diameters measured on thin sections of six greywackes and matrix of "correlations" between thin sections. Highest "correlation" in each column is indicated in boldface type.

Average diameters in mm

Specimen	Pore	Quartz	Rock fragment	Feldspar
A	0.24	1.78	0.69	3.32
B	0.48	2.07	2.41	4.78
C	0.76	4.05	1.2	3.21
D	0.23	2.98	0.85	2.06
E	0.04	3.33	3.39	2.63
F	1.98	0.98	2.01	2.02

"Correlations" on initial iteration

	A	B	C	D	E	F
A	1	**0.9110**	0.7671	0.7041	0.4401	−0.1067
B	**0.9110**	1	0.5393	0.4996	0.5704	**0.1680**
C	0.7671	0.5393	1	**0.9910**	0.5873	−0.7187
D	0.7041	0.4996	**0.9910**	1	**0.6647**	−0.7675
E	0.4401	0.5704	0.5873	0.6647	1	−0.3883
F	−0.1067	0.168	−0.7187	−0.7675	−0.3883	1

"Correlations" on second iteration

	AB	CD	E	F
AB	1	0.394	0.505	**0.031**
CD	0.394	1	**0.626**	−0.744
E	**0.505**	**0.626**	1	−0.388
F	0.031	−0.744	−0.388	1

"Correlations" on third iteration

	AB	CDE	F
AB	1	**0.450**	**0.031**
CDE	**0.450**	1	−0.566
F	0.031	−0.566	1

"Correlations" on fourth iteration

	ABCDE	F
ABCDE	1	−0.268
F	−0.268	1

the degree of their mutual similarity. In the same manner, A and B are connected at a level of $\hat{r} = 0.91$. This is the first step in the construction of a ***dendrogram***, or tree diagram, which is the most common way of displaying the results of clustering.

Next, the similarity matrix must be recomputed, treating grouped or clustered elements as a single element. There are several methods for doing this. In the simple technique we are considering, new correlations between all clusters and unclustered objects are recalculated by simple arithmetic averaging. For example, the new correlation between cluster CD and object E is equal to the sum of the correlations of the elements common to both CD and E, divided by 2 (that is, $\hat{r} = (0.5873 + 0.6647)/2 = 0.626$). **Table 6–8** contains the results of these

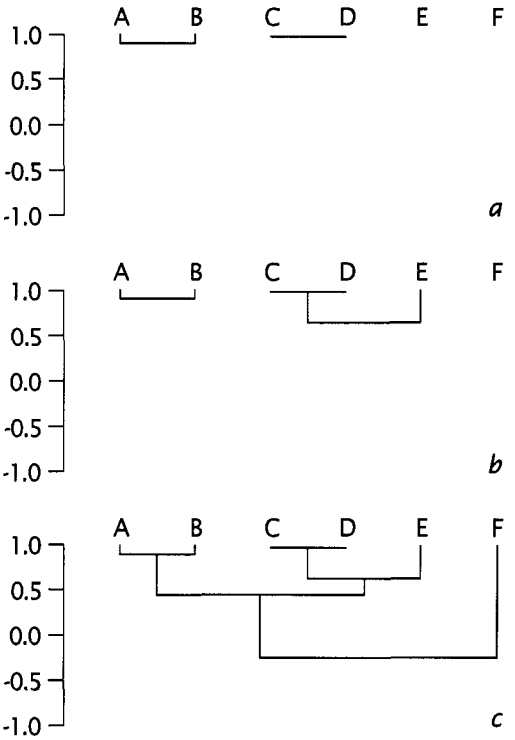


Figure 6–5. (*a*) Dendrogram with initial clusters, *CD* and *AB*. (*b*) Connection of object *E* to initial cluster *CD*. (*c*) Final connection of two clusters *AB* and *CDE*, and connection of isolated object *F* to *CDE*, completing dendrogram.

recalculations. Again, the highest correlations in each column are shown in boldface type.

The clustering procedure is now repeated; mutually high pairs are sought out and clustered. In this cycle, object *E* joins cluster *CD* (**Fig. 6–5 b**) to form cluster CDE. The correlations between cluster CDE and other clusters or individual objects such as *F* are again found by adding together the common elements and dividing by 2. This process is repeated again and again until all objects and clusters are joined together. The final matrix of similarities will be a 2×2 matrix between the last remaining object and everything else collected into a single cluster, as shown in **Table 6–8**. This indicates that cluster *ABCDE* has a resemblance of $\hat{r} = -0.27$ with object *F*. Our dendrogram can then be completed (**Fig. 6–5 c**).

Clustering is an efficient way of displaying complex relationships among many objects. However, the process of averaging together members of a cluster and treating them as a single new object introduces distortions into the dendrogram. This distortion becomes increasingly apparent as successive levels of clusters are averaged together. We can evaluate the severity of this distortion by examining what numerical taxonomists call the ***matrix of cophenetic values***. This is nothing more than a matrix of apparent correlations contained within the dendrogram. For example, the dendrogram in **Figure 6–5** implies that the correlations between *C*, *D*, and *E*, on one hand, with *A* and *B*, on the other, are all $\hat{r} = 0.45$. Similarly, the correlation between *F* and *E* is the same as the correlation between *F* and *D*, or between *F* and any of the other objects. Only the correlations between *A* and *B* and between

APPENDIX

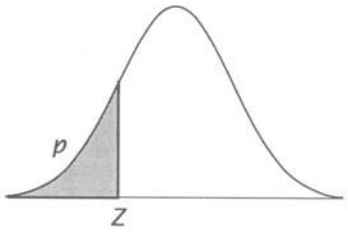


Table A.1. Cumulative probabilities for the standardized normal distribution. Z-scores are standard deviations from the mean. Probabilities are cumulative areas under the normal distribution. Especially useful critical values shown in bold italics.

Z	p	Z	p	Z	p	Z	p
−3.00	0.0013	−1.55	0.0606	0.05	0.5199	***1.64***	***0.9500***
−2.95	0.0016	−1.50	0.0668	0.10	0.5398	1.65	0.9505
−2.90	0.0019	−1.45	0.0735	0.15	0.5596	1.70	0.9554
−2.85	0.0022	−1.40	0.0808	0.20	0.5793	1.75	0.9599
−2.80	0.0026	−1.35	0.0885	0.25	0.5987	1.80	0.9641
−2.75	0.0030	−1.30	0.0968	0.30	0.6179	1.85	0.9678
−2.70	0.0035	***−1.28***	***0.1000***	0.35	0.6368	1.90	0.9713
−2.65	0.0040	−1.25	0.1056	0.40	0.6554	1.95	0.9744
−2.60	0.0047	−1.20	0.1151	0.45	0.6736	***1.96***	***0.9750***
−2.57	***0.0050***	−1.15	0.1251	0.50	0.6915	2.00	0.9772
−2.55	0.0054	−1.10	0.1357	0.55	0.7088	2.05	0.9798
−2.50	0.0062	−1.05	0.1469	0.60	0.7257	2.10	0.9821
−2.45	0.0071	−1.00	0.1587	0.65	0.7422	2.15	0.9842
−2.40	0.0082	−0.95	0.1711	0.70	0.7580	2.20	0.9861
−2.35	0.0094	−0.90	0.1841	0.75	0.7734	2.25	0.9878
−2.33	***0.0100***	−0.85	0.1977	0.80	0.7881	2.30	0.9893
−2.30	0.0107	−0.80	0.2119	0.85	0.8023	***2.33***	***0.9900***
−2.25	0.0122	−0.75	0.2266	0.90	0.8159	2.35	0.9906
−2.20	0.0139	−0.70	0.2420	0.95	0.8289	2.40	0.9918
−2.15	0.0158	−0.65	0.2578	1.00	0.8413	2.45	0.9929
−2.10	0.0179	−0.60	0.2743	1.05	0.8531	2.50	0.9938
−2.05	0.0202	−0.55	0.2912	1.10	0.8643	2.55	0.9946
−2.00	0.0228	−0.50	0.3085	1.15	0.8749	***2.57***	***0.9950***
−1.96	***0.0250***	−0.45	0.3264	1.20	0.8849	2.60	0.9953
−1.95	0.0256	−0.40	0.3446	1.25	0.8944	2.65	0.9960
−1.90	0.0287	−0.35	0.3632	***1.28***	***0.9000***	2.70	0.9965
−1.85	0.0322	−0.30	0.3821	1.30	0.9032	2.75	0.9970
−1.80	0.0359	−0.25	0.4013	1.35	0.9115	2.80	0.9974
−1.75	0.0401	−0.20	0.4207	1.40	0.9192	2.85	0.9978
−1.70	0.0446	−0.15	0.4404	1.45	0.9265	2.90	0.9981
−1.65	0.0495	−0.10	0.4602	1.50	0.9332	2.95	0.9984
−1.64	***0.0500***	−0.05	0.4801	1.55	0.9394	3.00	0.9987
−1.60	0.0548	0.00	0.5000	1.60	0.9452		

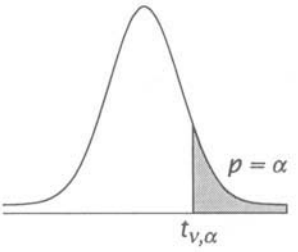


Table A.2. Critical values of t for ν degrees of freedom and selected levels of significance. For critical values in the left-hand tail, change the sign of the table value. Critical values are given for the right-hand tail.

	Significance Level, α, for:						
	One-tailed Test						
	.001	.005	.01	.025	.05	.1	.2
No. of Degrees	Two-tailed Test						
of Freedom, ν	.002	.010	.02	.05	.1	.2	.4
1	318.3088	63.6567	31.8205	12.7062	6.3138	3.0777	1.3764
2	22.3271	9.9248	6.9646	4.3027	2.9200	1.8856	1.0607
3	10.2145	5.8409	4.5407	3.1824	2.3534	1.6377	0.9785
4	7.1732	4.6041	3.7470	2.7764	2.1318	1.5332	0.9410
5	5.8934	4.0322	3.3649	2.5706	2.0150	1.4759	0.9195
6	5.2076	3.7074	3.1427	2.4469	1.9432	1.4398	0.9057
7	4.7853	3.4995	2.9980	2.3646	1.8946	1.4149	0.8960
8	4.5008	3.3554	2.8965	2.3060	1.8595	1.3968	0.8889
9	4.2968	3.2498	2.8214	2.2622	1.8331	1.3830	0.8834
10	4.1437	3.1693	2.7638	2.2281	1.8125	1.3722	0.8791
11	4.0247	3.1058	2.7181	2.2010	1.7959	1.3634	0.8755
12	3.9296	3.0545	2.6810	2.1788	1.7823	1.3562	0.8726
13	3.8520	3.0123	2.6503	2.1604	1.7709	1.3502	0.8702
14	3.7874	2.9768	2.6245	2.1448	1.7613	1.3450	0.8681
15	3.7328	2.9467	2.6025	2.1314	1.7531	1.3406	0.8662
16	3.6862	2.9208	2.5835	2.1199	1.7459	1.3368	0.8647
17	3.6458	2.8982	2.5669	2.1098	1.7396	1.3334	0.8633
18	3.6105	2.8784	2.5524	2.1009	1.7341	1.3304	0.8620
19	3.5794	2.8609	2.5395	2.0930	1.7291	1.3277	0.8610
20	3.5518	2.8453	2.5280	2.0860	1.7247	1.3253	0.8600
21	3.5272	2.8314	2.5176	2.0796	1.7207	1.3232	0.8591
22	3.5050	2.8188	2.5083	2.0739	1.7171	1.3212	0.8583
23	3.4850	2.8073	2.4999	2.0687	1.7139	1.3195	0.8575
24	3.4668	2.7969	2.4922	2.0639	1.7109	1.3178	0.8569
25	3.4502	2.7874	2.4851	2.0595	1.7081	1.3163	0.8562
26	3.4350	2.7787	2.4786	2.0555	1.7056	1.3150	0.8557

(Continued)

Table A.2. Concluded.

No. of Degrees of Freedom, ν	Significance Level, α, for: One-tailed Test .001 / Two-tailed Test .002	.005 / .010	.01 / .02	.025 / .05	.05 / .1	.1 / .2	.2 / .4
27	3.4210	2.7707	2.4727	2.0518	1.7033	1.3137	0.8551
28	3.4082	2.7633	2.4671	2.0484	1.7011	1.3125	0.8546
29	3.3962	2.7564	2.4620	2.0452	1.6991	1.3114	0.8542
30	3.3852	2.7500	2.4573	2.0423	1.6973	1.3104	0.8538
40	3.3069	2.7045	2.4233	2.0211	1.6839	1.3031	0.8507
50	3.2614	2.6778	2.4033	2.0086	1.6759	1.2987	0.8489
60	3.2317	2.6603	2.3901	2.0003	1.6706	1.2958	0.8477
70	3.2108	2.6479	2.3808	1.9944	1.6669	1.2938	0.8468
80	3.1953	2.6387	2.3739	1.9901	1.6641	1.2922	0.8461
90	3.1833	2.6316	2.3685	1.9867	1.6620	1.2910	0.8456
100	3.1737	2.6259	2.3642	1.9840	1.6602	1.2901	0.8452
110	3.1660	2.6213	2.3607	1.9818	1.6588	1.2893	0.8449
120	3.1595	2.6174	2.3578	1.9799	1.6577	1.2886	0.8446
130	3.1541	2.6142	2.3554	1.9784	1.6567	1.2881	0.8444
140	3.1495	2.6114	2.3533	1.9771	1.6558	1.2876	0.8442
150	3.1455	2.6090	2.3515	1.9759	1.6551	1.2872	0.8440
∞	3.0902	2.5758	2.2364	1.9600	1.6449	1.2816	0.8416

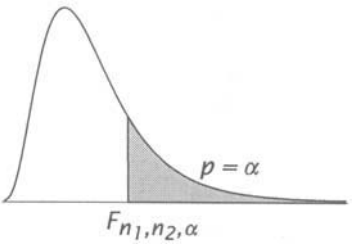


Table A.3a. Critical values of F for ν_1 and ν_2 degrees of freedom and 5% ($\alpha = 0.05$) level of significance.

df	1	2	3	4	5	6	7	8	9	10	15	20	25	∞
1	161.45	199.50	215.71	224.58	230.16	233.99	236.77	238.88	240.54	241.88	245.95	248.01	249.26	250.10
2	18.51	19	19.16	19.25	19.30	19.33	19.35	19.37	19.38	19.40	19.43	19.45	19.46	19.46
3	10.13	9.55	9.28	9.12	9.01	8.94	8.89	8.85	8.81	8.79	8.70	8.66	8.63	8.62
4	7.71	6.94	6.59	6.39	6.26	6.16	6.09	6.04	6.00	5.96	5.86	5.80	5.77	5.75
5	6.61	5.79	5.41	5.19	5.05	4.95	4.88	4.82	4.77	4.74	4.62	4.56	4.52	4.50
6	5.99	5.14	4.76	4.53	4.39	4.28	4.21	4.15	4.10	4.06	3.94	3.87	3.83	3.81

(Continued)

Table A.3a. Concluded.

df	1	2	3	4	5	6	7	8	9	10	15	20	25	∞
7	5.59	4.74	4.35	4.12	3.97	3.87	3.79	3.73	3.68	3.64	3.51	3.44	3.4	3.38
8	5.32	4.46	4.07	3.84	3.69	3.58	3.50	3.44	3.39	3.35	3.22	3.15	3.11	3.08
9	5.12	4.26	3.86	3.63	3.48	3.37	3.29	3.23	3.18	3.14	3.01	2.94	2.89	2.86
10	4.96	4.10	3.71	3.48	3.33	3.22	3.14	3.07	3.02	2.98	2.85	2.77	2.73	2.70
11	4.84	3.98	3.59	3.36	3.20	3.09	3.01	2.95	2.90	2.85	2.72	2.65	2.60	2.57
12	4.75	3.89	3.49	3.26	3.11	3.00	2.91	2.85	2.80	2.75	2.62	2.54	2.50	2.47
13	4.67	3.81	3.41	3.18	3.03	2.92	2.83	2.77	2.71	2.67	2.53	2.46	2.41	2.38
14	4.60	3.74	3.34	3.11	2.96	2.85	2.76	2.70	2.65	2.60	2.46	2.39	2.34	2.31
15	4.54	3.68	3.29	3.06	2.90	2.79	2.71	2.64	2.59	2.54	2.40	2.33	2.28	2.25
16	4.49	3.63	3.24	3.01	2.85	2.74	2.66	2.59	2.54	2.49	2.35	2.28	2.23	2.19
17	4.45	3.59	3.20	2.96	2.81	2.70	2.61	2.55	2.49	2.45	2.31	2.23	2.18	2.15
18	4.41	3.55	3.16	2.93	2.77	2.66	2.58	2.51	2.46	2.41	2.27	2.19	2.14	2.11
19	4.38	3.52	3.13	2.90	2.74	2.63	2.54	2.48	2.42	2.38	2.23	2.16	2.11	2.07
20	4.35	3.49	3.10	2.87	2.71	2.60	2.51	2.45	2.39	2.35	2.20	2.12	2.07	2.04
21	4.32	3.47	3.07	2.84	2.68	2.57	2.49	2.42	2.37	2.32	2.18	2.10	2.05	2.01
22	4.30	3.44	3.05	2.82	2.66	2.55	2.46	2.40	2.34	2.30	2.15	2.07	2.02	1.98
23	4.28	3.42	3.03	2.80	2.64	2.53	2.44	2.37	2.32	2.27	2.13	2.05	2.00	1.96
24	4.26	3.40	3.01	2.78	2.62	2.51	2.42	2.36	2.30	2.25	2.11	2.03	1.97	1.94
25	4.24	3.39	2.99	2.76	2.60	2.49	2.40	2.34	2.28	2.24	2.09	2.01	1.96	1.92
26	4.23	3.37	2.98	2.74	2.59	2.47	2.39	2.32	2.27	2.22	2.07	1.99	1.94	1.90
27	4.21	3.35	2.96	2.73	2.57	2.46	2.37	2.31	2.25	2.20	2.06	1.97	1.92	1.88
28	4.20	3.34	2.95	2.71	2.56	2.45	2.36	2.29	2.24	2.19	2.04	1.96	1.91	1.87
29	4.18	3.33	2.93	2.70	2.55	2.43	2.35	2.28	2.22	2.18	2.03	1.94	1.89	1.85
30	4.17	3.32	2.92	2.69	2.53	2.42	2.33	2.27	2.21	2.16	2.01	1.93	1.88	1.84
40	4.08	3.23	2.84	2.61	2.45	2.34	2.25	2.18	2.12	2.08	1.92	1.84	1.78	1.74
50	4.03	3.18	2.79	2.56	2.40	2.29	2.20	2.13	2.07	2.03	1.87	1.78	1.73	1.69
60	4.00	3.15	2.76	2.53	2.37	2.25	2.17	2.10	2.04	1.99	1.84	1.75	1.69	1.65
70	3.98	3.13	2.74	2.50	2.35	2.23	2.14	2.07	2.02	1.97	1.81	1.72	1.66	1.62
80	3.96	3.11	2.72	2.49	2.33	2.21	2.13	2.06	2.00	1.95	1.79	1.70	1.64	1.60
90	3.95	3.10	2.71	2.47	2.32	2.20	2.11	2.04	1.99	1.94	1.78	1.69	1.63	1.59
100	3.94	3.09	2.70	2.46	2.31	2.19	2.10	2.03	1.97	1.93	1.77	1.68	1.62	1.57
110	3.93	3.08	2.69	2.45	2.30	2.18	2.09	2.02	1.97	1.92	1.76	1.67	1.61	1.56
120	3.92	3.07	2.68	2.45	2.29	2.18	2.09	2.02	1.96	1.91	1.75	1.66	1.60	1.55
∞	3.85	3.00	2.61	2.38	2.22	2.11	2.02	1.95	1.89	1.84	1.68	1.58	1.52	1.47

Table A.3b. Critical values of F for ν_1 and ν_2 degrees of freedom and 2.5% ($\alpha = 0.025$) level of significance.

df	1	2	3	4	5	6	7	8	9	10	15	20	25	∞
1	647.79	799.50	864.16	899.58	921.85	937.11	948.22	956.66	963.28	968.63	984.87	993.10	998.08	1001.41
2	38.51	39.00	39.17	39.25	39.30	39.33	39.36	39.37	39.39	39.40	39.43	39.45	39.46	39.46
3	17.44	16.04	15.44	15.10	14.88	14.73	14.62	14.54	14.47	14.42	14.25	14.17	14.12	14.08
4	12.22	10.65	9.98	9.60	9.36	9.20	9.07	8.98	8.90	8.84	8.66	8.56	8.50	8.46
5	10.01	8.43	7.76	7.39	7.15	6.98	6.85	6.76	6.68	6.62	6.43	6.33	6.27	6.23
6	8.81	7.26	6.60	6.23	5.99	5.82	5.70	5.60	5.52	5.46	5.27	5.17	5.11	5.07
7	8.07	6.54	5.89	5.52	5.29	5.12	4.99	4.90	4.82	4.76	4.57	4.47	4.40	4.36
8	7.57	6.06	5.42	5.05	4.82	4.65	4.53	4.43	4.36	4.30	4.10	4.00	3.94	3.89
9	7.21	5.71	5.08	4.72	4.48	4.32	4.20	4.10	4.03	3.96	3.77	3.67	3.60	3.56
10	6.94	5.46	4.83	4.47	4.24	4.07	3.95	3.85	3.78	3.72	3.52	3.42	3.35	3.31
11	6.72	5.26	4.63	4.28	4.04	3.88	3.76	3.66	3.59	3.53	3.33	3.23	3.16	3.12
12	6.55	5.10	4.47	4.12	3.89	3.73	3.61	3.51	3.44	3.37	3.18	3.07	3.01	2.96
13	6.41	4.97	4.35	4.00	3.77	3.60	3.48	3.39	3.31	3.25	3.05	2.95	2.88	2.84
14	6.30	4.86	4.24	3.89	3.66	3.50	3.38	3.29	3.21	3.15	2.95	2.84	2.78	2.73
15	6.20	4.77	4.15	3.80	3.58	3.41	3.29	3.20	3.12	3.06	2.86	2.76	2.69	2.64
16	6.12	4.69	4.08	3.73	3.50	3.34	3.22	3.12	3.05	2.99	2.79	2.68	2.61	2.57
17	6.04	4.62	4.01	3.66	3.44	3.28	3.16	3.06	2.98	2.92	2.72	2.62	2.55	2.50
18	5.98	4.56	3.95	3.61	3.38	3.22	3.10	3.01	2.93	2.87	2.67	2.56	2.49	2.44
19	5.92	4.51	3.90	3.56	3.33	3.17	3.05	2.96	2.88	2.82	2.62	2.51	2.44	2.39
20	5.87	4.46	3.86	3.51	3.29	3.13	3.01	2.91	2.84	2.77	2.57	2.46	2.40	2.35
21	5.83	4.42	3.82	3.48	3.25	3.09	2.97	2.87	2.80	2.73	2.53	2.42	2.36	2.31
22	5.79	4.38	3.78	3.44	3.22	3.05	2.93	2.84	2.76	2.70	2.50	2.39	2.32	2.27
23	5.75	4.35	3.75	3.41	3.18	3.02	2.90	2.81	2.73	2.67	2.47	2.36	2.29	2.24
24	5.72	4.32	3.72	3.38	3.15	2.99	2.87	2.78	2.70	2.64	2.44	2.33	2.26	2.21
25	5.69	4.29	3.69	3.35	3.13	2.97	2.85	2.75	2.68	2.61	2.41	2.30	2.23	2.18
26	5.66	4.27	3.67	3.33	3.10	2.94	2.82	2.73	2.65	2.59	2.39	2.28	2.21	2.16
27	5.63	4.24	3.65	3.31	3.08	2.92	2.80	2.71	2.63	2.57	2.36	2.25	2.18	2.13
28	5.61	4.22	3.63	3.29	3.06	2.90	2.78	2.69	2.61	2.55	2.34	2.23	2.16	2.11
29	5.59	4.20	3.61	3.27	3.04	2.88	2.76	2.67	2.59	2.53	2.32	2.21	2.14	2.09
30	5.57	4.18	3.59	3.25	3.03	2.87	2.75	2.65	2.57	2.51	2.31	2.20	2.12	2.07
40	5.42	4.05	3.46	3.13	2.90	2.74	2.62	2.53	2.45	2.39	2.18	2.07	1.99	1.94
50	5.34	3.97	3.39	3.05	2.83	2.67	2.55	2.46	2.38	2.32	2.11	1.99	1.92	1.87
60	5.29	3.93	3.34	3.01	2.79	2.63	2.51	2.41	2.33	2.27	2.06	1.94	1.87	1.82
70	5.25	3.89	3.31	2.97	2.75	2.59	2.47	2.38	2.30	2.24	2.03	1.91	1.83	1.78
80	5.22	3.86	3.28	2.95	2.73	2.57	2.45	2.35	2.28	2.21	2.00	1.88	1.81	1.75
90	5.20	3.84	3.26	2.93	2.71	2.55	2.43	2.34	2.26	2.19	1.98	1.86	1.79	1.73
100	5.18	3.83	3.25	2.92	2.70	2.54	2.42	2.32	2.24	2.18	1.97	1.85	1.77	1.71
110	5.16	3.82	3.24	2.90	2.68	2.53	2.40	2.31	2.23	2.17	1.96	1.84	1.76	1.70
120	5.15	3.80	3.23	2.89	2.67	2.52	2.39	2.30	2.22	2.16	1.94	1.82	1.75	1.69
∞	5.04	3.70	3.13	2.80	2.58	2.42	2.30	2.20	2.13	2.06	1.85	1.72	1.64	1.58

Table A.3c. Critical values of F for ν_1 and ν_2 degrees of freedom and 1% ($\alpha = 0.01$) level of significance.

df	1	2	3	4	5	6	7	8	9	10	15	20	25	∞
1	4052.18	4999.50	5403.35	5624.58	5763.65	5858.99	5928.36	5981.07	6022.47	6055.85	6157.28	6208.73	6239.83	6260.65
2	98.50	99.00	99.17	99.25	99.30	99.33	99.36	99.37	99.39	99.40	99.43	99.45	99.46	99.47
3	34.12	30.82	29.46	28.71	28.24	27.91	27.67	27.49	27.35	27.23	26.87	26.69	26.58	26.50
4	21.20	18.00	16.69	15.98	15.52	15.21	14.98	14.80	14.66	14.55	14.20	14.02	13.91	13.84
5	16.26	13.27	12.06	11.39	10.97	10.67	10.46	10.29	10.16	10.05	9.72	9.55	9.45	9.38
6	13.75	10.92	9.78	9.15	8.75	8.47	8.26	8.10	7.98	7.87	7.56	7.40	7.30	7.23
7	12.25	9.55	8.45	7.85	7.46	7.19	6.99	6.84	6.72	6.62	6.31	6.16	6.06	5.99
8	11.26	8.65	7.59	7.01	6.63	6.37	6.18	6.03	5.91	5.81	5.52	5.36	5.26	5.20
9	10.56	8.02	6.99	6.42	6.06	5.80	5.61	5.47	5.35	5.26	4.96	4.81	4.71	4.65
10	10.04	7.56	6.55	5.99	5.64	5.39	5.20	5.06	4.94	4.85	4.56	4.41	4.31	4.25
11	9.65	7.21	6.22	5.67	5.32	5.07	4.89	4.74	4.63	4.54	4.25	4.10	4.01	3.94
12	9.33	6.93	5.95	5.41	5.06	4.82	4.64	4.50	4.39	4.30	4.01	3.86	3.76	3.70
13	9.07	6.70	5.74	5.21	4.86	4.62	4.44	4.30	4.19	4.10	3.82	3.66	3.57	3.51
14	8.86	6.51	5.56	5.04	4.69	4.46	4.28	4.14	4.03	3.94	3.66	3.51	3.41	3.35
15	8.68	6.36	5.42	4.89	4.56	4.32	4.14	4.00	3.89	3.80	3.52	3.37	3.28	3.21
16	8.53	6.23	5.29	4.77	4.44	4.20	4.03	3.89	3.78	3.69	3.41	3.26	3.16	3.10
17	8.40	6.11	5.18	4.67	4.34	4.10	3.93	3.79	3.68	3.59	3.31	3.16	3.07	3.00
18	8.29	6.01	5.09	4.58	4.25	4.01	3.84	3.71	3.60	3.51	3.23	3.08	2.98	2.92
19	8.18	5.93	5.01	4.50	4.17	3.94	3.77	3.63	3.52	3.43	3.15	3.00	2.91	2.84
20	8.10	5.85	4.94	4.43	4.10	3.87	3.70	3.56	3.46	3.37	3.09	2.94	2.84	2.78
21	8.02	5.78	4.87	4.37	4.04	3.81	3.64	3.51	3.40	3.31	3.03	2.88	2.79	2.72
22	7.95	5.72	4.82	4.31	3.99	3.76	3.59	3.45	3.35	3.26	2.98	2.83	2.73	2.67
23	7.88	5.66	4.76	4.26	3.94	3.71	3.54	3.41	3.30	3.21	2.93	2.78	2.69	2.62
24	7.82	5.61	4.72	4.22	3.90	3.67	3.50	3.36	3.26	3.17	2.89	2.74	2.64	2.58
25	7.77	5.57	4.68	4.18	3.85	3.63	3.46	3.32	3.22	3.13	2.85	2.70	2.60	2.54
26	7.72	5.53	4.64	4.14	3.82	3.59	3.42	3.29	3.18	3.09	2.81	2.66	2.57	2.50
27	7.68	5.49	4.60	4.11	3.78	3.56	3.39	3.26	3.15	3.06	2.78	2.63	2.54	2.47
28	7.64	5.45	4.57	4.07	3.75	3.53	3.36	3.23	3.12	3.03	2.75	2.60	2.51	2.44
29	7.60	5.42	4.54	4.04	3.73	3.50	3.33	3.20	3.09	3.00	2.73	2.57	2.48	2.41
30	7.56	5.39	4.51	4.02	3.70	3.47	3.30	3.17	3.07	2.98	2.70	2.55	2.45	2.39
40	7.31	5.18	4.31	3.83	3.51	3.29	3.12	2.99	2.89	2.80	2.70	2.55	2.45	2.39
50	7.17	5.06	4.20	3.72	3.41	3.19	3.02	2.89	2.78	2.70	2.52	2.37	2.27	2.20
60	7.08	4.98	4.13	3.65	3.34	3.12	2.95	2.82	2.72	2.63	2.42	2.27	2.17	2.10
70	7.01	4.92	4.07	3.60	3.29	3.07	2.91	2.78	2.67	2.59	2.35	2.20	2.10	2.03
80	6.96	4.88	4.04	3.56	3.26	3.04	2.87	2.74	2.64	2.55	2.31	2.15	2.05	1.98
90	6.93	4.85	4.01	3.53	3.23	3.01	2.84	2.72	2.61	2.52	2.27	2.12	2.01	1.94
100	6.90	4.82	3.98	3.51	3.21	2.99	2.82	2.69	2.59	2.50	2.24	2.09	1.99	1.92
110	6.87	4.80	3.96	3.49	3.19	2.97	2.81	2.68	2.57	2.49	2.22	2.07	1.97	1.89
120	6.85	4.79	3.95	3.48	3.17	2.96	2.79	2.66	2.56	2.47	2.21	2.05	1.95	1.88
∞	6.66	4.63	3.80	3.34	3.04	2.82	2.66	2.53	2.43	2.34	2.06	1.90	1.79	1.72

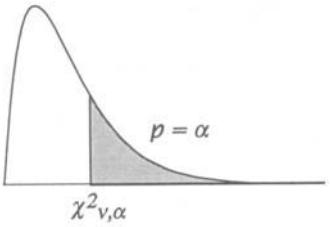


Table A.4. Critical values of χ^2 for ν degrees of freedom and selected levels of significance.

No. of Degrees of Freedom, ν	Significance Level, α 0.20	0.10	0.05	0.025	0.01
1	1.64	2.71	3.84	5.02	6.63
2	3.22	4.61	5.99	7.38	9.21
3	4.64	6.25	7.81	9.35	11.34
4	5.99	7.78	9.49	11.14	13.28
5	7.29	9.24	11.07	12.83	15.09
6	8.56	10.64	12.59	14.45	16.81
7	9.80	12.02	14.07	16.01	18.48
8	11.03	13.36	15.51	17.53	20.09
9	12.24	14.68	16.92	19.02	21.67
10	13.44	15.99	18.31	20.48	23.21
11	14.63	17.28	19.68	21.92	24.72
12	15.81	18.55	21.03	23.34	26.22
13	16.98	19.81	22.36	24.74	27.69
14	18.15	21.06	23.68	26.12	29.14
15	19.31	22.31	25.00	27.49	30.58
16	20.47	23.54	26.30	28.85	32.00
17	21.61	24.77	27.59	30.19	33.41
18	22.76	25.99	28.87	31.53	34.81
19	23.90	27.20	30.14	32.85	36.19
20	25.04	28.41	31.41	34.17	37.57
21	26.17	29.62	32.67	35.48	38.93
22	27.30	30.81	33.92	36.78	40.29
23	28.43	32.01	35.17	38.08	41.64
24	29.55	33.20	36.42	39.36	42.98
25	30.68	34.38	37.65	40.65	44.31
26	31.79	35.56	38.89	41.92	45.64
27	32.91	36.74	40.11	43.19	46.96
28	34.03	37.92	41.34	44.46	48.28
29	35.14	39.09	42.56	45.72	49.59
30	36.25	40.26	43.77	46.98	50.89
40	47.27	51.81	55.76	59.34	63.69
50	58.16	63.17	67.50	71.42	76.15
60	68.97	74.40	79.08	83.30	88.38

(Continued)

Table A.4. Concluded.

No. of Degrees of Freedom, ν	Significance Level, α 0.20	0.10	0.05	0.025	0.01
70	79.71	85.53	90.53	95.02	100.43
80	90.41	96.58	101.88	106.63	112.33
90	101.05	107.57	113.15	118.14	124.12
100	111.67	118.50	124.34	129.56	135.81
110	122.25	129.39	135.48	140.92	147.41
120	132.81	140.23	146.57	152.21	158.95

Table A.5. Probabilities of occurrence of specified values of the Mann–Whitney W_x statistic for testing the equality to two samples of size n and m, where $m \leq n \leq 8$. C_L is the lower critical value and C_U is the upper critical value.[1]

$m = 3$	n											
C_L	3	C_U	4	C_U	5	C_U	6	C_U	7	C_U	8	C_U
6	.0500	15	.0286	18	.0179	21	.0119	24	.0083	27	.0061	30
7	.1000	14	.0571	17	.0357	20	.0238	23	.0167	26	.0121	29
8	.2000	13	.1143	16	.0714	19	.0476	22	.0333	25	.0242	28
9	.3500	12	.2000	15	.1250	18	.0833	21	.0583	24	.0424	27
10	.5000	11	.3143	14	.1964	17	.1310	20	.0917	23	.0667	26
11	.6500	10	.4286	13	.2857	16	.1905	19	.1333	22	.0970	25
12	.8000	9	.5714	12	.3929	15	.2738	18	.1917	21	.1394	24
13	.9000	8	.6857	11	.5000	14	.3571	17	.2583	20	.1879	23
14	.9500	7	.8000	10	.6071	13	.4524	16	.3333	19	.2485	22
15	1.0000	6	.8857	9	.7143	12	.5476	15	.4167	18	.3152	21
16			.942	8	.8036	11	.6429	14	.5000	17	.3879	20
17			.9714	7	.8750	10	.7262	13	.5833	16	.4606	19
18			1.0000	6	.9286	9	.8095	12	.6667	15	.5394	18
19					.9643	8	.8690	11	.7417	14	.6121	17
20					.9821	7	.9167	10	.8083	13	.6848	16
21					1.0000	6	.9524	9	.8667	12	.7515	15
22							.9762	8	.9083	11	.8121	14
23							.9881	7	.9417	10	.8606	13
24							1.0000	6	.9667	9	.9030	12

[1] Adapted from S. Siegel and N.J. Castellan, Jr., 1988, *Nonparametric Statistics for the Behavioral Sciences*, 2ed. Reproduced by permission of The McGraw-Hill Companies, New York.

(Continued)

Table A.5. Continued.

$m = 4$					n					
C_L	4	C_U	5	C_U	6	C_U	7	C_U	8	C_U
10	.0143	*26*	.0079	*30*	.0048	*34*	.0030	*38*	.0020	*42*
11	.0286	*25*	.0159	*29*	.0095	*33*	.0061	*37*	.0040	*41*
12	.0571	*24*	.0317	*28*	.0190	*32*	.0121	*36*	.0081	*40*
13	.1000	*23*	.0556	*27*	.0333	*31*	.0212	*35*	.0141	*39*
14	.1714	*22*	.0952	*26*	.0571	*30*	.0364	*34*	.0242	*38*
15	.2429	*21*	.1429	*25*	.0857	*29*	.0545	*33*	.0364	*37*
16	.3429	*20*	.2063	*24*	.1286	*28*	.0818	*32*	.0545	*36*
17	.4429	*19*	.2778	*23*	.1762	*27*	.1152	*31*	.0768	*35*
18	.5571	*18*	.3651	*22*	.2381	*26*	.1576	*30*	.1071	*34*
19	.6571	*17*	.4524	*21*	.3048	*25*	.2061	*29*	.1414	*33*
20	.7571	*16*	.5476	*20*	.3810	*24*	.2636	*28*	.1838	*32*
21	.8286	*15*	.6349	*19*	.4571	*23*	.3242	*27*	.2303	*31*
22	.9000	*14*	.7222	*18*	.5429	*22*	.3939	*26*	.2848	*30*
23	.9429	*13*	.7937	*17*	.6190	*21*	.4636	*25*	.3414	*29*
24	.9714	*12*	.8571	*16*	.6952	*20*	.5364	*24*	.4040	*28*
25	.9857	*11*	.9048	*15*	.7619	*19*	.6061	*23*	.4667	*27*
26	1.0000	*10*	.9444	*14*	.8238	*18*	.6758	*22*	.5333	*26*
27			.9683	*13*	.8714	*17*	.7364	*21*	.5960	*25*
28			.9841	*12*	.9143	*16*	.7939	*20*	.6586	*24*
29			.9921	*11*	.9429	*15*	.8424	*19*	.7152	*23*
30			1.0000	*10*	.9667	*14*	.8848	*18*	.7697	*22*
31					.9810	*13*	.9182	*17*	.8162	*21*
32					.9905	*12*	.9455	*16*	.8586	*20*
33					.9952	*11*	.9636	*15*	.8929	*19*
34					1.0000	*10*	.9788	*14*	.9232	*18*

(Continued)

Table A.5. Continued.

$m = 5$	n							
C_L	5	C_U	6	C_U	7	C_U	8	C_U
15	.0040	40	.0022	45	.0013	50	.0008	55
16	.0079	39	.0043	44	.0025	49	.0016	54
17	.0159	38	.0087	43	.0051	48	.0031	53
18	.0278	37	.0152	42	.0088	47	.0054	52
19	.0476	36	.0260	41	.0152	46	.0093	51
20	.0754	35	.0411	40	.0240	45	.0148	50
21	.1111	34	.0628	39	.0366	44	.0225	49
22	.1548	33	.0887	38	.0530	43	.0326	48
23	.2103	32	.1234	37	.0745	42	.0466	47
24	.2738	31	.1645	36	.1010	41	.0637	46
25	.3452	30	.2143	35	.1338	40	.0855	45
26	.4206	29	.2684	34	.1717	39	.1111	44
27	.5000	28	.3312	33	.2159	38	.1422	43
28	.5794	27	.3961	32	.2652	37	.1772	42
29	.6548	26	.4654	31	.3194	36	.2176	41
30	.7262	25	.5346	30	.3775	35	.2618	40
31	.7897	24	.6039	29	.4381	34	.3108	39
32	.8452	23	.6688	28	.5000	33	.3621	38
33	.8889	22	.7316	27	.5619	32	.4165	37
34	.9246	21	.7857	26	.6225	31	.4716	36
35	.9524	20	.8355	25	.6806	30	.5284	35
36	.9722	19	.8766	24	.7348	29	.5835	34
37	.9841	18	.9113	23	.7841	28	.6379	33
38	.9921	17	.9372	22	.8283	27	.6892	32
39	.9960	16	.9589	21	.8662	26	.7382	31
40	1.0000	15	.9740	20	.8990	25	.7824	30

(Continued)

Table A.5. Continued.

$m = 6$	n					
C_L	6	C_U	7	C_U	8	C_U
21	.0011	*57*	.0006	*63*	.0003	*69*
22	.0022	*56*	.0012	*62*	.0007	*68*
23	.0043	*55*	.0023	*61*	.0013	*67*
24	.0076	*54*	.0041	*60*	.0023	*66*
25	.0130	*53*	.0070	*59*	.0040	*65*
26	.0206	*52*	.0111	*58*	.0063	*64*
27	.0325	*51*	.0175	*57*	.0100	*63*
28	.0465	*50*	.0256	*56*	.0147	*62*
29	.0660	*49*	.0367	*55*	.0213	*61*
30	.0898	*48*	.0507	*54*	.0296	*60*
31	.1201	*47*	.0688	*53*	.0406	*59*
32	.1548	*46*	.0903	*52*	.0539	*58*
33	.1970	*45*	.1171	*51*	.0709	*57*
34	.2424	*44*	.1474	*50*	.0906	*56*
35	.2944	*43*	.1830	*49*	.1142	*55*
36	.3496	*42*	.2226	*48*	.1412	*54*
37	.4091	*41*	.2669	*47*	.1725	*53*
38	.4686	*40*	.3141	*46*	.2068	*52*
39	.5314	*39*	.3654	*45*	.2454	*51*
40	.5909	*38*	.4178	*44*	.2864	*50*
41	.6504	*37*	.4726	*43*	.3310	*49*
42	.7056	*36*	.5274	*42*	.3773	*48*
43	.7576	*35*	.5822	*41*	.4259	*47*
44	.8030	*34*	.6346	*40*	.4749	*46*
45	.8452	*33*	.6859	*39*	.5251	*45*
46	.8799	*32*	.7331	*38*	.5741	*44*
47	.9102	*31*	.7774	*37*	.6227	*43*
48	.9340	*30*	.8170	*36*	.6690	*42*
49	.9535	*29*	.8526	*35*	.7136	*41*
50	.9675	*28*	.8829	*34*	.7546	*40*
51	.9794	*27*	.9097	*33*	.7932	*39*

(Continued)

Table A.5. Concluded.

$m = 7$			n		$m = 8$		
	7		8			8	
C_L		C_U		C_U	C_L		C_U
28	.0003	77	.0002	84	36	.0001	100
29	.0006	76	.0003	83	37	.0002	99
30	.0012	75	.0006	82	38	.0003	98
31	.0020	74	.0011	81	39	.0005	97
32	.0035	73	.0019	80	40	.0009	96
33	.0055	72	.0030	79	41	.0015	95
34	.0087	71	.0047	78	42	.0023	94
35	.0131	70	.0070	77	43	.0035	93
36	.0189	69	.0103	76	44	.0052	92
37	.0265	68	.0145	75	45	.0074	91
38	.0364	67	.0200	74	46	.0103	90
39	.0487	66	.0270	73	47	.0141	89
40	.0641	65	.0361	72	48	.0190	88
41	.0825	64	.0469	71	49	.0249	87
42	.1043	63	.0603	70	50	.0325	86
43	.1297	62	.0760	69	51	.0415	85
44	.1588	61	.0946	68	52	.0524	84
45	.1914	60	.1159	67	53	.0652	83
46	.2279	59	.1405	66	54	.0803	82
47	.2675	58	.1678	65	55	.0974	81
48	.3100	57	.1984	64	56	.1172	80
49	.3552	56	.2317	63	57	.1393	79
50	.4024	55	.2679	62	58	.1641	78
51	.4508	54	.3063	61	59	.1911	77
52	.5000	53	.3472	60	60	.2209	76
53	.5492	52	.3894	59	61	.2527	75
54	.5976	51	.4333	58	62	.2869	74
55	.6448	50	.4775	57	63	.3227	73
56	.6900	49	.5225	56	64	.3605	72
57	.7325	48	.5667	55	65	.3992	71
58	.7721	47	.6106	54	66	.4392	70
59	.8086	46	.6528	53	67	.4796	69
60	.8412	45	.6937	52	68	.5204	68
61	.8703	44	.7321	51	69	.5608	67
62	.8957	43	.7683	50	70	.6008	66
63	.9175	42	.8016	49	71	.6395	65
					72	.6773	64
					73	.7131	63
					74	.7473	62
					75	.7791	61
					76	.8089	60

Table A.6. Critical values of Spearman's ρ for testing the significance of a rank correlation. Table gives upper critical value of Spearman's ρ for specified level of significance. Lower critical values are equal to $-\rho$.

	Significance, α, for One-tailed Test					
	.10	.05	.025	.01	.005	.001
	Significance, α, for Two-tailed Test					
	.20	.10	.05	.02	.01	.002
n						
4	.8000	.8000				
5	.7000	.8000	.9000	.9000		
6	.6000	.7714	.8286	.8857	.9429	
7	.5357	.6786	.7450	.8571	.8929	.9643
8	.5000	.6190	.7143	.8095	.8571	.9286
9	.4667	.5833	.6833	.7667	.8167	.9000
10	.4424	.5515	.6364	.7333	.7818	.8667
11	.4182	.5273	.6091	.7000	.7455	.8364
12	.3986	.4965	.5804	.6713	.7273	.8182
13	.3791	.4780	.5549	.6429	.6978	.7912
14	.3626	.4593	.5341	.6220	.6747	.7670
15	.3500	.4429	.5179	.6000	.6536	.7464
16	.3382	.4265	.5000	.5824	.6324	.7265
17	.3260	.4118	.4853	.5637	.6152	.7083
18	.3148	.3994	.4716	.5480	.5975	.6904
19	.3070	.3895	.4579	.5333	.5825	.6737
20	.2977	.3789	.4451	.5203	.5684	.6586
21	.2909	.3688	.4351	.5078	.5545	.6455
22	.2829	.3597	.4241	.4963	.5426	.6318
23	.2767	.3518	.4150	.4852	.5306	.6186
24	.2704	.3435	.4061	.4748	.5200	.6070
25	.2646	.3362	.3977	.4654	.5100	.5962
26	.2588	.3299	.3894	.4564	.5002	.5856
27	.2540	.3236	.3822	.4481	.4915	.5757
28	.2490	.3175	.3749	.4401	.4828	.5660
29	.2443	.3113	.3685	.4320	.4744	.5567
30	.2400	.3059	.3620	.4251	.4665	.5479

Table A.7. Critical values of D in the Kolmogorov–Smirnov goodness-of-fit test.

	Significance, α, for One-tailed Test					
	0.1	0.05	0.025	0.05	0.02	0.01
	Significance, α, for Two-tailed Test					
	0.2	0.1	0.05	0.025	0.01	0.005
n						
1	0.7275	0.8721	0.9950	0.9999	0.9999	0.9999
2	0.5551	0.6655	0.7592	0.8425	0.9413	0.9999
3	0.4671	0.5600	0.6389	0.7090	0.7922	0.8497
4	0.4114	0.4932	0.5627	0.6244	0.6977	0.7483
5	0.3720	0.4460	0.5088	0.5646	0.6309	0.6767
6	0.3422	0.4103	0.4681	0.5195	0.5804	0.6226
7	0.3187	0.3821	0.436	0.4838	0.5405	0.5798
8	0.2995	0.3591	0.4097	0.4546	0.5080	0.5448
9	0.2834	0.3398	0.3877	0.4302	0.4807	0.5156
10	0.2697	0.3234	0.3689	0.4094	0.4575	0.4907
11	0.2579	0.3092	0.3527	0.3914	0.4373	0.4691
12	0.2474	0.2967	0.3385	0.3756	0.4196	0.4501
13	0.2382	0.2856	0.3258	0.3616	0.4040	0.4333
14	0.2299	0.2757	0.3145	0.3490	0.3900	0.4183
15	0.2225	0.2668	0.3043	0.3377	0.3773	0.4048
16	0.2157	0.2586	0.2951	0.3274	0.3659	0.3924
17	0.2096	0.2513	0.2866	0.3181	0.3554	0.3812
18	0.2039	0.2444	0.2789	0.3095	0.3458	0.3709
19	0.1986	0.2382	0.2717	0.3015	0.3369	0.3614
20	0.1938	0.2323	0.2651	0.2942	0.3287	0.3526
21	0.1893	0.2270	0.2589	0.2873	0.3211	0.3443
22	0.1851	0.2219	0.2532	0.2810	0.3139	0.3367
23	0.1812	0.2172	0.2478	0.2750	0.3072	0.3296
24	0.1775	0.2128	0.2428	0.2694	0.3010	0.3228
25	0.1740	0.2086	0.2380	0.2641	0.2951	0.3166
26	0.1707	0.2047	0.2335	0.2591	0.2895	0.3106
27	0.1676	0.2010	0.2293	0.2544	0.2843	0.3049
28	0.1647	0.1975	0.2253	0.2500	0.2793	0.2996
29	0.1619	0.1941	0.2215	0.2458	0.2746	0.2946
30	0.1593	0.1910	0.2179	0.2418	0.2701	0.2897
31	0.1568	0.1880	0.2144	0.2379	0.2659	0.2852
32	0.1544	0.1851	0.2112	0.2343	0.2618	0.2808
33	0.1521	0.1823	0.2080	0.2308	0.2579	0.2766
34	0.1499	0.1797	0.2050	0.2275	0.2542	0.2726
35	0.1478	0.1772	0.2021	0.2243	0.2506	0.2688
36	0.1458	0.1748	0.1994	0.2212	0.2472	0.2652
37	0.1438	0.1725	0.1967	0.2183	0.2439	0.2616
38	0.1420	0.1702	0.1942	0.2155	0.2408	0.2582
39	0.1402	0.1681	0.1917	0.2128	0.2377	0.2550
40	0.1385	0.1660	0.1894	0.2102	0.2348	0.2519

(Continued)

Table A.7. Continued.

	Significance, α, for One-tailed Test					
	0.1	0.05	0.025	0.05	0.02	0.01
	Significance, α, for Two-tailed Test					
	0.2	0.1	0.05	0.025	0.01	0.005
41	0.1368	0.1640	0.1871	0.2076	0.2320	0.2489
42	0.1352	0.1621	0.1849	0.2052	0.2293	0.2460
43	0.1337	0.1602	0.1828	0.2029	0.2267	0.2431
44	0.1322	0.1585	0.1808	0.2006	0.2241	0.2404
45	0.1307	0.1567	0.1788	0.1984	0.2217	0.2378
46	0.1293	0.1551	0.1769	0.1963	0.2193	0.2353
47	0.1280	0.1534	0.1751	0.1942	0.2170	0.2328
48	0.1267	0.1519	0.1732	0.1923	0.2148	0.2304
49	0.1254	0.1503	0.1715	0.1903	0.2126	0.2281
50	0.1242	0.1488	0.1698	0.1885	0.2106	0.2259
51	0.1230	0.1474	0.1682	0.1866	0.2085	0.2237
52	0.1218	0.1460	0.1666	0.1849	0.2065	0.2216
53	0.1206	0.1447	0.1650	0.1831	0.2046	0.2195
54	0.1196	0.1433	0.1635	0.1815	0.2028	0.2175
55	0.1185	0.1421	0.1621	0.1798	0.2010	0.2155
56	0.1174	0.1408	0.1606	0.1783	0.1992	0.2137
57	0.1164	0.1396	0.1592	0.1767	0.1975	0.2118
58	0.1155	0.1384	0.1579	0.1753	0.1958	0.2100
59	0.1145	0.1373	0.1566	0.1738	0.1941	0.2082
60	0.1135	0.1361	0.1553	0.1723	0.1926	0.2065
61	0.1126	0.1350	0.1540	0.1709	0.1910	0.2049
62	0.1117	0.1340	0.1528	0.1696	0.1895	0.2033
63	0.1108	0.1329	0.1516	0.1683	0.1880	0.2017
64	0.1100	0.1319	0.1505	0.1670	0.1866	0.2001
65	0.1092	0.1309	0.1493	0.1657	0.1851	0.1986
66	0.1084	0.1299	0.1482	0.1645	0.1838	0.1971
67	0.1075	0.1290	0.1471	0.1633	0.1824	0.1957
68	0.1068	0.1280	0.1460	0.1621	0.1811	0.1942
69	0.1060	0.1271	0.1450	0.1609	0.1798	0.1928
70	0.1053	0.1262	0.1440	0.1598	0.1785	0.1915
71	0.1045	0.1253	0.1430	0.1587	0.1773	0.1901
72	0.1038	0.1245	0.1420	0.1576	0.1761	0.1888
73	0.1031	0.1236	0.1411	0.1565	0.1749	0.1876
74	0.1024	0.1228	0.1401	0.1555	0.1737	0.1863
75	0.1017	0.1220	0.1392	0.1544	0.1726	0.1851
76	0.1011	0.1212	0.1383	0.1534	0.1714	0.1839
77	0.1004	0.1204	0.1374	0.1525	0.1703	0.1827
78	0.0998	0.1197	0.1365	0.1515	0.1693	0.1816
79	0.0992	0.1189	0.1357	0.1506	0.1682	0.1805
80	0.0986	0.1182	0.1348	0.1496	0.1672	0.1793

(Continued)

Table A.7. Concluded.

	Significance, α, for One-tailed Test					
	0.1	0.05	0.025	0.05	0.02	0.01
	Significance, α, for Two-tailed Test					
	0.2	0.1	0.05	0.025	0.01	0.005
81	0.0980	0.1175	0.1340	0.1487	0.1662	0.1782
82	0.0974	0.1168	0.1332	0.1478	0.1652	0.1772
83	0.0968	0.1161	0.1324	0.1470	0.1642	0.1761
84	0.0962	0.1154	0.1316	0.1461	0.1632	0.1751
85	0.0957	0.1147	0.1309	0.1452	0.1623	0.1741
86	0.0951	0.1141	0.1301	0.1444	0.1613	0.1730
87	0.0946	0.1134	0.1294	0.1436	0.1604	0.1721
88	0.0941	0.1128	0.1287	0.1428	0.1595	0.1711
89	0.0935	0.1121	0.1279	0.1420	0.1586	0.1702
90	0.0930	0.1115	0.1272	0.1412	0.1578	0.1692
91	0.0925	0.1109	0.1265	0.1404	0.1569	0.1683
92	0.0920	0.1103	0.1259	0.1397	0.1561	0.1674
93	0.0915	0.1097	0.1252	0.1390	0.1552	0.1665
94	0.0911	0.1092	0.1245	0.1382	0.1544	0.1656
95	0.0906	0.1086	0.1239	0.1375	0.1536	0.1648
96	0.0901	0.1081	0.1233	0.1368	0.1528	0.1639
97	0.0897	0.1075	0.1226	0.1361	0.1520	0.1631
98	0.0892	0.1069	0.1220	0.1354	0.1513	0.1623
99	0.0888	0.1064	0.1214	0.1347	0.1505	0.1614
100	0.0883	0.1059	0.1208	0.1341	0.1498	0.1607

Table A.8. Critical values of the Lilliefors test statistic, T, for testing goodness-of-fit to a normal distribution.

	Level of Significance, α				
	.20	.15	.10	.05	.01
Sample size,					
n = 4	.300	.319	.352	.381	.417
5	.285	.299	.315	.337	.405
6	.265	.277	.294	.319	.364
7	.247	.258	.276	.300	.348
8	.233	.244	.261	.285	.331
9	.223	.233	.249	.271	.311
10	.215	.224	.239	.258	.294
11	.206	.217	.230	.249	.284
12	.199	.212	.223	.242	.275
13	.190	.202	.214	.234	.268
14	.183	.194	.207	.227	.261
15	.177	.187	.201	.220	.257
16	.173	.182	.195	.213	.250
17	.169	.177	.189	.206	.245
18	.166	.173	.184	.200	.239
19	.163	.169	.179	.195	.235
20	.160	.166	.174	.190	.231
25	.142	.147	.158	.173	.200
30	.131	.136	.144	.161	.187
>30	$\frac{.736}{\sqrt{n}}$	$\frac{.768}{\sqrt{n}}$	$\frac{.805}{\sqrt{n}}$	$\frac{.886}{\sqrt{n}}$	$\frac{1.031}{\sqrt{n}}$

Table A.9. Maximum likelihood estimates of the concentration parameter κ for calculated values of $\overline{R}$ (adapted from Batschelet, 1965; and Gumbel, Greenwood, and Durand, 1953).

$\overline{R}$	κ	$\overline{R}$	κ	$\overline{R}$	κ
0.00	0.00000	0.35	0.74783	0.70	2.01363
.01	.02000	.36	.77241	.71	2.07685
.02	.04001	.37	.79730	.72	2.14359
.03	.06003	.38	.82253	.73	2.21425
.04	.08006	.39	.84812	.74	2.28930
.05	.10013	.40	.87408	.75	2.36930
.06	.12022	.41	.90043	.76	2.45490
.07	.14034	.42	.92720	.77	2.54686
.08	.16051	.43	.95440	.78	2.64613
.09	.18073	.44	.98207	.79	2.75382
.10	.20101	.45	1.01022	.80	2.87129
.11	.22134	.46	1.03889	.81	3.00020
.12	.24175	.47	1.06810	.82	3.14262
.13	.26223	.48	1.09788	.83	3.30114
.14	.28279	.49	1.12828	.84	3.47901
.15	.30344	.50	1.15932	.85	3.68041
.16	.32419	.51	1.19105	.86	3.91072
.17	.34503	.52	1.22350	.87	4.17703
.18	.36599	.53	1.25672	.88	4.48876
.19	.38707	.54	1.29077	.89	4.85871
.20	.40828	.55	1.32570	.90	5.3047
.21	.42962	.56	1.36156	.91	5.8522
.22	.45110	.57	1.39842	.92	6.5394
.23	.47273	.58	1.43635	.93	7.4257
.24	.49453	.59	1.47543	.94	8.6104
.25	.51649	.60	1.51574	.95	10.2716
.26	.53863	.61	1.55738	.96	12.7661
.27	.56097	.62	1.60044	.97	16.9266
.28	.58350	.63	1.64506	.98	25.2522
.29	.60625	.64	1.69134	.99	50.2421
.30	.62922	.65	1.73945	1.00	∞
.31	.65242	.66	1.78953		
.32	.67587	.67	1.84177		
.33	.69958	.68	1.89637		
.34	.72356	.69	1.95357		

Table A.10. Critical values of $\overline{R}$ for Rayleigh's test for the presence of a preferred trend. From Mardia (1972).

	Level of Significance, α			
	.10	.05	.025	.01
Sample size,				
n = 4	0.768	0.847	0.905	0.960
5	.677	.754	.816	.879
6	.618	.690	.753	.825
7	.572	.642	.702	.771
8	.535	.602	.660	.725
9	.504	.569	.624	.687
10	.478	.540	.594	.655
11	.456	.516	.567	.627
12	.437	.494	.544	.602
13	.420	.475	.524	.580
14	.405	.458	.505	.560
15	.391	.443	.489	.542
16	.379	.429	.474	.525
17	.367	.417	.460	.510
18	.357	.405	.447	.496
19	.348	.394	.436	.484
20	.339	.385	.425	.472
21	.331	.375	.415	.461
22	.323	.367	.405	.451
23	.316	.359	.397	.441
24	.309	.351	.389	.432
25	.303	.344	.381	.423
30	.277	.315	.348	.387
35	.256	.292	.323	.359
40	.240	.273	.302	.336
45	.226	.257	.285	.318
50	.214	.244	.270	.301

Table A.11. Critical values of $\overline{R}$ for the test of uniformity of a spherical distribution.

	Level of Significance, α			
	.10	.05	.02	.01
Sample size,				
n = 5	0.637	0.700	0.765	0.805
6	.583	.642	.707	.747
7	.541	.597	.659	.698
8	.506	.560	.619	.658
9	.478	.529	.586	.624
10	.454	.503	.558	.594
11	.433	.480	.533	.568
12	.415	.460	.512	.546
13	.398	.442	.492	.526
14	.384	.427	.475	.507
15	.371	.413	.460	.491
16	.359	.400	.446	.476
17	.349	.388	.443	.463
18	.339	.377	.421	.450
19	.330	.367	.410	.438
20	.322	.358	.399	.428
21	.314	.350	.390	.418
22	.307	.342	.382	.408
23	.300	.334	.374	.400
24	.294	.328	.366	.392
25	.288	.321	.359	.384
30	.26	.29	.33	.36
35	.24	.27	.31	.33
40	.23	.26	.29	.31
45	.22	.24	.27	.29
50	.20	.23	.26	.28
100	.14	.16	.18	.19

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