Multivariate Analysis for the Behavioral Sciences

Second Edition

Kimmo Vehkalahti
Brian S. Everitt

CRC Press
Taylor & Francis Group
Boca Raton London New York

CRC Press is an imprint of the
Taylor & Francis Group, an **informa** business

“MABS for IODS”

Selected excerpts of the textbook *Multivariate Analysis for the Behavioral Sciences*, Second Edition (Vehkalahti and Everitt, 2019), produced exclusively for the students of IODS (Introduction to Open Data Science, University of Helsinki), with a permission from Chapman and Hall/CRC, London, UK.

Contents

Preface

In some respects this book is a second edition of *Multivariable Modeling and Multivariate Analysis for the Behavioral Sciences* but in others it is largely a new book with new chapters on missing values and the analysis of longitudinal data where the response variable can not be assumed to be normally distributed. The book also includes a wider account of generalized linear models as well as a new chapter on multidimensional scaling and correspondence analysis and separate chapters on exploratory and confirmatory factor analysis; in the latter there is also new coverage of structural equation models. A number of interesting, new examples and exercises have been added in several chapters.

The original lengthy title tried to explain that the book covered situations where the variables of interest consisted of a response variable and explanatory variables and where interest lies in finding suitable models relating the response to the explanatory variables, hence *multivariable modeling*, in addition to techniques that can be applied to what has historically been termed *multivariate data* where there is no division of the variables and the aim is to find a parsimonious description of the structure of the data. The current book contains extended coverage of both situations but has been given a somewhat shorter title, *Multivariate Analysis for the Behavioral Sciences*, because both types of data mentioned can be represented symbolically by an $n \times q$ matrix $\mathbf{X}$ containing the q variable values for n number of units (often subjects) in the data set. Chapters 3–11 will describe methods for dealing with data when one of the q variables is a response and the others explanatory, while the remaining chapters deal with methods for the analysis of data sets where there is no such division of the variables. We hope this makes it clear that this book covers accounts of a wider range of statistical methodology than covered in the conventional ‘multivariate analysis’ textbook.

The ‘we’ opening the last sentence above brings us to the most important change between this book and that mentioned in the first line of this Preface, namely the arrival of a co-author Dr. Kimmo Vehkalahti. It is Kimmo who is responsible for many of the changes and most of the new material in this book compared with the original on which it is based.

Most chapters include ‘technical detail’ sections which briefly describe the theory behind the methods of concern in the chapter. These sections often require a familiarity with some relatively advanced mathematics, for example, matrix algebra, for their understanding (see Puntanen et al., 2011, 2013). Readers without the necessary grounding in maths can largely ignore such sections and instead concentrate on the examples given to help them understand the practical implications of the methods.

There are exercises at the end of each chapter, some of which are ‘starred’ (*) to indicate that they are more challenging and could perhaps be used as the basis of student projects. Data sets for most exercises are not given in the text but are available on the associated web sites (see later) where they are identified by the relevant exercise number. For the starred exercises the web sites also contain pointers to the appropriate analysis.

The web site for the book is www.crcpress.com and in addition the book has a GitHub repository (https://github.com/KimmoVehkalahti/MABS) for distributing the complete data sets and the R code for reproducing the examples and for answering the exercises; consequently this allows us to abbreviate the listings of most data sets in the text.

We hope that this book will be found useful in a number of different ways, including:

- As the main part of a formal statistics course for advanced undergraduates and postgraduates in all areas of the behavioral sciences,
- As a supplement to an existing course,
- For self-study,
- For researchers in the behavioral sciences undertaking statistical analyses on their data,
- For statisticians teaching statistics to psychologists and others,
- For statisticians using R when teaching intermediate statistics courses both in the behavioral sciences and in other areas.

Brian S. Everitt
Dulwich, London

Kimmo Vehkalahti
Vuosaari, Helsinki

Preface to Multivariable Modeling and Multivariate Analysis for the Behavioral Sciences

The *Encyclopedia of Statistics in Behavioral Science* (Everitt and Howell, 2005) opens with the following paragraph:

> Forty years ago there was hardly a field called "behavioral science." In fact, psychology largely was the behavioral sciences, with some help from group theory in sociology and decision making in economics. Now, of course, psychology has expanded and developed in a myriad of ways, to the point where behavioral science is often the most useful term. Physiological psychology has become neuroscience, covering areas not previously part of psychology. Decision-making has become decision science, involving people from economics, marketing, and other disciplines. Learning theory has become cognitive science, again exploring problems that were not even considered 40 years ago. And developments in computing have brought forth a host of new techniques that were not possible in the days of manual and electronic calculators. With all these changes, there have been corresponding changes in the appropriate statistical methodologies.

Despite the changes mentioned in the last sentence of this quotation, many statistical books aimed at psychologists and others working in the behavioral sciences continue to cover primarily simple hypothesis testing, using a variety of parametric and nonparametric significance tests, simple linear regression, and analysis of variance. Such statistical methodology remains important in introductory courses, but represents only the first step in equipping behavioral science students with enough statistical tools to help them on their way to success in their later careers. The aim of this book is to encourage students and others to learn a little more about statistics and, equally important, how to apply statistical methods in a sensible fashion. It is hoped that the following features of the text will help it reach its target:

- The central theme is that statistics is about solving problems; data relevant to these problems are collected and analyzed to provide useful answers. To this end, the book contains a large number of real data sets arising from real problems. Numerical examples of the type that involve the skiing activities of belly dancers and politicians are avoided as far as possible.

- Mathematical details of methods are confined to numbered and separated Technical Sections. For the mathematically challenged, the most difficult of these displays can, at least as a last resort, be ignored. But the study of the relevant mathematical material (which on occasion will include the use of vectors and matrices) will undoubtedly help in the reader's appreciation of the corresponding technique.

- Although many statistical methods require considerable amounts of arithmetic for their application, the burden of actually performing the necessary calculations has been almost entirely removed by the development and wide availability of powerful and relatively cheap personal computers and associated statistical software packages. It is assumed, therefore, that all students will be using such tools when undertaking their own analyses. Consequently, arithmetic details are noticeable largely by their absence, although a little arithmetic is included where it is considered helpful in explaining a technique.

- There are many challenging data sets both in the text and in the exercises provided at the end of each chapter. All data sets, both in the body of the text and in the exercises, are given on the Web site associated with the book, as are the answers to all the exercises. (Because the majority of data sets used in the book are available on the book's Web site (http://www.crcpress.com/product/isbn/9781439807699), tables of data in the text only give a small subset of each data set.)

As mentioned in the penultimate bullet point above, the text assumes that readers will be using one or another of the many available statistical software packages for data analysis. This raises the thorny question for the author of what information should be provided in the text about software. Would, for example, screen dumps from SPSS be useful, or listings of STATA code? Perhaps, but neither are included here. Instead, all the computer code used to analyze the many examples to be found in the text is given on the book's Web site, and this code is in the R language, where R is a software system for statistical computing, data analysis, and graphics. This may appear a strange choice for a book aimed at behavioral scientists, but the rationale behind the choice is first that the author uses R in preference to other statistical software, second that R can be used to produce many interesting and informative graphics that are difficult if not impossible to produce with other software, third that R is free and can be easily downloaded by students, and fourth, R has a very active user community and recently developed statistical methods become available far more quickly than they do with other packages. The only downside with R is that it takes a little more time to learn than say using "point-and-click" SPSS. The initial extra effort, however, is rapidly rewarded. A useful book for learning more about R is Everitt and Hothorn (2009).

The material covered in the book assumes the reader is familiar with the topics covered in introductory statistics courses, for example, population, sample, variable, parameter, significance test, p-value, confidence interval, correlation, simple regression, and analysis of variance. The book is primarily about methods for analyzing data but some comments are made in Chapter 1 about the various types of study that behavioral researchers may use and their design. And it is in Chapter 1 that the distinction between multivariable and multivariate—both of which appear in the book's title—will be explained.

It is hoped that the text will be useful in a number of different ways, including:

- As the main part of a formal statistics course for advanced undergraduates and postgraduates in all areas of the behavioral sciences.
- As a supplement to an existing course.
- For self-study.
- For researchers in the behavioral sciences undertaking statistical analyses on their data.
- For statisticians teaching statistics to psychologists and others.
- For statisticians using R when teaching intermediate statistics courses both in the behavioral sciences and in other areas.

B. S. Everitt
Dulwich, U.K.

Authors

Kimmo Vehkalahti is a fellow of the Teachers' Academy, University of Helsinki, Finland. He has been a part of the faculty of Social Sciences for over 25 years, currently as senior lecturer of the Social Data Science in the Centre for Research Methods. He is author of a Finnish textbook on measurement and survey methods. The present book is his first international textbook on statistics. His research and teaching activities are related to open data science, multivariate analysis, and introductory statistics. His spare time is divided (unequally) between jogging and trail running, reading, watching ice hockey, holidays with his wife, and singing tenor in choir.

Brian S. Everitt is professor emeritus, King's College, London, UK. He worked at the Institute of Psychiatry, University of London for over 35 years, finally as head of the Biostatistics and Computing Department and professor of behavioural statistics. He is author or co-author of over 70 books on statistics and approximately 100 papers and other articles, and was a section editor for the *Encyclopedia of Biostatistics*, published by Wiley. In retirement, he divides his time between working as editor-in-chief of *Statistical Methods in Medical Research*, playing tennis, watching cricket, long walking holidays with his wife, and playing classical guitar in private.

Acknowledgments

Kimmo would like to thank the faculty of Social Sciences at the University of Helsinki for granting him a six-month sabbatical without which this book could not have been written. Three months of this sabbatical were spent at the Universitat Pompeu Fabra in Barcelona at the kind invitation and hospitality of Professor Michael Greenacre. The hard work needed to get to grips with R and LaTeX was greatly aided by the sharing of an office (and coffee breaks) with Michael at Campus de la Ciutadella. Gràcies!

Kimmo's thanks are also given to Maria Anna Donati, Ulla Palotie, Juha Törmänen, Raimo Hämäläinen, Esa Saarinen, and Seppo Mustonen, all of whom gave their permission to use their interesting data sets in this book; he has the warmest memories of staying in the beautiful home of the lovely Firenze family. Grazie Caterina Primi, Michele e Luisa!

Thanks are given to Dr. Deepayan Sarkar, the author of *Lattice: Multivariate Data Visualization with R*, and Springer, the publishers of the book, for permission to use Figures 2.8, 2.9, 4.5, 4.6, 4.7, and 5.16 in Chapter 2 of this book.

Brian and Kimmo thank each other for an extremely smooth collaboration that allowed this book to be completed on time whilst allowing them to become and remain good friends; they also agree that sincere thanks are given to Rob Calver of Taylor & Francis, who has been, as always, supportive and encouraging during the writing of the book.

Part I

Prerequisites and introductory material ("MABS for IODS")

Selected excerpts of the textbook *Multivariate Analysis for the Behavioral Sciences*, Second Edition (Vehkalahti and Everitt, 2019), produced exclusively for the students of IODS (Introduction to Open Data Science, University of Helsinki), with a permission from Chapman and Hall/CRC, London, UK.

1 Data, Measurement, and Models

This chapter discusses the various types of studies used in behavioral research and the various levels of measurements that are made. The use of p-values by behavioral researchers is considered and the advantages of confidence intervals made clear.

2 Looking at Data

Graphical displays are very popular in many areas and graphical presentation of data often leads to unexpected insights. In this chapter a variety of graphical techniques are described including histograms, bar charts, boxplots and scatterplots. The use of these methods is illustrated by a number of examples taken from behavioral studies. The possibility of graphical deception is also considered in the chapter.

1

Data, Measurement, and Models

1.1 Introduction

> Statistics is a general intellectual method that applies wherever data, variation, and chance appear. It is a fundamental method because data, variation and chance are omnipresent in modern life. It is an independent discipline with its own core ideas, rather than, for example, a branch of mathematics ... Statistics offers general, fundamental and independent ways of thinking.
>
> ***Journal of the American Statistical Association***

Quintessentially, statistics is about solving problems; data (measurements or observations) relevant to these problems are collected, and statistical analyses are used to provide useful answers. But the path from data collection to analysis and interpretation is often not straightforward. Most real-life applications of statistical methodology have one or more nonstandard features, meaning in practice that there are few routine statistical questions, although there are questionable statistical routines. Many statistical pitfalls lie in wait for the unwary. Indeed, statistics is perhaps more open to misuse than most other subjects, particularly by the nonstatistician with access to powerful statistical software. The misleading average, the graph with "fiddled axes," the inappropriate p-value, and the linear regression fitted to nonlinear data are just four examples of horror stories that are part of statistical folklore.

Statisticians often complain that many of those working in the behavioral sciences put undue faith in significance tests, use complex methods of analysis when the data merit only a relatively simple approach, and sometimes abuse the statistical techniques they are employing. Statisticians become upset (and perhaps feel a little insecure) when their advice to, say, "plot a few simple graphs," is ignored in favor of a multivariate analysis of covariance or similar statistical extravagance.

However, if statisticians are at times horrified by the way in which behavioral scientists apply statistical techniques, behavioral scientists may be no less horrified by many statisticians' apparent lack of awareness of what stresses behavioral research can place on an investigator. A statistician may, for example, demand a balanced design with 30 subjects in each cell so as to achieve some appropriate power for the analysis. But it is not the statistician who is faced with the frustration caused by a last-minute phone call from a subject who cannot take part in an experiment that has taken several hours to arrange. Again, the statistician advising on a longitudinal study may call for more effort in carrying out follow-up interviews so that the study avoids statistical problems produced by the presence of missing data. It is, however, the behavioral researcher who must continue to persuade people to talk about potentially distressing aspects of their lives, who must confront possibly dangerous respondents, or who arrives at a given (and often remote) address to conduct an interview, only to find that the person is not at home. Many statisticians often do not appear to appreciate the complex stories behind each data point in many behavioral studies. One way of improving the possible communication problems between behavioral scientist and statistician is for each to learn more about the language of the other. There is already available a plethora of, for example, "Statistics for Psychologists" books, but sadly, (as far as we know) no "Psychology for Statisticians" equivalent. Perhaps there should be?

Having outlined briefly a few caveats about the possible misuse of statistics and the equally possible conflict between statistician and behavioral scientist, it is time to move on to consider some of the basics of behavioral science studies and their implications for statistical analysis.

1.2 Types of Study

It is said that, when Gertrude Stein lay dying, she roused briefly and asked her assembled friends, "Well, what's the answer?" They remained uncomfortably quiet, at which she sighed, "In that case, what's the question?"

Research in the behavioral science, as in science in general, is about searching for the answers to particular questions of interest. Do politicians have higher IQs than university lecturers? Do men have faster reaction times than women? Should phobic patients be treated by psychotherapy or by a behavioral treatment such as flooding? Do children who are abused have more problems later in life than children who are not abused? Do children of divorced parents suffer more marital breakdowns themselves than children from more stable family backgrounds?

In more general terms, scientific research involves a sequence of asking and answering questions about the nature of relationships among variables (e.g., How does A affect B? Do A and B vary together? Is A significantly different from B? and so on). Scientific research is carried out at many levels that differ in the types of question asked and therefore in the procedures used to answer them. Thus, the choice of which methods to use in research is largely determined by the kinds of questions that are asked.

Of the many types of investigation used in behavioral research, the most common are perhaps the following:

- Surveys
- Experiments
- Observational studies
- Quasi-experiments

Some brief comments about each of these four types are given below; a more detailed account is available in the papers by Stretch, Raulin, and Graziano, and by Dane, all of which appear in the second volume of the excellent *Companion Encyclopedia of Psychology* (see Colman, 1994).

1.2.1 Surveys

Survey methods are based on the simple discovery that "asking questions is a remarkably efficient way to obtain information from and about people" (Schuman and Kalton, 1985, p. 635). Surveys involve an exchange of information between researcher and respondent; the researcher identifies topics of interest, and the respondent provides knowledge or opinion about these topics. Depending upon the length and content of the survey as well as the facilities available, this exchange can be accomplished via written questionnaires, in-person interviews, or telephone conversations; and, in the 21st century, surveys via the Internet are increasingly common.

Surveys conducted by behavioral scientists are usually designed to elicit information about the respondents' opinions, beliefs, attitudes, and values. Perhaps one of the most famous surveys of the 20th century was that conducted by Alfred Charles Kinsey, a student of human sexual behavior in the 1940s and 1950s. The first Kinsey report, *Sexual Behavior in the Human Male*, appeared in 1948 (see Kinsey et al., 1948), and the second, *Sexual Behavior in the Human Female*, in 1953 (see Kinsey et al., 1953). It is no exaggeration to say that both reports caused a sensation, and the first quickly became a bestseller.

Surveys are often a flexible and powerful approach to gathering information of interest, but careful consideration needs to be given to several aspects of the survey if the information is to be accurate, particularly when dealing with a sensitive topic. Having a representative sample, having a large-enough sample, minimizing nonresponse, and ensuring that the questions asked elicit accurate responses are just a few of the issues that the researcher thinking of carrying out a survey needs to consider. Readers are referred to Bradburn et al. (2004) and Tourangeau et al. (2000) for a broad coverage of practical advice for questionnaire construction and Laaksonen (2018), Groves et al. (2009), de Leeuw et al. (2008) and Lehtonen and Pahkinen (2004) for detailed accounts of survey sampling and survey methodology.

Examples of data collected in surveys and their analysis are given in several later chapters.

1.2.2 Experiments

According to Sir Ronald Fisher, perhaps the greatest statistician of the 20th century, “experiments are only experience carefully planned in advance and designed to form a secure basis of new knowledge.” The essential feature of an experiment is the large degree of control in the hands of the experimenters, and in designed experiments the goal is to allow inferences to be drawn about the effects of an intervention of interest that are logically compelled by the data and hence allow assessment of a *causal relationship*. In many cases the “intervention” will be some form of therapy in which case the experiment is usually called a clinical trial.

In an experiment, the researcher controls the manner in which subjects are allocated to the different levels of the experimental factors. In a comparison of a new treatment with one used previously, for example, the researcher would have control over the scheme for allocating subjects to the two treatments. The manner in which this control is exercised is of vital importance if the results of the experiment are to lead to a largely unambiguous assessment of the effect of treatment. The objective in allocation is that the groups to be compared should be alike in all respects except the intervention (treatment) received. Comparable groups prior to the intervention ensure that differences in outcomes after the intervention reflect effects of the intervention in an unbiased fashion. Let us begin by considering two flawed allocation procedures that are unlikely to achieve the desired degree of similarity of the two groups.

- Perhaps the first subjects to volunteer to take part in the experiment should all be given the new treatment, for example, and the later ones the old treatment? The two groups formed in this way may differ in level of motivation and so subsequently in performance. Observed treatment differences would be confounded with differences produced by the allocation procedure. Alternatively, early volunteers might be more seriously ill, those desperate to find a new remedy that works, and again, this might lead to a bias in the measured difference between the two treatments.

- So what about putting alternate subjects into each group? The objection to this is that the experimenter will know who is receiving what treatment and may be tempted to “tinker” with the scheme to ensure that those patients who are most ill receive the new treatment.

So, how should we form the groups that will be used to assess an experimental intervention? The answer is deceptively simple—use randomization. The group to which a participant in the experiment is allocated is decided by chance. It could be arranged by flipping a coin each time a new eligible patient arrives, and allocating the patient to the new treatment if the result is a head, or to the old treatment if a tail appears. In practice, of course, a more sophisticated randomization procedure will be used. The essential feature, however, is randomization, rather than the mechanism used to achieve it. Randomization was introduced into scientific experiments far more recently, when in 1926 Fisher randomly assigned individual blocks or plots of land in agricultural experiments to receive particular types of "treatment"—different amounts of fertilizer. The primary benefit that randomization has is the chance (and therefore impartial) assignment of extraneous influences among the groups to be compared, and it offers this control over such influences whether or not they are known by the experimenter to exist. Note that randomization does not claim to render the two samples equal with regard to these influences; if, however, the same procedure was applied to repeated samples from the population, equality would be achieved in the long run. Thus, randomization ensures a lack of bias, whereas other methods of assignment may not. In a properly conducted, randomized, experiment the interpretation of an observed group difference is largely unambiguous; its cause is very likely to be the different treatments or conditions received by the groups.

Several of the data sets introduced and analyzed in later chapters arise from experimental studies, often clinical trials.

1.2.3 Observational Studies

Suppose a researcher is interested in investigating how smoking cigarettes affects a person's systolic blood pressure. Using the experimental approach described earlier, people would have to be allocated at random to two groups, the members of one group being asked to smoke some quantity of cigarettes per day, and the members of the other group required not to smoke at all. Clearly, no ethical committee would approve of such a study. So, what can be done? An approach that would get ethical approval is to measure the systolic blood pressure of naturally occurring groups of individuals who smoke, and those who do not, and then compare the results. This would then be what is known as an observational study, defined by Cochran (1965) as follows:

> An empiric comparison of "treated" and "control" groups in which the objective is to elucidate cause-and-effect relationships but where it is not possible to use controlled experimentation, in the sense of being able to impose the procedures or treatments whose effects it is desired to discover, or to assign patients at random to different procedures.

Many observational studies involve recording data on the members of naturally occurring groups, generally over a period of time, and comparing the rate at which a particular event of interest occurs in the different groups (such studies are often referred to as prospective). If, for example, an investigator was interested in the health effects of a natural disaster such as an earthquake, those who experienced the earthquake could be compared, on some outcome variable of interest, with a group of people who did not.

Another commonly used type of observational study is the case-control investigation. Here, a group of people (the cases) all having a particular characteristic (a certain disease perhaps) are compared with a group of people who do not have the characteristic (the controls), in terms of their past exposure to some event or risk factor. The cases and controls are usually matched one-to-one for possible confounding variables. An example of such a study is reported in Lehman et al. (1987). Here the researchers collected data following the sudden death of a spouse or a child in a car crash. They matched 80 bereaved spouses and parents to 80 controls drawn from 7582 individuals who came to renew their driver's license. Specifically, they matched for gender, age, family income before crash, education level, and number and ages of children.

The types of analyses suitable for observational studies are often the same as those used for experimental studies. Unlike experiments, however, the lack of control over the groups to be compared in an observational study makes the interpretation of any difference between the groups detected in the study open to a variety of interpretations. In the smoking and systolic blood pressure study, for example, any difference found between the blood pressures of the two groups would be open to three possible interpretations:

- Smoking causes a change in systolic blood pressure.
- Level of blood pressure has a tendency to encourage or discourage smoking.
- Some unidentified factors play a part in determining both the level of blood pressure and whether or not a person smokes.

In the design of an observational study, an attempt is made to reconstruct some of the structure and strengths of an experiment. But the possible ambiguity in interpretation of the results from an observational study, however well designed, means that the observational approach is not as powerful as a designed experiment. A detailed account of observational studies is given in Rosenbaum (2002).

1.2.4 Quasi-Experiments

Quasi-experimental designs resemble experiments proper but are weak on some of the characteristics. In particular (and as in the observational study), the ability to manipulate the groups to be compared is not under the investigator's control. But, unlike the observational study, the quasi-experiment involves the intervention of the investigator in the sense that he or she applies a variety of different "treatments" to naturally occurring groups. In investigating the effectiveness of three different methods of teaching mathematics to 15 year olds, for example, a method might be given to all the members of a particular class in a school. The three classes that receive the different teaching methods would be selected to be similar to each other on most relevant variables, and the methods would be assigned to classes on a chance basis.

For more details of quasi-experiments see Shadish et al. (2002).

1.3 Types of Measurement

The measurements and observations made on a set of subjects comprise the basic material that is the foundation of all behavioral science investigations. These measurements provide the data for statistical analysis from which the researcher will draw his or her conclusions. Clearly, not all measurements are the same. Measuring an individual's weight is qualitatively different from measuring that person's response to some treatment on a two-category scale: "improved" and "not improved," for example. Whatever measurements are made, they need to be objective, precise, and reproducible for reasons nicely summarized in the following quotation from Fleiss (1986):

> The most elegant design of a study will not overcome the damage caused by unreliable or imprecise measurement. The requirement that one's data be of high quality is at least as important a component of a proper study design as the requirement for randomization, double blinding, controlling where necessary for prognostic factors, and so on. Larger sample sizes than otherwise necessary, biased estimates, and even biased samples are some of the untoward consequences of unreliable measurements that can be demonstrated.

Measurements are often differentiated according to the degree of precision involved. If it is said that an individual has a high IQ, it is not as precise as the statement that the individual has an IQ of 151. The comment that a woman is tall is not as accurate as specifying that her height is 1.88 m. Certain characteristics of interest are more amenable to precise measurement than others. Given an accurate thermometer, a subject's temperature can be measured very precisely. Quantifying the level of anxiety or depression of a psychiatric patient or assessing the degree of pain of a migraine sufferer are, however, more difficult measurement tasks.

Four levels of measurement scales are generally distinguished.

1.3.1 Nominal or Categorical Measurements

Nominal measurements allow classification with respect to some characteristic. Examples of such measurements are marital status, sex, and blood group. The properties of a nominal measurement are

- The categories are mutually exclusive (an individual can belong to only one category).
- The categories have no logical order—numbers may be assigned to categories but merely as convenient labels.

1.3.2 Ordinal Scale Measurements

The next level of measurement is the ordinal scale. This scale has one additional property over those of a nominal measurement—a logical ordering of the categories. With such measurements, the numbers assigned to the categories indicate the amount of a characteristic possessed. A psychiatrist may, for example, grade patients on an anxiety scale as "not anxious," "mildly anxious," "moderately anxious," or "severely anxious," and use the numbers 0, 1, 2, and 3 to label the categories, with lower numbers indicating less anxiety. The psychiatrist cannot infer, however, that the difference in anxiety between patients with scores of, say, 0 and 1 is the same as the difference between patients assigned scores 2 and 3. The scores on an ordinal scale do, however, allow patients to be ranked with respect to the characteristic being assessed.

The following are the properties of an ordinal scale:

- The categories are mutually exclusive.
- The categories have some logical order.
- The categories are scaled according to the amount of a particular characteristic they indicate.

1.3.3 Interval Scales

The third level of measurement is the interval scale. Such scales possess all the properties of an ordinal scale plus the additional property that equal differences between category levels, on any part of the scale, reflect equal differences in the characteristic being measured. An example of such a scale is temperature on the Celsius (C) or Fahrenheit (F) scale; the difference between temperatures of 80°F and 90°F represents the same difference in heat as that between temperatures of 30° and 40° on the Fahrenheit scale. An important point to make about interval scales is that the zero point is simply another point on the scale; it does not represent the starting point of the scale or the total absence of the characteristic being measured. The properties of an interval scale are as follows:

- The categories are mutually exclusive.
- The categories have a logical order.
- The categories are scaled according to the amount of the characteristic they indicate.
- Equal differences in the characteristic are represented by equal differences in the numbers assigned to the categories.
- The zero point is completely arbitrary.

1.3.4 Ratio Scales

The final level of measurement is the ratio scale. This type of scale has one further property in addition to those listed for interval scales, namely, the possession of a true zero point that represents the absence of the characteristic being measured. Consequently, statements can be made about both the differences on the scale and the ratio of points on the scale. An example is weight, where not only is the difference between 100 and 50 kg the same as between 75 and 25 kg, but an object weighing 100 kg can be said to be twice as heavy as one weighing 50 kg. This is not true of, say, temperature on the Celsius or Fahrenheit scales, where a reading of 100° on either scale does not represent twice the warmth of a temperature of 50°. If, however, two temperatures are measured on the Kelvin scale, which does have a true zero point (absolute zero or $-273°$C), then statements about the ratio of the two temperatures can be made.

The properties of a ratio scale are

- The categories are mutually exclusive.
- The data categories have a logical order.
- The categories are scaled according to the amount of the characteristic they possess.
- Equal differences in the characteristic being measured are represented by equal differences in the numbers assigned to the categories.
- The zero point represents an absence of the characteristic being measured.

In many statistical textbooks, discussion of different types of measurements is often followed by recommendations as to which statistical techniques are suitable for each type. For example, analyses on nominal data should be limited to summary statistics such as the number of cases, the mode, etc., and for ordinal data, means and standard deviations are said to be not suitable. But Velleman and Wilkinson (1993) make the important point that restricting the choice of statistical methods in this way may be a dangerous practice for data analysis. In essence, the measurement taxonomy described is often too strict to apply to real-world data. This is not the place for a detailed discussion of measurement, but we take a fairly pragmatic approach to such problems. For example, we would not agonize too long over treating variables such as measures of depression, anxiety, or intelligence as if they were interval scaled, although strictly, they fit into the ordinal level described earlier.

1.3.5 Response and Explanatory Variables

This is a convenient point to mention a further classification of measurements that is used in many studies, and that is the division of measured variables into response or dependent variables (often also referred to as outcome variables), and independent (a misnomer; the variables are not independent of one another, and therefore a term to be avoided) or explanatory variables (also occasionally called predictor variables); in this book we shall stick to explanatory. Essentially, response variables are those that appear on the left-hand side of the equation defining the proposed model for the data, with the explanatory variables, thought to possibly affect the response variable, appearing on the right-hand side of the model equation. With such data sets only the response is considered to be a random variable and the analysis of the data aims to assess how the explanatory variables are related to the response. (In practice, of course, explanatory variables will also usually be random variables, so any analysis performed will be *conditional* on the observed values of these explanatory variables.)

But there are many data sets gathered in the behavioral sciences where the variables measured or observed are not divided into response and explanatory variables and in which all are random variables. In those types of research settings, analyses are carried out to discover how the variables relate to one another and to try to determine the underlying structure of the data.

Both these types of data are multivariate although to distinguish between them the term *multivariable* is often used for the response/explanatory variable type of data. In this book, methods for analysing both data types will be described.

1.4 Missing Values

Most researchers in the behavioral sciences undertake studies that involve human subjects and many of them will be able to immediately relate to much of the following quotation from Efron (1998) which was originally made in the context of clinical trials in medicine:

> There could be no worse experimental animals on earth than human beings; they complain, they go on vacations, they take things they are not supposed to take, they lead incredibly complicated lives, and sometimes, they do not take their medicine.

So, situations will occur in almost all studies that observations or measurements that should have been recorded for a subject, but for some reason or another are not, for example, a subject may simply not turn up for a planned measurement session. The result is a missing value. When faced with missing values, many researchers simply resort to analyzing only complete cases since this is what most statistical software packages do automatically. If data are being collected on several variables, for example, the researcher might omit any case with a missing value on any of the variables. When the incomplete cases comprise only a small fraction of all cases (say, 5% or less), then case deletion may be a perfectly reasonable solution to the missing data problem. But when there are many cases with missing values, omitting them may cause large amounts of information, that is, the variable values on which a case has been measured, to be discarded, which would clearly be very inefficient. However, the main problem with complete-case analysis is that it can lead to serious biases in both estimation and inference unless the missing data are missing completely at random in the sense that the probabilities of response do not depend on any data values observed or missing (see Chapter 11 and Little and Rubin, 2002, for more details). In other words, complete-case analysis implicitly assumes that the discarded cases are like a random subsample. So, at the very least, complete-case analysis leads to a loss, and perhaps a substantial loss, in power (see Section 1.6), but worse, analyses based just on complete cases might in some cases be misleading.

Fortunately, there are now sophisticated techniques for dealing with missing values, and some of these will be the subject of Chapter 11. But researchers should remember that despite their sophistication, such methods will not rescue a study where a substantial proportion of subjects have missing values; in such a study it should perhaps be questioned whether any form of statistical analysis is worth undertaking. And it also still worth paying attention to that old axiom from the past, now largely forgotten in the growing enthusiasm for modern techniques for handling missing values, namely, the best solution to missing values is not to have any.

1.5 The Role of Models in the Analysis of Data

Models attempt to imitate the properties of “real” objects or situations in a simpler or more convenient form. A road map, for example, models part of the earth’s surface, attempting to reproduce the relative positions of towns, roads, and other features. Chemists use models of molecules to mimic their theoretical properties, which, in turn, can be used to predict the behavior of real compounds. A good model follows as accurately as possible the relevant properties of the real object while being convenient to use.

Statistical models allow inferences to be made about an object, or activity, or a process by representing some associated observable data. Suppose, for example, a child has scored 20 points on a test of verbal ability, and after studying a dictionary for some time, scores 24 points on a similar test. If it is believed that studying the dictionary has caused an improvement, then a possible model of what is happening is

$$20 = \{\text{person's initial score}\}$$

$$24 = \{\text{person's initial score}\} + \{\text{improvement}\}$$

The improvement can now be found by simply subtracting the first score from the second. Such a model is, of course, very naive since it assumes that verbal ability can be measured exactly. A more realistic representation of the two scores, which allows for possible measurement error, is

$$x_1 = \gamma + \varepsilon_1$$

$$x_2 = \gamma + \delta + \varepsilon_1$$

where x_1 and x_2 represent the two verbal ability measurements, γ represents the "true" initial measure of verbal ability, and δ is the value of the improvement made in verbal ability. The terms ε_1 and ε_2 represent the measurement error for verbal ability made on the two occasions of testing. Here the improvement score can only be estimated as $\hat{\delta} = x_2 - x_1$. (The "hat" over a parameter indicates an estimate of that parameter.)

A model gives a precise description of what the investigator assumes is occurring in a particular situation; in the foregoing case it says that the improvement, δ, is considered to be independent of γ and is simply added to it. (An important point that needs to be noted here is that if you do not believe in a model, you should not perform operations and analyses on the data that assume the model to be true.)

Suppose now that it is believed that studying the dictionary does more good if a child already has a fair degree of verbal ability, so that the initial ability effect is multiplied by the dictionary effect and that the various random influences that affect the test scores are also dependent on the true scores, so also enter the model multiplicatively. Then an appropriate model would be

$$x_1 = \gamma\varepsilon_1$$

$$x_2 = \gamma\delta\varepsilon_2$$

Now the parameters are multiplied rather than added to give the observed scores x_1 and x_2. Here, δ might be estimated by dividing x_1 by x_2.

A further possibility is that there is a limit, λ, to improvement, and studying the dictionary improves performance on the verbal ability test by some proportion of the child's possible improvement, $\lambda - \gamma$. Here, a suitable model would be

$$x_1 = \gamma + \varepsilon_1$$

$$x_2 = \gamma + (\lambda - \gamma)\delta + \varepsilon_2$$

With this model there is no way to estimate δ from the data unless a value of λ

is given or assumed. One of the principal uses of statistical models is to attempt to explain variation in measurements. This variation may be due to a variety of factors, including variation from the measurement system, variation due to environmental conditions that change over the course of a study, variation from individual to individual (or experimental unit to experimental unit), etc.

The decision about an appropriate model should be largely based on the investigator's prior knowledge of an area. In many situations, however, additive linear models are invoked by default since such models allow many powerful and informative statistical techniques to be applied to the data. Such models appear in several later chapters.

Formulating an appropriate model can be a difficult problem. The general principles of model formulation are covered in detail in books on scientific method but include the need to collaborate with appropriate experts, to incorporate as much background theory as possible, etc. Apart from those models formulated entirely on a priori theoretical grounds, most models are, to some extent at least, based on an initial examination of the data, although completely empirical models are rare. The more usual intermediate case arises when a class of models is entertained a priori, but the initial data analysis is crucial in selecting a subset of models from the class. In regression analysis, for example, the general approach is determined a priori, but a scatter diagram (see Chapter 2) will be of crucial importance in indicating the "shape" of the relationship, and residual plots (see Chapter 3) will be essential for checking assumptions such as normality, etc.

The formulation of a preliminary model from an initial examination of the data is the first step in the iterative, formulation/criticism cycle of model building. This can produce some problems since formulating a model and testing it on the same data is not generally considered good science. It is always preferable to confirm whether a derived model is sensible by testing on new data. But when data are difficult or expensive to obtain, some model modification and assessment of fit on the original data are almost inevitable. Investigators need to be aware of the possible dangers of such a process.

Perhaps the most important principle to have in mind when testing models on data is that of parsimony, that is, the "best" model is one that provides an adequate fit to data with the fewest number of parameters. This principle is often known as *Occam's razor*, which in its original form in Latin is *entia non stunt multiplicanda praeter necessitatem*, which translates roughly as "a plurality of reasons should not be posited without necessity."

One last caveat about statistical models: according to George Box, "all models are wrong, but some are useful." Statistical models are always simplifications, but some models are useful in providing insights into what is happening in complex, real-world situations.

1.6 Determining Sample Size

One of the most frequent questions faced by a statistician dealing with investigators planning a study is, "How many participants do I need to recruit?" Answering the question requires consideration of a number of factors, for example, the amount of time available for the study, the likely ease or difficulty in recruiting the type of subject required, and the possible financial constraints that may be involved. But the statistician may, initially at least, largely ignore these important aspects of the problem and apply a statistical procedure for calculating sample size. To make things simpler, we will assume that the investigation the researcher is planning is an experimental intervention with two treatment groups. To calculate the sample size, the statistician and the researcher will first need to identify the response variable of most interest and the appropriate statistical test to be used in the analysis of the chosen response; then they will need to decide on values for the following quantities:

- The size of the type I error, that is, the significance level.
- The likely variance of the response variable.
- The power they would like to achieve. (For those readers who have forgotten, or perhaps never knew, the power of a statistical test is the probability of the test rejecting the null hypothesis when the null hypothesis is false.)
- A size of treatment effect that the researcher feels is important, that is, a treatment difference that the investigators would not like to miss being able to declare to be statistically significant.

Given such information, the calculation of the corresponding sample size is often relatively straightforward, although the details will depend on the type of response variable and the type of test involved (see the following text for an example). In general terms, the sample size will increase as the variability of the response variable increases, and decrease as the chosen clinically relevant treatment effect increases. In addition, the sample size will need to be larger to achieve a greater power and a more stringent significance level.

As an example of the calculations involved in sample-size determination, consider a trial involving the comparison of two treatments for anorexia nervosa. Anorexic women are to be randomly assigned to each treatment, and the gain in weight in kilograms after three months is to be used as the outcome measure. From previous experience gained in similar trials, it is known that the standard deviation (σ) of weight gain is likely to be about 4 kg. The investigator feels that a difference in weight gain of 1 kg (Δ) would be of clinical importance and wishes to have a power of 90% when the appropriate two-sided test is used with significance level of 0.05 (α). The formula for calculating the number of women required in each treatment group (n) is

$$n = \frac{2\left(Z_{\alpha/2} + Z_{\beta}\right)^2 \sigma^2}{\Delta^2}$$

where β is $1 -$ Power, and

- $Z_{\alpha/2}$ is the value of the normal distribution that cuts off an upper tail probability of $\alpha/2$. So, for $\alpha = 0.05, Z_{\alpha/2} = 1.96$.
- Z_{β} is the value of the normal distribution that cuts off an upper tail probability of β. So, for a power of 0.90, $\beta = 0.10$ and $Z_{\beta} = 1.28$.

Therefore, for the anorexia trial,

$$n = \frac{2 \times (1.96 + 1.28)^2 \times 4^2}{1} = 336 \text{ women per treatment group.}$$

The foregoing example is clearly simplistic in the context of most psychiatric clinical trials in which measurements of the response variable are likely to be made at several different time points, during which time some patients may drop out of the trial (see Chapter 9 for a discussion of such longitudinal data and the drop out problem). Fortunately, there is a large volume of methodology useful in planning the size of randomized clinical trials with a variety of different types of outcome measures and with the complications outlined; some examples are to be found in Lee (1984), McHugh and Le (1984), Schoenfeld (1983), Hsieh (1987), and Wittes and Wallenstein (1987). In many cases, tables are available that enable the required sample size for chosen power, significance level, effect size, etc., to be simply read off. Increasingly, these are being replaced by computer software for determining sample size for many standard and nonstandard designs and outcome measures.

An obvious danger with the sample size determination procedure just mapped out is that investigators (and, in some cases, even their statisticians) may occasionally be led to specify an effect size that is unrealistically extreme (what Senn, 1997, has described with his usual candor as “a cynically relevant difference”) so that the calculated sample size looks feasible in terms of possible pressing temporal and financial constraints. Such a possibility may be what led Senn (1997) to describe power calculations as “a guess masquerading as mathematics,” and Pocock (1996) to comment that they are “a game that can produce any number you wish with manipulative juggling of the parameter values.” Statisticians advising on behavioral investigations need to be active in estimating the degree of difference that can be realistically expected for a study based on previous studies of a similar type or, when such information is lacking, perhaps based on subjective opinions of investigators not involved in the putative study.

Getting the sample size right in a scientific study is generally believed to be critical; indeed, according to Simon (1991), discussing in particular clinical trials,

> An effective clinical trial must ask an important question and provide a reliable answer. A major determinant of the reliability of the answer is the sample size of the trial. Trials of inadequate size may cause contradictory and erroneous results and thereby lead to an inappropriate treatment of patients. They also divert limited resources from useful applications and cheat the patients who participated in what they thought was important clinical research. Sample size planning is, therefore, a key component of clinical trial methodology.

Studies with inadequate sample sizes risk missing important intervention differences, a risk nicely summarized in the phrase "absence of evidence is not evidence of absence." The case against studies with inadequate numbers of subjects appears strong, but as Senn (1997) points out, sometimes only a small study is possible. Also, misinterpreting a nonsignificant effect as an indication that a treatment effect is not effective, rather than as a failure to prove that it is effective, suggests trying to improve statistical education rather than totally abandoning small studies. In addition, with the growing use of systematic reviews and meta-analysis (see, for example, Everitt and Wessely, 2008), the results from small studies may prove valuable in contributing to an overview of the evidence of intervention effectiveness, a view neatly summarized by Senn in the phrase "some evidence is better than none." Perhaps size really is not always everything.

1.7 Significance Tests, *p*-Values, and Confidence Intervals

Although we are assuming that readers have had an introductory course in statistics that covered simple significance tests, *p*-values, and confidence intervals, a few more words about these topics here will hopefully not go amiss.

For many behavioral science students and researchers the still-ubiquitous *p*-value continues to be the Holy Grail of their research efforts, and many see it as the *raison d'etre* of statistics and statisticians. Despite the numerous caveats about *p*-values in the literature (e.g., Gardner and Altman, 1986), many behavioral scientists still seem determined to experience a "eureka moment" on finding a *p*-value of 0.049, and despair on finding one of 0.051. The *p*-value retains a powerful hold over the average behavioral researcher and student; there are a number of reasons why it should not.

The first is that the *p*-value is poorly understood. Although *p*-values appear in almost every account of behavioral science research findings, there is evidence that the general degree of understanding of the true meaning of the term is very low. Oakes (1986), for example, put the following test to 70 academic psychologists:

> Suppose you have a treatment which you suspect may alter performance on a certain task. You compare the means of your control and experimental groups (say 20 subjects in each sample). Further suppose you use a simple independent means t-test and your result is t = 2.7, df = 18, P = 0.01. Please mark each of the following statements as true or false.

- You have absolutely disproved the null hypothesis that there is no difference between the population means.
- You have found the probability of the null hypothesis being true.
- You have absolutely proved your experimental hypothesis.
- You can deduce the probability of the experimental hypothesis being true.
- You know, if you decided to reject the null hypothesis, the probability that you are making the wrong decision.
- You have a reliable experiment in the sense that if, hypothetically, the experiment were repeated a great number of times, you would obtain a significant result on 99% of occasions.

The subjects were all university lecturers, research fellows, or postgraduate students. The results presented in Table 1.1 are illuminating. Under a relative frequency view of probability, all six statements are in fact false. Only 3 out of the 70 subjects came to this conclusion. The correct interpretation of the probability associated with the observed t-value is:

> The probability of obtaining the observed data (or data that represent a more extreme departure from the null hypothesis) if the null hypothesis is true.

TABLE 1.1
Frequencies and Percentages of "True" Responses in Test of Knowledge about *p*-values

Statement	**Frequency**	**Percentage**
1. The null hypothesis is absolutely disproved.	1	1.4
2. The probability of the null hypothesis has been found.	25	35.7
3. The experimental hypothesis is absolutely proved.	4	5.7
4. The probability of the experimental hypothesis can be deduced.	46	65.7
5. The probability that the decision taken is wrong is known.	60	85.7
6. A replication has a 0.99 probability of being significant.	42	60.0

Clearly, the number of false statements described as true in this experiment would have been reduced if the true interpretation of a p-value had been included with the six others. Nevertheless, the exercise is extremely interesting in highlighting the misguided appreciation of p-values held by a group of behavioral researchers.

The second reason for researchers and students to be careful using p-values is that a p-value represents only limited information about the results from a study. Gardner and Altman (1986) make the point that the excessive use of p-values in hypothesis testing, simply as a means of rejecting or accepting a particular hypothesis at the expense of other ways of assessing results, has reached such a degree that levels of significance are often quoted alone in the main text and abstracts of papers with no mention of other more relevant and important quantities. The implications of hypothesis testing—that there can always be a simple "yes" or "no" answer as the fundamental result from a research study—is clearly false and, used in this way, hypothesis testing is of limited value; indeed, according to Siegfried (2010) "It's science's dirtiest secret: The 'scientific method' of testing hypotheses by statistical analysis stands on a flimsy foundation." And in 2016 in *The American Statistician* the American Statistical Association (ASA) made a lengthy statement mostly critical of the way p-values are used (see Wasserstein and Lazar, 2016).

The most common alternative to presenting results in terms of p-values in relation to a statistical null hypothesis is to estimate the magnitude of some parameter of interest along with some interval that includes the population value of the parameter with a specified probability. Such confidence intervals can be found relatively simply for many quantities of interest (see Gardner and Altman, 1986, for details), and although the underlying logic of interval estimation is essentially similar to that of significance tests, they do not carry with them the pseudoscientific hypothesis testing language of such tests. Instead, they give a plausible range of values for the unknown parameter. As Oakes (1986) rightly comments: "The significance test relates to what the population parameter is not: the confidence interval gives a plausible range for what the parameter is."

So, should the p-value be abandoned completely? Many statisticians would, grumpily, answer yes, but we think a more sensible response, at least for behavioral scientists, would be a resounding "maybe." The p-value should rarely be used in a purely confirmatory way, but in an exploratory fashion, p-values can be useful in giving some informal guidance on the possible existence of an interesting effect even when the required assumptions of whatever test is being used are known to be invalid. It is often possible to assess whether a p-value is likely to be an under- or overestimate, and whether the result is clear one way or the other. In this text, both p-values and confidence intervals will be used; purely from a pragmatic point-of-view, the former are needed by behavioral science students since they remain of central importance in the bulk of the behavioral science literature.

1.8 Summary

- Statistical principles are central to most aspects of a psychological investigation.
- Data and their associated statistical analyses form the evidential parts of behavioral science arguments.
- Significance testing is far from the be-all and end-all of statistical analyses, but it does still matter because evidence that can be discounted as an artifact of sampling will not be particularly persuasive. But p-values should not be taken too seriously; confidence intervals are often more informative.
- Good statistical analysis should highlight those aspects of the data that are relevant to the substantive arguments; do so clearly and fairly, and be resistant to criticisms.
- Although randomised controlled experiments are largely considered as the gold standard in behavioral research because they are generally considered to lead to the clearest conclusions about causal relationships, Yarkoni and Westfall (2017) argue that more emphasis should be placed of methods that accurately forecast/predict behaviours that have not yet been observed.
- Variable type often determines the most appropriate method of analysis, although some degree of flexibility should be allowed.
- Sample size determination to achieve some particular power is an important exercise when designing a study, but the result of the statistical calculation involved needs to be considered in terms of what is feasible from a practical viewpoint.
- Statisticians giving advise to behavioral scientists and behavioral scientists seeking advise from a statistician might like to take a look at the small book, *Talking about Statistics* (Everitt and Hay, 1992) to see ideal examples of how such consultations should develop.
- Three small books, one by Hand (2008), one by Magnello and van Loon (2009), and one by Stigler (2016) give brief, but useful accounts of the basics of statistics, measurement, and models, along with interesting snippets of the history of these topics.

1.9 Exercises

(excluded from MABS for IODS)

2

Looking at Data

2.1 Introduction

According to Chambers et al. (1983), “there is no statistical tool that is as powerful as a well-chosen graph.” Certainly, graphical display has a number of advantages over tabular displays of numerical results, not least in creating interest and attracting the attention of the viewer.

But just what is a graphical display? A concise description is given by Tufte (1983):

> Data graphics visually display measured quantities by means of the combined use of points, lines, a coordinate system, numbers, symbols, words, shading and color.

Graphical displays are very popular; it has been estimated that between 900 billion (9×10^{11}) and 2 trillion (2×10^{12}) images of statistical graphics are printed each year. Perhaps one of the main reasons for such popularity is that graphical presentation of data often provides the vehicle for discovering the unexpected; the human visual system is very powerful in detecting patterns, although the following caveat from the late Carl Sagan should be kept in mind:

> Humans are good at discerning subtle patterns that are really there, but equally so at imagining them when they are altogether absent.

Some of the advantages of graphical methods have been listed by Spear (1952) and Schmid (1954):

- In comparison with other types of presentation, well-designed charts are more effective in creating interest and in appealing to the attention of the reader.
- Visual relationships as portrayed by charts and graphs are more easily grasped and more easily remembered.
- The use of charts and graphs saves time since the essential meaning of large measures of statistical data can be visualized at a glance.

- Charts and graphs provide a comprehensive picture of a problem that makes for a more complete and better-balanced understanding than could be derived from tabular or textual forms of presentation.

- Charts and graphs can bring out hidden facts and relationships, and can stimulate, as well as aid, analytical thinking and investigation.

The last point is reiterated by the legendary John Tukey in his observation that "the greatest value of a picture is when it forces us to notice what we never expected to see."

The prime objective of a graphical display is to communicate to ourselves and others. Graphic design must do everything it can to help people understand. In some cases a graphic is required to give an overview of the data and perhaps to tell a story about the data. In other cases a researcher may want a graphical display to suggest possible hypotheses for testing on new data and, after some model has been fitted to the data, a graphic that criticizes the model may be what is needed. In this chapter we will consider graphics primarily from the story-telling angle; graphics that help check model assumption will be discussed in later chapters.

Since the 1970s, a wide variety of new methods for displaying data graphically have been developed; these will hunt for special effects in data, indicate outliers, identify patterns, diagnose models, and generally search for novel and perhaps unexpected phenomena. Large numbers of graphs may be required, so computers are needed to supply them for the same reasons they are used for numerical analyses, namely, they are fast and they are accurate.

So, because the machine is doing the work, the question is no longer "shall we plot?" but rather "what shall we plot?" There are many exciting possibilities, including *dynamic graphics* (see Cleveland and McGill, 1988), and the related area of *infographics* (also called information visualization or *infovis*, see Gelman and Unwin, 2013 and Vehkalahti et al., 2018), but graphical exploration of data usually begins with some simpler, well-known methods, and it is these that we deal with in the next section.

2.2 Simple Graphics—Pie Charts, Bar Charts, Histograms, and Boxplots

2.2.1 Categorical Data

Newspapers, television, and the media in general are very fond of two very simple graphics for displaying categorical data, namely, the pie chart and the bar chart. Both can be illustrated using the data shown in Table 2.1, which show the percentage of people convicted of five different types of crime. In the pie charts for drinkers and abstainers (see Figure 2.1), the sections of the circle have areas proportional to the observed percentages. In the correspond-

TABLE 2.1
Crime Rates for Drinkers and Abstainers

Crime	Drinkers	Abstainers
Arson	6.6	6.4
Rape	11.7	9.2
Violence	20.6	16.3
Stealing	50.3	44.6
Fraud	10.8	23.5

Note: Figures are percentages.

ing bar charts (see Figure 2.2), percentages are represented by rectangles of appropriate size placed along a horizontal axis.

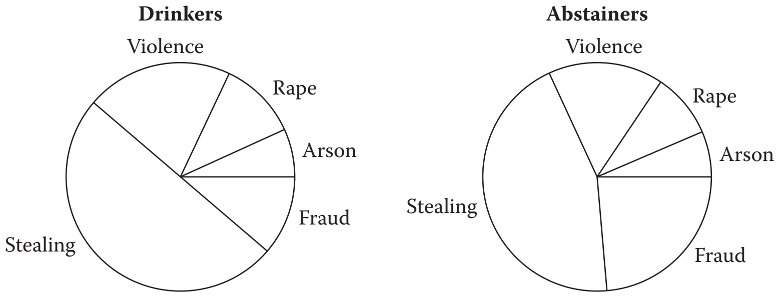


FIGURE 2.1
Pie charts for drinkers' and abstainers' crime percentages.

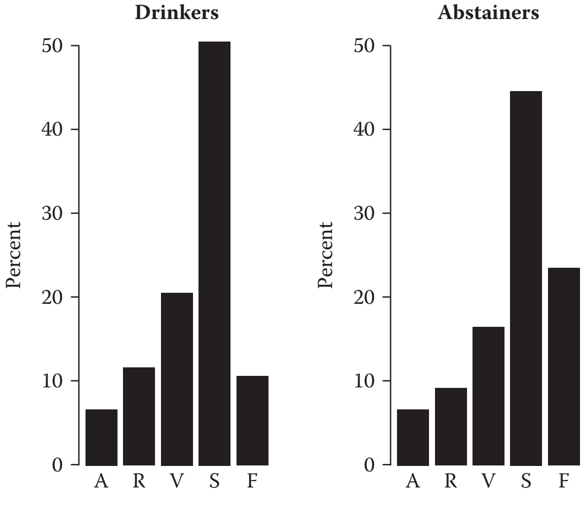


FIGURE 2.2
Bar charts for drinkers' and abstainers' crime percentages.

Despite their widespread popularity, both the general and, in particular, the scientific use of pie charts has been severely criticized. Tufte (1983), for example, comments that "tables are preferable to graphics for many small data sets. A table is nearly always better than a dumb pie chart; the only worse design than a pie chart is several of them . . . pie charts should never be used." A similar lack of affection is shown by Bertin (1981), who declares that "pie charts are completely useless," and by Wainer (1997), who claims that "pie charts are the least useful of all graphical forms." Certainly in regard to the data in Table 2.1, the numerical data in the table are as informative, or perhaps even more informative, than the associated pie charts in Figure 2.1, and the bar chart in Figure 2.2 seems no more necessary than the pie chart for these data.

Two examples that illustrate why both pie charts and bar charts are often (but not always—as will be seen later) of little more help in understanding categorical data than the numerical data themselves and how other graphics are frequently more useful are given in Cleveland (1994). The first example compares the pie chart of 10 percentages with an alternative graphic, the dot plot. The plots are shown in Figures 2.3 and 2.4. The 10 percentages represented by the two graphics have a bimodal distribution; odd-numbered observations cluster around 8%, and even-numbered observations cluster around 12%. Furthermore, each even value is shifted with respect to the preceding odd value by about 4%. This pattern is far easier to spot in the dot plot than in the pie chart.

Dot plots for the crime data in Table 2.1 are shown in Figure 2.5, and these are also more informative than the corresponding pie charts in Figure 2.1.

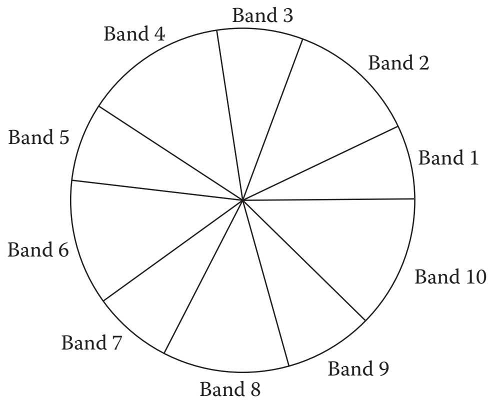


FIGURE 2.3
Pie chart for 10 percentages. (Suggested by Cleveland, 1994. Used with permission from Hobart Press.)

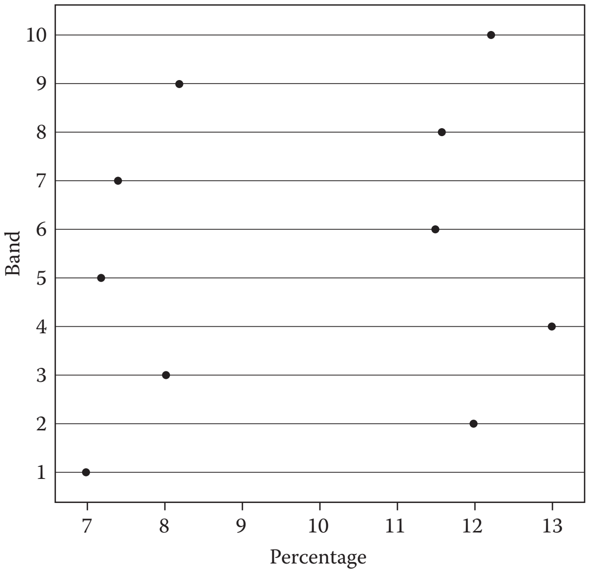


FIGURE 2.4
Dot plot for 10 percentages.

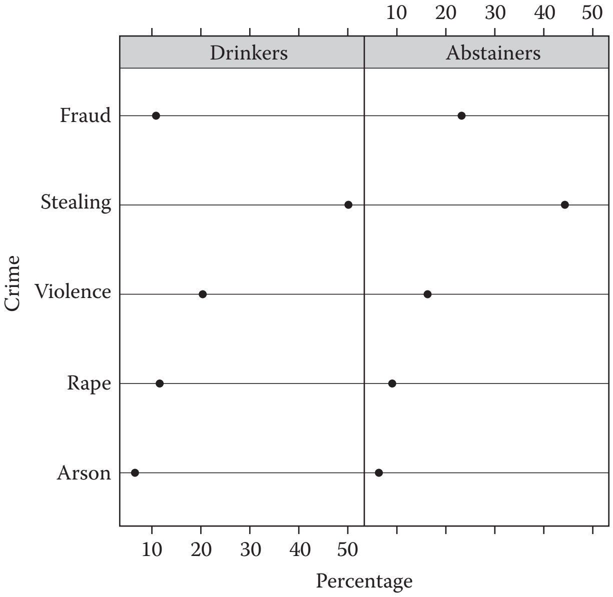


FIGURE 2.5
Dot plots for drinkers' and abstainers' crime percentages.

The second example given by Cleveland begins with the diagram shown in Figure 2.6, which originally appeared in Vetter (1980). The aim of the diagram is to display the percentages of degrees awarded to women in several disciplines of science and technology during three time periods. At first glance the labels on the diagram suggest that the graph is a standard divided bar chart with the length of the bottom division of each bar showing the percentage for doctorates, the length of the middle division showing the percentage for master's degrees, and the top division showing the percentage for bachelor's degrees. A little reflection shows that this interpretation is not correct since it would imply that, in most cases, the percentage of bachelor's degrees given to women is lower than the percentage of doctorates. Closer examination of the diagram reveals that the three values of the data for each discipline during each time period are determined by the three adjacent vertical dotted lines. The top of the left-hand line indicates the value for doctorates, the top end of the middle line indicates the value for master's degrees, and the top end of the right-hand line indicates the value for bachelor's degrees.

Cleveland (1994) discusses other problems with the diagram in Figure 2.6; in particular, he points out that the manner of the diagram's construction makes it hard to connect visually the three values of a particular type of degree for a specific discipline, thus making it difficult to see changes over time.

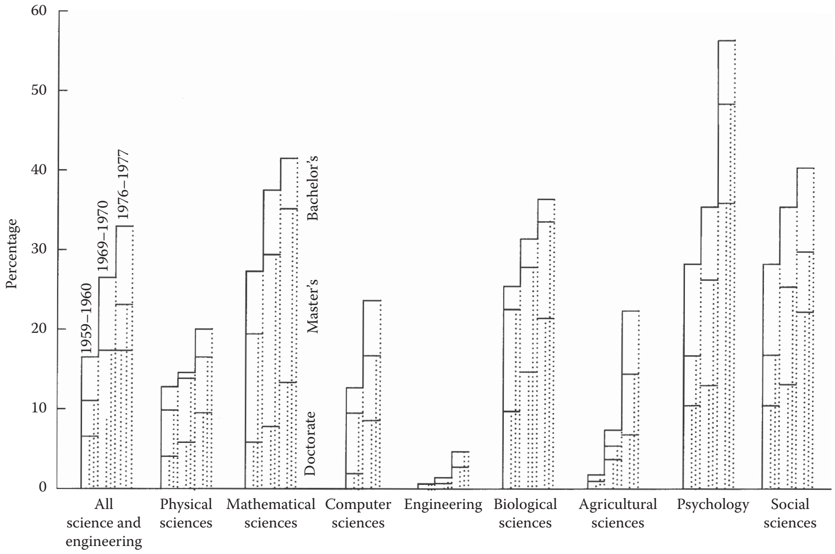


FIGURE 2.6
Proportion of degrees in science and technology earned by women in the periods 1959–1960, 1969–1970, and 1976–1977. (Reproduced with permission from Vetter, B. M., 1980, Science, 207, 28–34. ©1980 American Association for the Advancement of Society.)

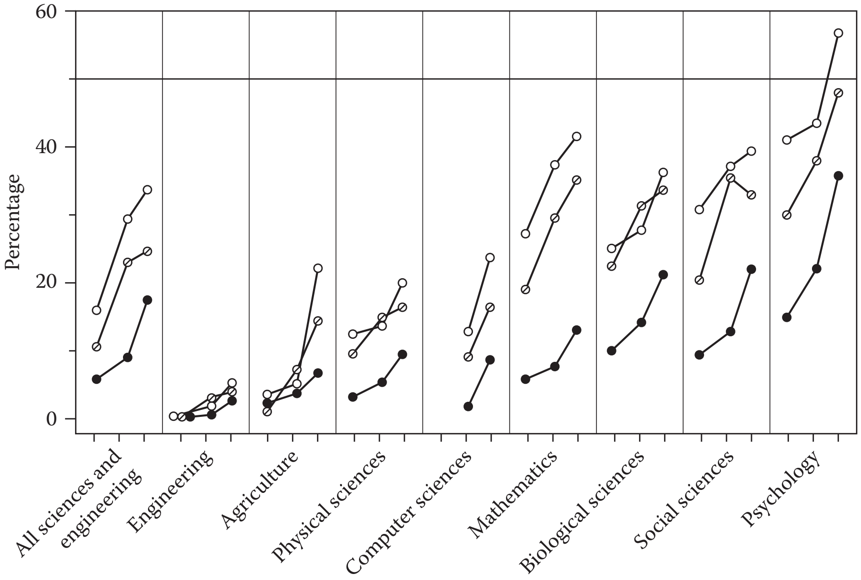


FIGURE 2.7
Percentage of degrees earned by women for three degrees (○ bachelor's degree; ϕ master's degree; • doctorate), three time periods, and nine disciplines. The three points for each discipline and degree indicate the periods 1959–1960, 1969–1970, and 1976–1977.

Figure 2.7 shows the data represented by Figure 2.6 replotted by Cleveland in a bid to achieve greater clarity. It is now clear how the data are represented, and this diagram allows viewers to see easily the percentages corresponding to each degree, in each discipline, over time. Finally the figure caption explains the content of the diagram in a comprehensive and clear fashion. All in all Cleveland appears to have produced a graphic that would satisfy even that doyen of graphical presentation, Edward R. Tufte, in his demand that "excellence in statistical graphics consists of complex ideas communicated with clarity, precision and efficiency."

Wainer (1997) gives a further demonstration of how displaying data as a bar chart can disguise rather than reveal important points about data. Figure 2.8 shows a bar chart of life expectancies in the middle 1970s, divided by sex, for ten industrialized nations. The order of presentation is alphabetical (with the U.S.S.R. positioned as Russia). The message we get from this diagram is that there is little variation and women live longer than men. But by displaying the data in the form of a simple stem-and-leaf plot (see Figure 2.9), the magnitude of the sex difference (7 years) is immediately clear as is the unusually short life expectancy for men in the U.S.S.R., whereas Russian women have life expectancy similar to women in other countries.

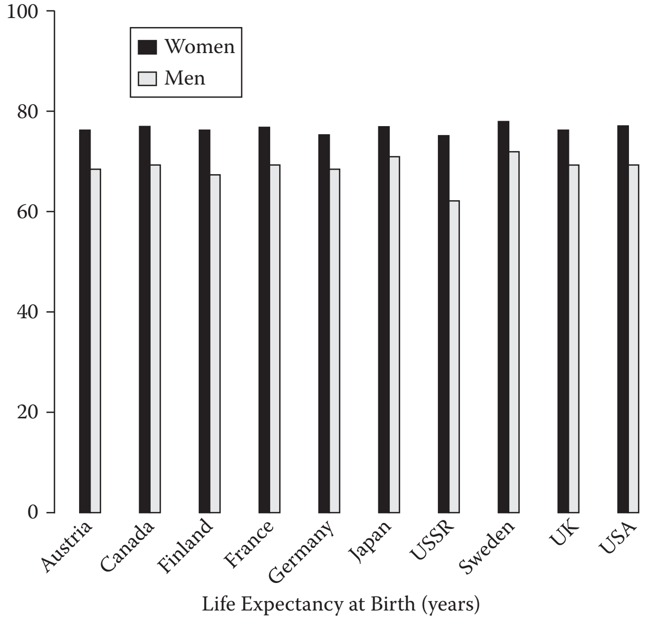


FIGURE 2.8
Bar chart showing life expectancies at birth by sex and by country.

Women	Age	Men
Sweden	78	
France, US, Japan, Canada	77	
Finland, Austria, UK	76	
USSR, Germany	75	
	74	
	73	
	72	Sweden
	71	Japan
	70	
	69	Canada, UK, US, France
	68	Germany, Austria
	67	Finland
	66	
	65	
	64	
	63	
	62	USSR

FIGURE 2.9
An alternative display of life expectancies at birth by sex and by country.

To be fair to the poor old bar chart, we will end this subsection by illustrating how a sophisticated adaptation of the graphic can become an extremely effective tool for displaying a complex set of categorical data. The example is taken from Sarkar (2008) and uses data summarizing the fates of the 2201 passengers on the Titanic. The data are categorized by economic status (class of ticket: 1st, 2nd, or 3rd, or crew), sex (male or female), age (adult or child), and whether they survived or not. The first diagram produced by Sarkar is shown in Figure 2.10. This plot looks impressive but is dominated by the third "panel" (adult males) as heights of bars represent counts, and all panels have the same limits. So, sadly, all the plot tells us is that there were many more males than females aboard (particularly among the crew, which is the largest group), and that there were even fewer children. The plot becomes more illuminating about what really happened to the passengers if the proportion of survivors is plotted and by allowing independent horizontal scales

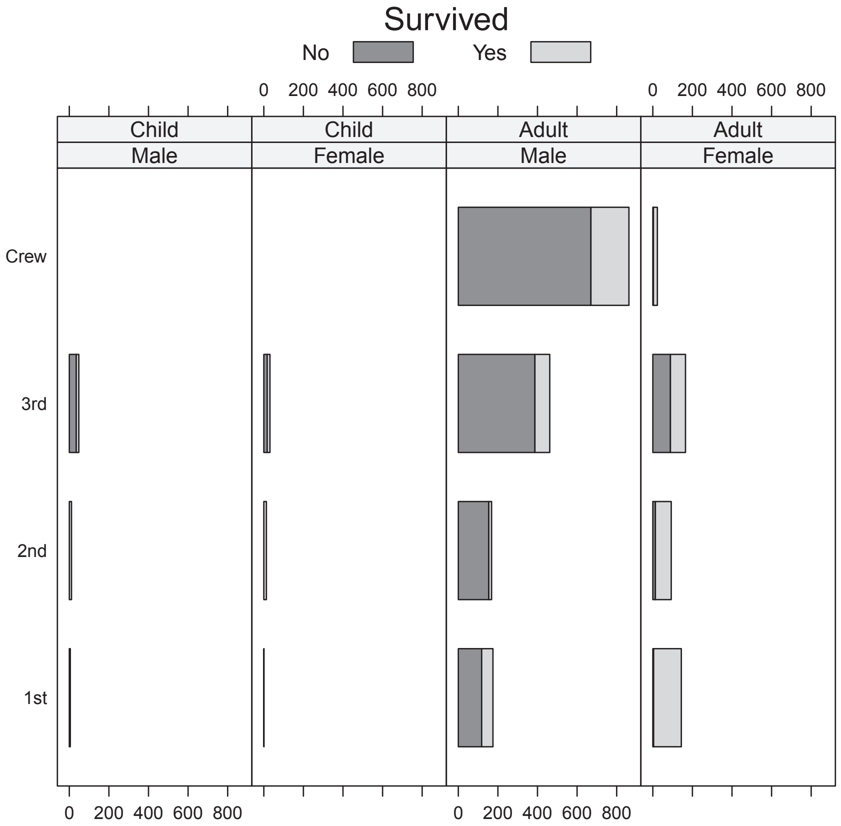


FIGURE 2.10
A bar chart summarizing the fate of passengers of the Titanic, classified by sex, age, and whether they survived or not.

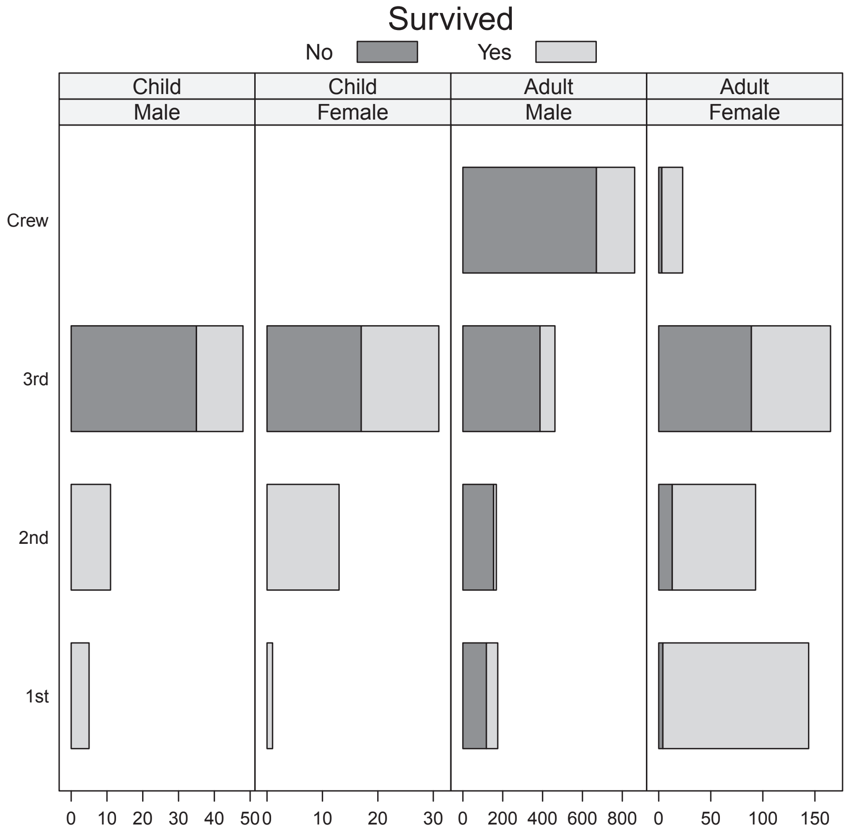


FIGURE 2.11
Survival among different subgroups of passengers on the Titanic, with a different horizontal scale in each panel.

for the different "panels" in the plot; this plot is shown in Figure 2.11. This plot emphasizes the proportion of survivors within each subgroup rather than the absolute numbers. The proportion of survivors is lowest among third-class passengers, and the diagram makes it very clear that the "women and children first" policy did not work very well for this class of passengers.

2.2.2 Interval/Quasi-Interval Data

The data shown in Table 2.2 come from an observational study described in Howell and Huessy (1981, 1985), in which a researcher asked 50 children to tell her about a given movie. For each child the researcher recorded the number of "and then ..." statements.

Let us begin by constructing that old favorite, the histogram, for these data; it is shown in Figure 2.12. Here the histogram is based on a relatively

TABLE 2.2
Number of "and Then . . . " Statements Made by 50 Children Recalling the Story of a Movie They Had Just Seen

18	15	22	19	18	17	18	20	17	12	16	16	17	21	23	18	20	21	20	20	15	18	17	19	20
23	22	10	17	19	19	21	20	18	18	24	11	19	31	16	17	15	19	20	18	18	40	18	19	16

small number of observations and tells us little about the data except that there is some degree of skewness perhaps and possibly two "outliers."

The histogram is a widely used graphical method that is at least a 100 years old. But Cleveland (1994) makes the point that "maturity and ubiquity do not guarantee the efficacy of a tool." The histogram is generally used for two purposes: counting and displaying the distribution of a variable. However, according to Wilkinson (1992), "it is effective for neither." Histograms can often be misleading about a variable's distribution because of their dependence on the number of classes chosen, and simple tallies of the observations to give a numerical frequency distribution table are usually preferable for counting. Finally, the histogram is a poor method for comparing groups of univariate measurements (Cleveland, 1994).

A more useful graphical display of a variable's distributional properties is the boxplot. This is obtained from the five-number summary of a data set, the five numbers in question being the minimum, the lower quartile (LQ), the median, the upper quartile (UQ), and the maximum. The distance between the upper and lower quartiles, the interquartile range (IQR), is a measure of the spread of a variable's distribution. The relative distances from the

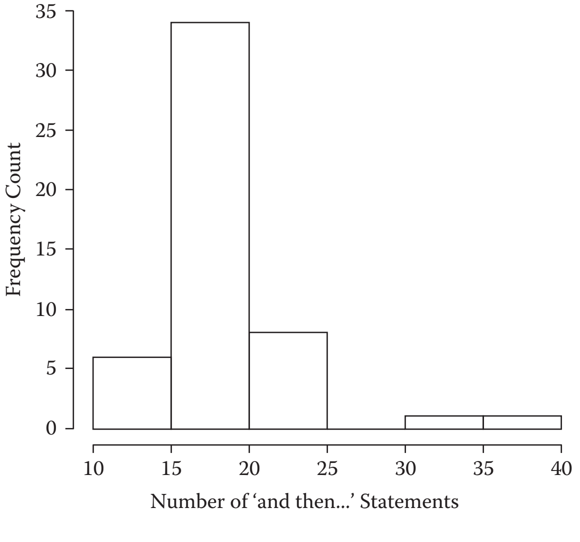


FIGURE 2.12
Histogram of count of "and then . . . " statements by 50 children.

median of the upper and lower quartiles give information about the shape of a variable's distribution; for example, if one distance is much greater than the other, the distribution is skewed. In addition, the median and the upper and lower quartiles can be used to define arbitrary but often useful limits, L and U, that maybe helpful in identifying possible outliers. The two limits are calculated as follows:

$$\mathrm{U} = \mathrm{UQ} + 1.5\,\mathrm{IQR}$$

$$\mathrm{L} = \mathrm{LQ} - 1.5\,\mathrm{IQR}$$

Observations outside the limits can be regarded as potential outliers (they are sometimes referred to specifically as outside observations), and such observations may merit careful attention before undertaking any analysis of a data set because there is always the possibility that they can have undue influence on the results of the analysis.

The construction of a boxplot is described in Figure 2.13.

The boxplot of the data in Table 2.2 is shown in Figure 2.14. The diagram indicates a number of possible outliers and also highlights the skewness in the data.

In Table 2.3, there is a similar data set as in Table 2.2, but here the observations were collected from adults. A question of interest is whether children and adults recall stories in the same way. At some stage this may require a formal procedure such as the construction of a confidence interval for, say, the mean difference in the number of "and then ... " statements between children and adults. But here we will see how far we can get with a

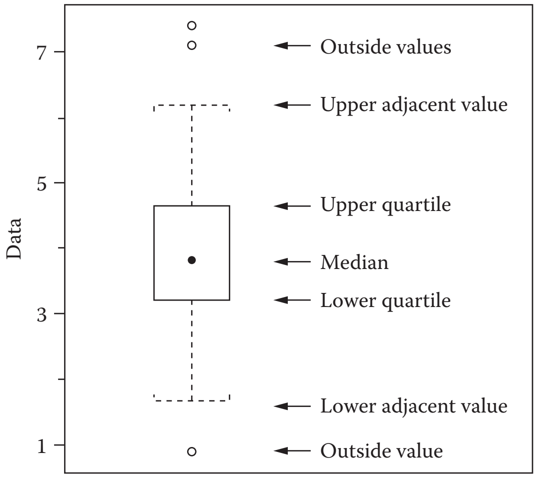


FIGURE 2.13
The construction of a boxplot.

TABLE 2.3
Number of "and Then . . . " Statements Made by 50 Adults Recalling the Story of a Movie They had just Seen

10	12	5	8	13	10	12	8	7	11	11	10	9	9	11	15	12	17	14	10	9	8	15	16	10
14	7	16	9	1	4	11	12	7	9	10	3	11	14	8	12	5	10	9	7	11	14	10	15	9

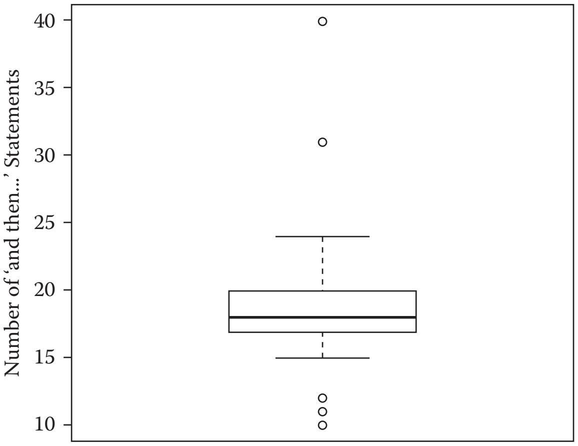


FIGURE 2.14
Boxplot of count of "and then . . . " statements by children.

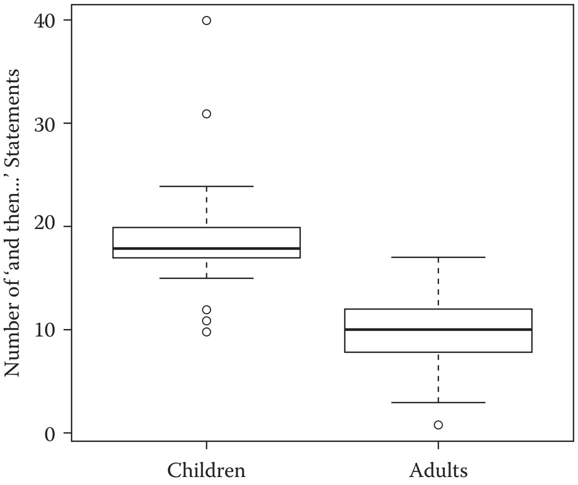


FIGURE 2.15
Side-by-side boxplots of counts of "and then . . . " statements by children and adults.

graphical approach namely comparing the boxplots of each data set. The side-by-side boxplots are shown in Figure 2.15. The diagram clearly demonstrates that the adults generally use less "and then ... " statements than children and also suggests that the distribution of the adults' observations is closer to being symmetric that that of the children.

Although the boxplots in Figure 2.15 give some information about the distributions of the observations in each group, it may useful to delve a little further and use probability plots to assess the normality of the observations for both children and adults. Probability plots are described in Technical Section 2.1.

Technical Section 2.1: Probability Plots

The classic example of a probability plot is that for investigating the assumption that a set of data is from a normal distribution; here the ordered sample values, $y_{(1)} \leq y_{(2)} \leq \cdots \leq y_{(n)}$ are plotted against the quantiles of a standard normal distribution, that is, $\Phi^{-1}(p_i)$, where

$$p_i = \frac{i - \frac{1}{2}}{n}, \quad \text{and} \quad \Phi(x) = \int_{-\infty}^{x} \frac{1}{\sqrt{2\pi}} e^{-\frac{1}{2}u^2} du$$

Departures from linearity in the plot indicate that the data do not have a normal distribution.

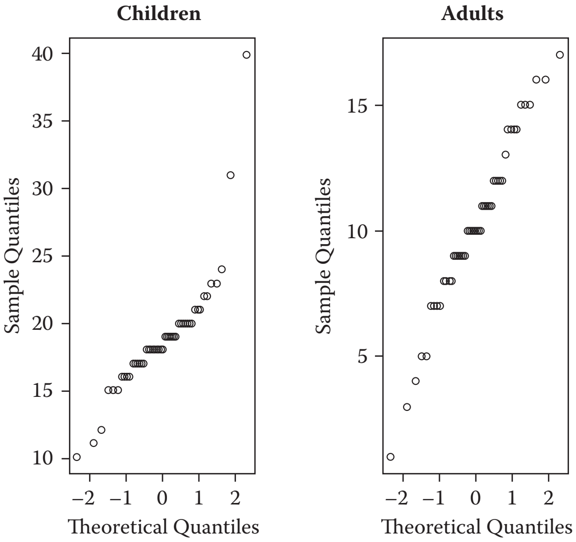


FIGURE 2.16
Probability plots of counts of "and then ... " statements by children and adults.

The normal probability plots for the children and the adults are shown in Figure 2.16. The plot for the children's observations shows a marked departure from linearity but the plot for the adults' data looks linear. These findings might need to be considered before any formal test or procedure is applied to the data set, although here constructing the usual normality based confidence interval is unlikely to be misleading.

Probability plots have been around for a long time, but they remain a useful technique for assessing distributional assumptions in some cases as here for the raw data, but also for the residuals that are used to assess the assumptions when fitting models to data, as we shall see in Chapter 3.

2.3 The Scatterplot and Beyond

The simple *xy* scatterplot has been in use since at least the 18th century and has many advantages for an initial exploration of data. Indeed, according to Tufte (1983):

> The relational graphic—in its barest form the scatterplot and its variants—is the greatest of all graphical designs. It links at least two variables encouraging and even imploring the newer to assess the possible causal relationship between the plotted variables. It confronts causal theories that *x* causes *y* with empirical evidence as to the actual relationship between *x* and *y*.

Let us begin by looking at a straightforward use of the scatterplot using some of the data in Table 2.4. These data were collected from a sample of 24 primary school children in Sydney, Australia. Part of the data is given in Table 2.4. Each child completed the Embedded Figures Test (EFT), which measures "field dependence," that is, the extent to which a person can abstract the logical structure of a problem from its context. Then the children were allocated to one of two experimental groups, and they were timed as they constructed a 3 × 3 pattern from nine colored blocks, taken from the Wechsler Intelligence Scale for Children (WISC). The two groups differed in the instructions they were given for the task: the "row" group was told to start with a row of

TABLE 2.4
Field Dependence Measure and Time to Complete a Task from the WISC for Children in Two Experimental Groups

Row Group			**Corner Group**		
Child	**Time**	**EFT**	**Child**	**Time**	**EFT**
1	317	59	1	342	43
2	464	33	2	222	23
3	525	49	3	219	9
4	298	69	4	513	128
5	491	65	5	295	44

three blocks, and the "corner" group was told to start with a corner of three blocks. The experimenter was interested in whether the different instructions produced any change in the average time to complete the picture and whether this time was affected by field dependence.

So, to begin, Figure 2.17 shows the scatterplots of completion time against EFT for both the row and the corner groups. The first thing to notice about the two plots is the obvious outlier in the plot for the row experimental group, and the relationship between time to completion and EFT appears to be stronger in the row group than in the corner group although the outlier in the row group may be entirely responsible for this apparent difference. Other than this, the plots are not particularly informative, and we perhaps cannot expect too much from them given the rather small samples involved. It should be remembered that calculating a correlation coefficient between two variables without looking at the corresponding scatterplot is very poor data analysis practice because a correlation coefficient can, on occasions, be badly affected by outliers, and the scatterplot is needed to spot the offending observations.

To make the scatterplots a little more informative, we can add the linear regression fit (see Chapter 3) of time to completion against EFT to each plot. The result is Figure 2.18. The plots now demonstrate more clearly that completion time appears to have a stronger linear relationship to EFT in the row group than in the corner group (but remember that outlier).

Another possible way to plot the data in Table 2.4 is to simply combine all the data in one scatterplot, identifying the row and corner group observations in some way. This is what we have done in Figure 2.19.

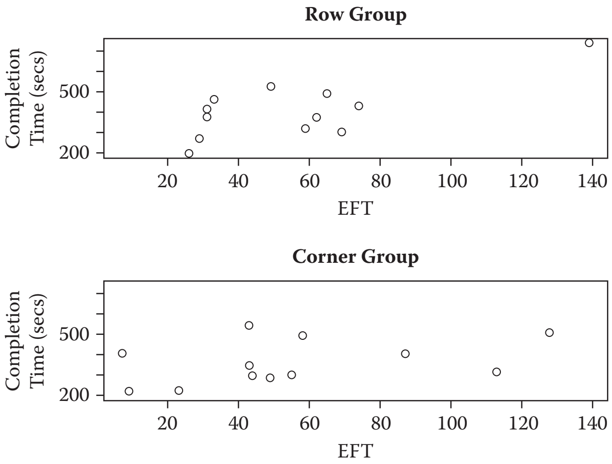


FIGURE 2.17
Scatterplots of time to completions against EFT score for row and corner groups.

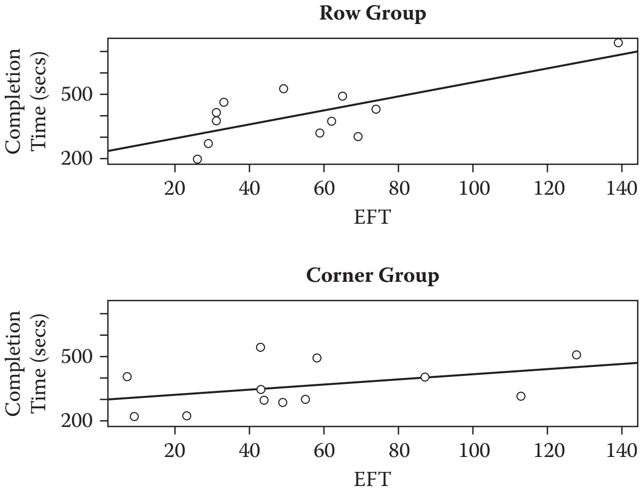


FIGURE 2.18
Scatterplots of time to completion against EFT for row and corner groups with added linear regression fit.

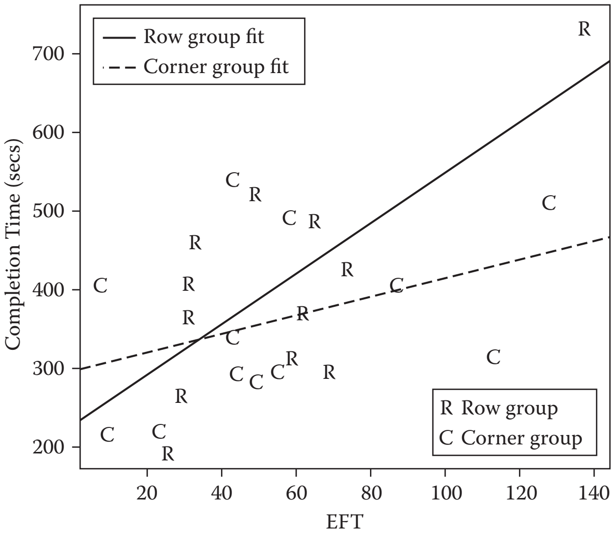


FIGURE 2.19
Scatterplot of completion time against EFT with observations labeled as row or corner group and linear regression fits for each group shown.

TABLE 2.5
Data Collected About Time Spent Looking After Car for First Five Subjects Out of 40

Subject	Sex	Age	Extro	Time
1	Male	55	40	46
2	Male	43	45	79
3	Female	57	52	33
4	Male	26	62	63
5	Female	22	31	20

Now let us move on to consider a larger set of data, part of which is given in Table 2.5. These data are taken from Miles and Shevlin (2001), and give the sex, age, extroversion score, and the average number of minutes per week a person spends looking after his or her car, for 40 people. People may project their self-image through themselves or through the objects they own, such as their cars. Therefore, a theory could be developed that predicts that people who score higher on a measure of extroversion are likely to spend more time looking after their cars. This possibility will be examined in Chapter 4; here we will see how much information about the data we can derive from some scatterplots. Any information about the data collected at this point may be very helpful in fitting formal models to the data.

To begin, we shall construct scatterplots of time spent by people looking after their cars, against age and extroversion score. Often when using scatterplots to look at data, it is helpful to add something about the marginal distributions of the two variables, and this we will do here. Further, we will add to each plot the appropriate linear regression fits separately for men and women. The two plots are shown in Figures 2.20 and 2.21. The plot in Figure 2.20 shows that the relationship between time spent looking after car and age is approximately the same for men and women and time increases a little with age. Figure 2.21 shows that time spent looking after car increases with an increase in extroversion score for both men and women, but that the increase appears greater for men. This has implications for how these data might be modeled as we shall see in Chapter 4.

2.3.1 The Bubbleplot

The scatterplot can only display two variables. However, there have been a number of suggestions as to how extra variables may be included. In this subsection we shall illustrate one of these, the bubbleplot, in which three variables are displayed; two are used to form the scatterplot itself, and then the values of the third variable are represented by circles with radii proportional to these values and centered on the appropriate point in the scatterplot.

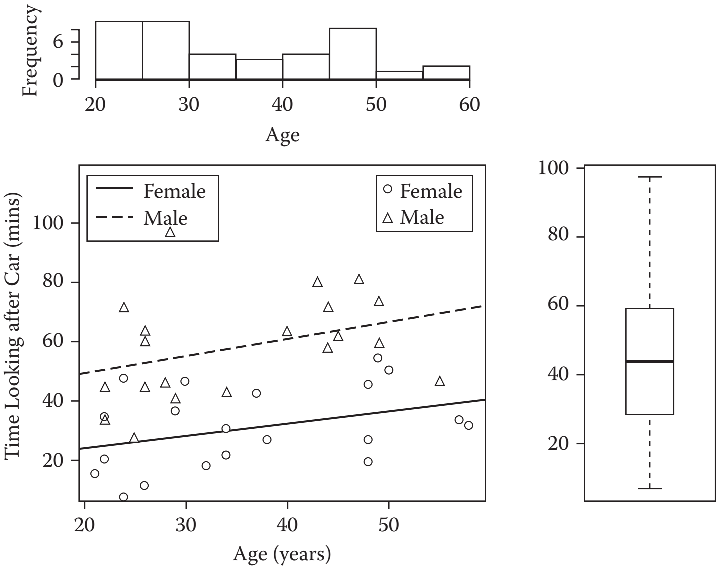


FIGURE 2.20
Scatterplot of time spent looking after car, against age, showing marginal distributions of the two variables and fitted linear regressions for men and women.

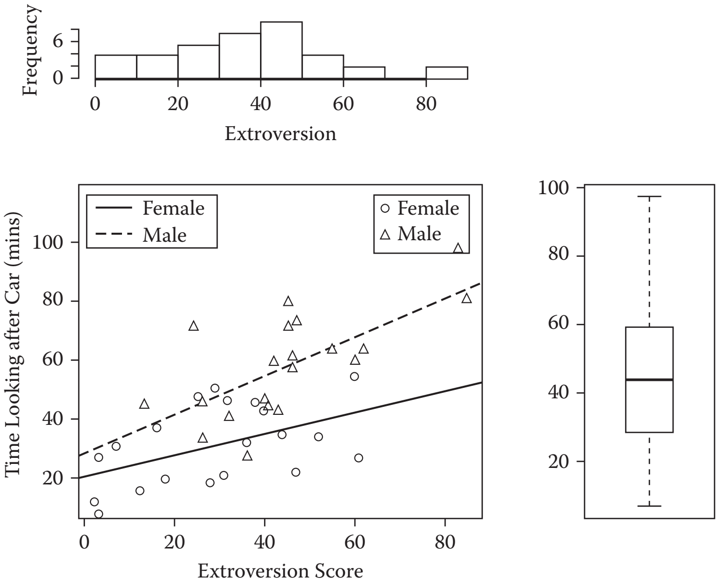


FIGURE 2.21
Scatterplot of time spent looking after car, against extroversion, showing marginal distributions of the two variables and fitted linear regressions for men and women.

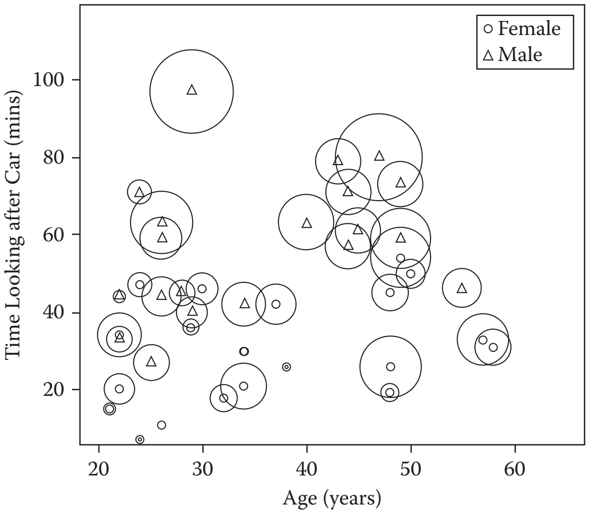


FIGURE 2.22
Bubbleplot of time spent looking after car, against age, with extroversion represented as circles.

For the data in Table 2.5, Figure 2.22 shows a bubbleplot with time spent looking after the car, against age as the scatterplot, and the extroversion scores represented by circles with appropriate radii. Gender is also displayed on the plot, so essentially, Figure 2.22 displays all four variables in the data set. Whether more information can be gleaned from this than from the plots given earlier is perhaps a moot point. But one observation does stand out: an approximately 30-year-old, extroverted man who spends almost 100 min per week looking after his car. Perhaps some counseling might be in order!

A plot a little like a bubbleplot is used by Bickel et al. (1975) to analyze the relationship between admission rate and the proportion of women applying to various academic departments at the University of California at Berkeley. The scatterplot of percentage of women applicants against percentage of applicants admitted is shown in Figure 2.23; the plots are enhanced by "boxes," the sizes of which indicate the relative number of applicants. The negative correlation indicated by the scatterplot is due almost exclusively to a trend for the large departments. If only a simple scatterplot had been used here, vital information about the relationship would have been lost.

2.3.2 The Bivariate Boxplot

A further helpful enhancement to the scatterplot is often provided by the two-dimensional analog of the boxplot for univariate data, known as the bivariate boxplot (Goldberg and Iglewicz, 1992). This type of boxplot may be useful in indicating the distributional properties of the data and in identi-

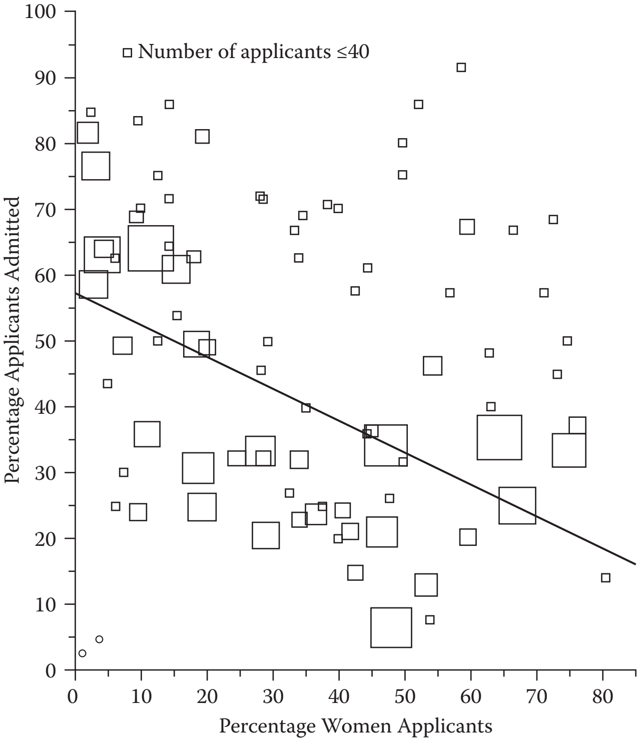


FIGURE 2.23
Scatterplot of the percentage of female applicants versus percentage of applicants admitted to 85 departments at the University of California at Berkeley. (Reproduced with permission from Bickel, P. J. et al., 1975, *Science*, 187, 398–404.)

fying possible outliers. The bivariate boxplot is based on calculating robust measures of location, scale, and correlation; it consists essentially of a pair of concentric ellipses, one of which (the "hinge") includes 50% of the data, and the other (called the "fence") which delineates potential troublesome outliers. In addition, resistant regression lines of both y on x and x on y are shown, with their intersection showing the bivariate locations estimator. The acute angle between the regression lines will be small for a large absolute value of correlations and large for a small one.

Figure 2.24 shows the bivariate boxplot of time spent looking after car and age, and Figure 2.25 shows the corresponding diagram for time and extroversion. Neither diagram shows any clear outliers, that is, observations that fall outside the dotted ellipse. But in both diagrams there is one observation that lies on the dotted ellipse.

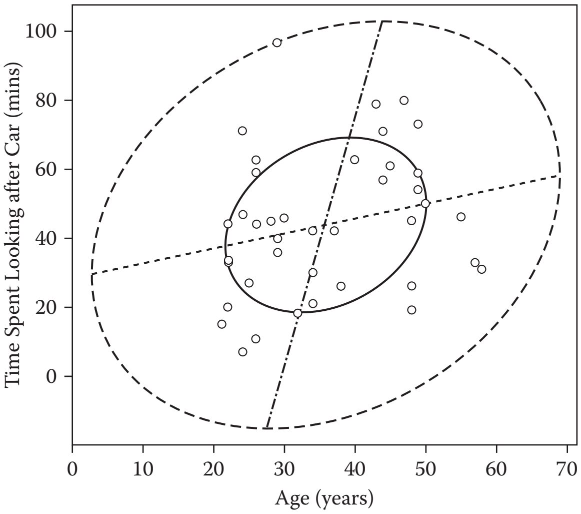


FIGURE 2.24
Bivariate boxplot of time spent looking after car and age.

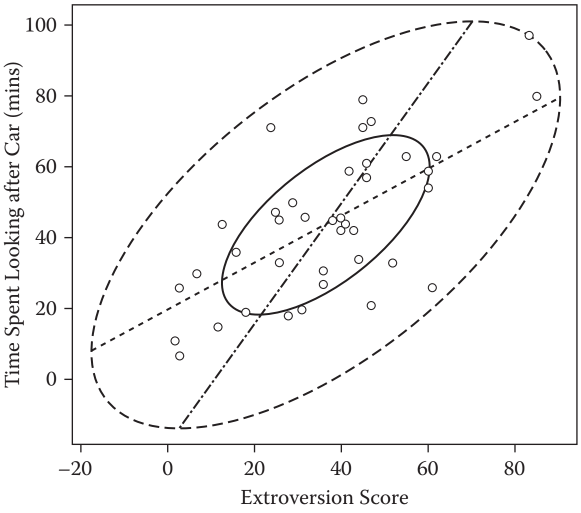


FIGURE 2.25
Bivariate boxplot of time spent looking after car and extroversion.

2.4 Scatterplot Matrices

When there are many variables measured on all the individuals in a study, an initial examination of all the separate pairwise scatterplots becomes difficult. For example, if 10 variables are available, there are 45 possible scatterplots. But all these scatterplots can be conveniently arranged into a scatterplot matrix that then aids in the overall comprehension and understanding of the data.

A scatterplot matrix is defined as a square, symmetric grid of bivariate scatterplots. The grid has q rows and columns, each one corresponding to a different variable. Each of the grid's cells shows a scatterplot of two variables. Variable j is plotted against variable i in the ijth cell, and the same variables appear in cell ji with the x- and y-axes of the scatterplots interchanged. The reason for including both the upper and lower triangles of the grid, despite the seeming redundancy, is that it enables a row and a column to be visually scanned to see one variable against all others, with the scales for the one variable lined up along the horizontal or the vertical.

To illustrate the use of a scatterplot matrix, we shall use the data shown in Table 2.6. These data arise from an experiment in which five different types of electrode were applied to the arms of 16 subjects and the resistance measured (in kilohms). The experiment was designed to see whether all electrode types performed similarly. The scatterplot matrix for the data is shown in Figure 2.26; each of the scatterplots in the diagram has been enhanced by the addition of the linear fit of the y variable on the x variable. The diagram suggests the presence of several outliers, the most extreme of which is subject 15; the reason for the two extreme readings on this subject was that he had very hairy arms. Figure 2.26 also indicates that the readings on particular pairs of electrodes, for example, electrode 1 and electrode 4, are hardly related at all.

We can use the plot of results for the first and second electrodes to demonstrate how the bivariate boxplot looks when there are probable outliers in the data (see Figure 2.27). Three outliers are identified by the bivariate boxplot. If we calculate the correlation coefficient between the two variables using all the

TABLE 2.6
Measure of Resistance (Kilohms) Made on Five Different Types of Electrode for Five of the 16 Subjects

Subject	E1	E2	E3	E4	E5
1	500	400	98	200	250
2	660	600	600	75	310
3	250	370	220	250	220
4	72	140	240	33	54
5	135	300	450	430	70

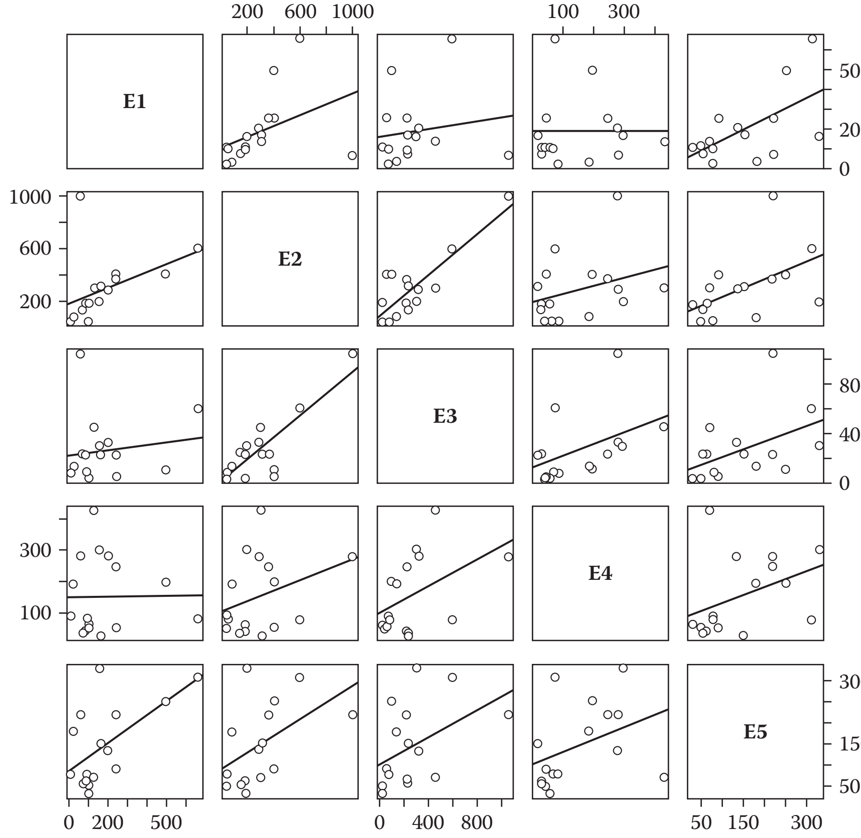


FIGURE 2.26
Scatterplot matrix for data on measurements of skin resistance made with five different types of electrodes.

data, we get a value of 0.41; if we recalculate the correlation after removing subjects 1, 2, and 15, we get a value of 0.88—more than double the previous value. This example underlines how useful the bivariate boxplot can be, and also underlines the danger of simply calculating a correlation coefficient without examining the relevant scatterplot.

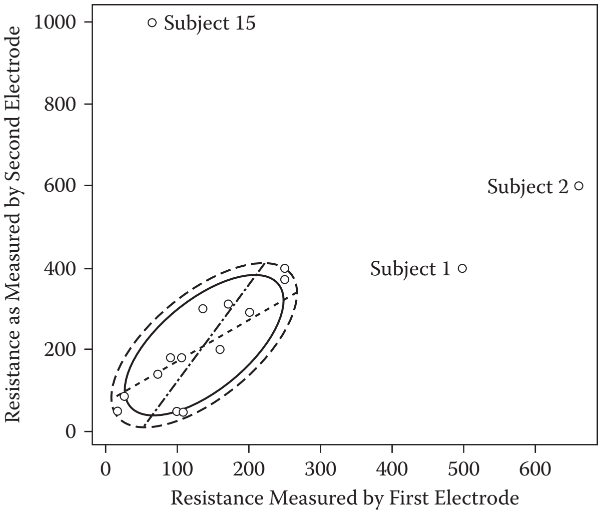


FIGURE 2.27
Bivariate boxplot for data on electrodes one and two.

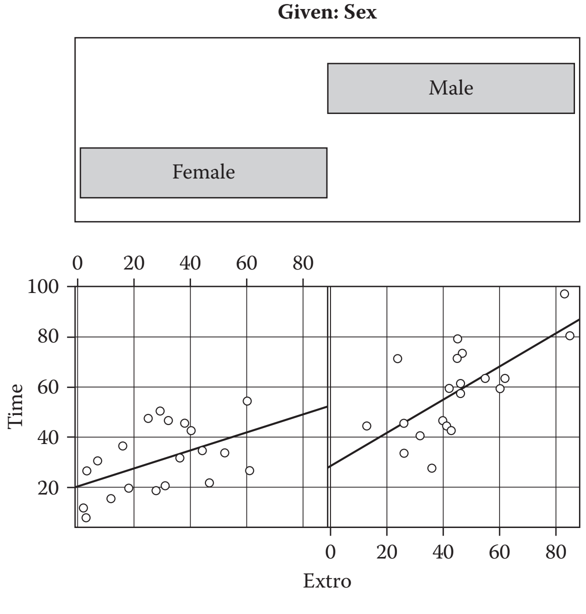


FIGURE 2.28
Coplot of time spent looking after car against extroversion conditioned on sex.

2.5 Conditioning Plots and Trellis Graphics

The conditioning plot or coplot is a potentially powerful visualization tool for studying how, say, a response variable depends on two or more explanatory variables. In essence, such plots display the bivariate relationship between two variables while holding constant (or "conditioning upon") the values of one or more other variables. If the conditioning variable is categorical, then the coplot is no more than, say, a scatterplot of two variables for each level of the categorical variable. As an example of this type of simple coplot, Figure 2.28 shows plots of time spent looking after car against extroversion score conditioned on sex; each scatterplot is enhanced by a linear regression fit. The plot highlights what was found in an earlier plot (Figure 2.21)—that the relationship between time spent looking after car and extroversion is different for men and women.

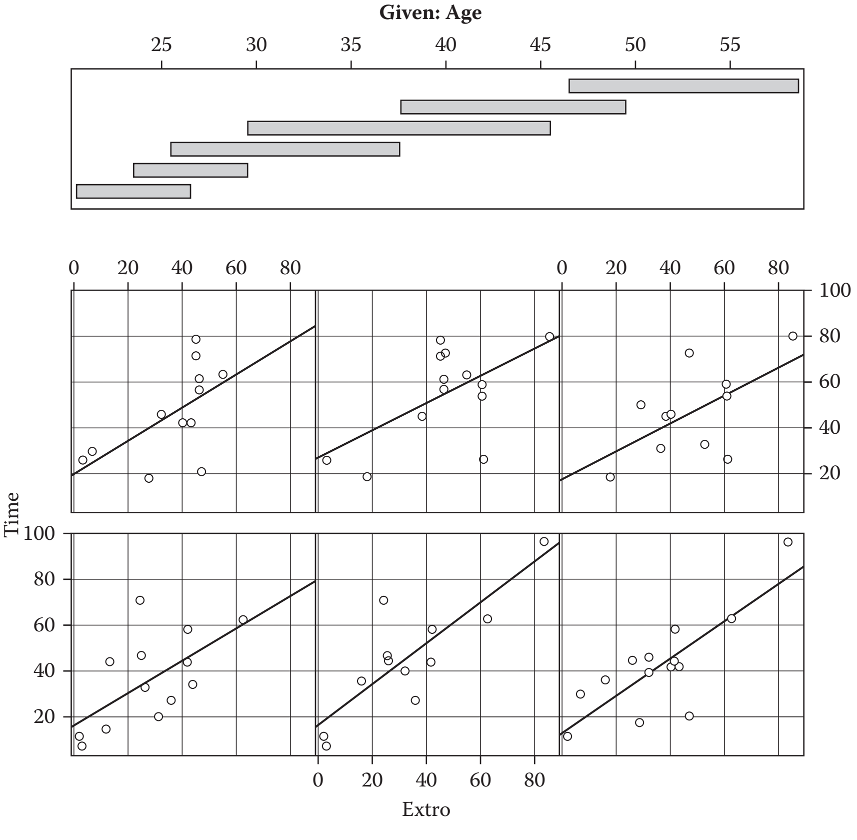


FIGURE 2.29
Coplot of time against extroversion conditioned on age.

As a more complicated coplot, Figure 2.29 shows time spent looking after car against extroversion conditioned on age. In this diagram, the panel at the top of the figure is known as the given panel; the panels below are dependence panels. Each rectangle in the given panel specifies a range of values of population size. On a corresponding dependence panel, time is plotted against age for those people whose ages lie in the particular interval. To match age intervals to dependence panels, the latter are examined in order from left to right in the bottom row and, then again, from left to right in subsequent rows. The plot suggests that the relationship between time and extroversion is much the same over the age range observed in the data set.

Conditional graphical displays are simple examples of a more general scheme known as *trellis graphics* (Cleveland, 1993). This is an approach to examining high-dimensional structure in data by means of one-, two-, and three-dimensional graphs. The problem addressed is how observations of one or more variables depend on the observations of the other variables. The essential feature of this approach is the multiple conditioning that allows some type of plot to be displayed for different values of a given variable (or variables). The aim is to help in understanding both the structure of the data and how well proposed models describe the structure. Excellent examples of the application of trellis graphics are found in Sarkar (2008).

As a relatively simple example of what can be done with trellis graphics, we will again use the data on time spent looking after car and produce a three-dimensional scatter plot for time, age, and extroversion conditioned on sex (see Figure 2.30). This diagram makes the generally longer times spent looking after their cars by men very apparent, although whether it adds anything to earlier plots is a question we leave for the reader.

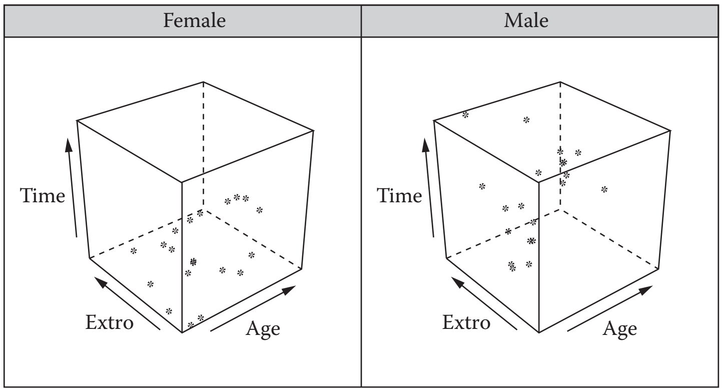


FIGURE 2.30
Three-dimensional scatterplot of time, age, and extroversion conditioned on sex.

Let us now look at two more complex examples of trellis graphics, taken from Sarkar (2008). The first involves data collected in a survey of doctorate degree recipients in the United States. The data are shown in Table 2.7. Any graphic for the data has to involve the proportions of reasons across fields of study rather than the counts because the latter do not tell us very much, except, for example, that the "Biological Sciences" subject area contributes the majority of postdocs. A stacked bar chart of the data based on the proportions rather than the counts in Table 2.7 is shown in Figure 2.31. An alternative display for the proportions, a multipanel dot plot, is shown in Figure 2.32. For comparing the proportions of reasons across areas of study, the dot plot seems preferable because it is more easily judged by eye. The multipanel dot plot becomes even more informative if the proportions are ordered from low to high within each panel, as shown in Figure 2.33. We see that the most popular reason for choosing a postdoctoral position is "Expected or Additional Training," and that this applies to all areas of study. For "Earth, Atmospheric, and Ocean Sciences," postdocs appear to mostly take a job because other employment is not available. Figure 2.33 provides an easy-to-use and informative display of the data.

TABLE 2.7
Reasons for Choosing a Postdoctoral Position After Graduating from U.S. Universities by Area of Study

Subject	Expected or Additional Training	Work with Specific Person	Training Outside PhD Field	Other Employment not Available	Other
Biological sciences	6404	2427	1950	1779	602
Chemistry	865	308	292	551	168
Earth, Atmospheric, and Ocean Sciences	343	75	75	238	80
Engineering	586	464	288	517	401
Medical sciences	205	137	82	68	74
Physics and astronomy	1010	347	175	399	162
Social and behavioral sciences	1368	564	412	514	305
All postdoctorates	11197	4687	3403	4406	1914

The last example is also taken from Sarkar (2008) and is shown in Figure 2.34. The diagram gives the scatterplot matrix of violent crime rates in the 50 states of the United States in 1973, conditioned on geographical region. Each scatterplot in the diagram is enhanced by a locally weighted regression fit, an alternative to linear regression, to be discussed in Chapter 3. The relationship between each pair of crimes appears to be pretty similar in all four regions.

Trellis graphics is a potentially very exciting and powerful tool for the exploration of data from behavioral studies. However, a word of caution is perhaps in order. With small or moderately sized data sets, the number of

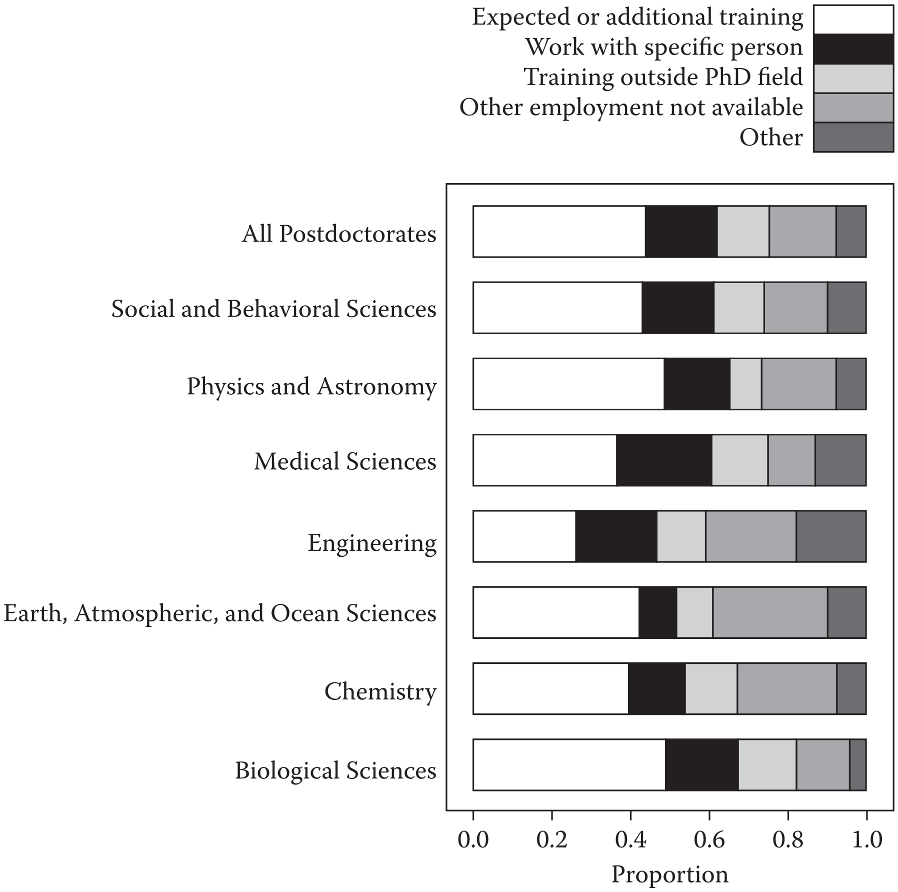


FIGURE 2.31
A stacked bar chart showing the proportion of reasons for choosing a postdoc by field of study.

observations in each panel may be too few to make the panel graphically acceptable. A further caveat is that trellis graphics can be seductive with the result that simpler graphics, which in many cases may be equally informative about a data set, may be ignored.

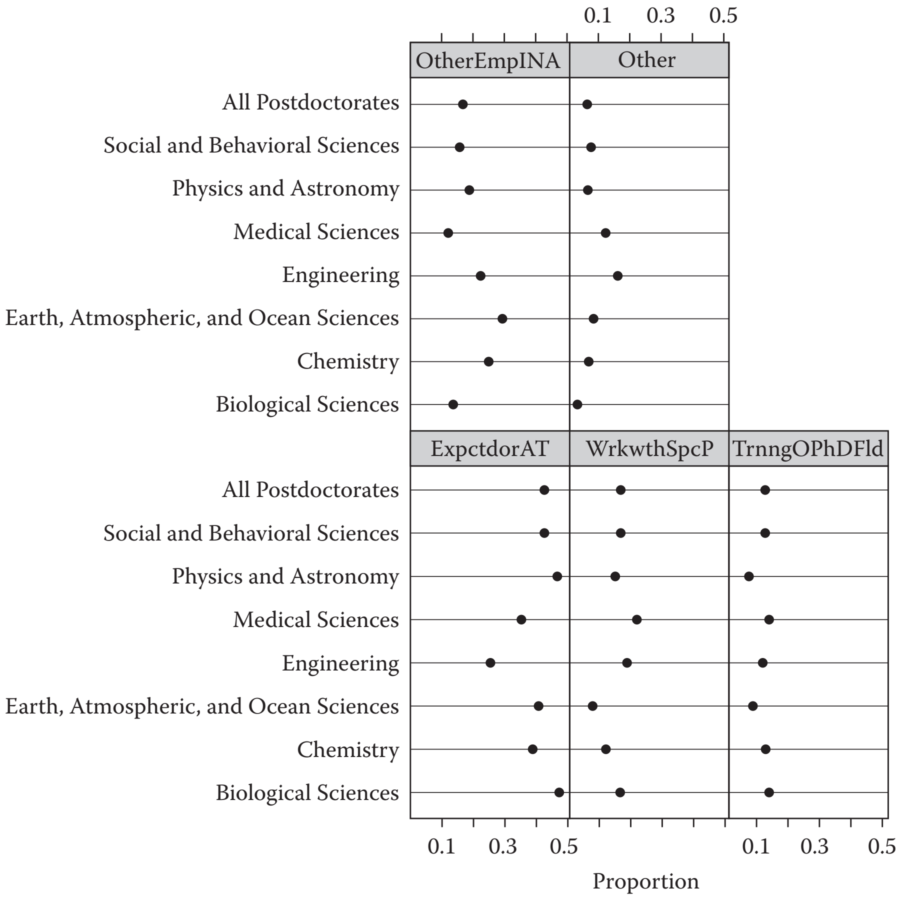


FIGURE 2.32
A multipanel dot plot showing the proportion of reasons for choosing a postdoc by field of study.

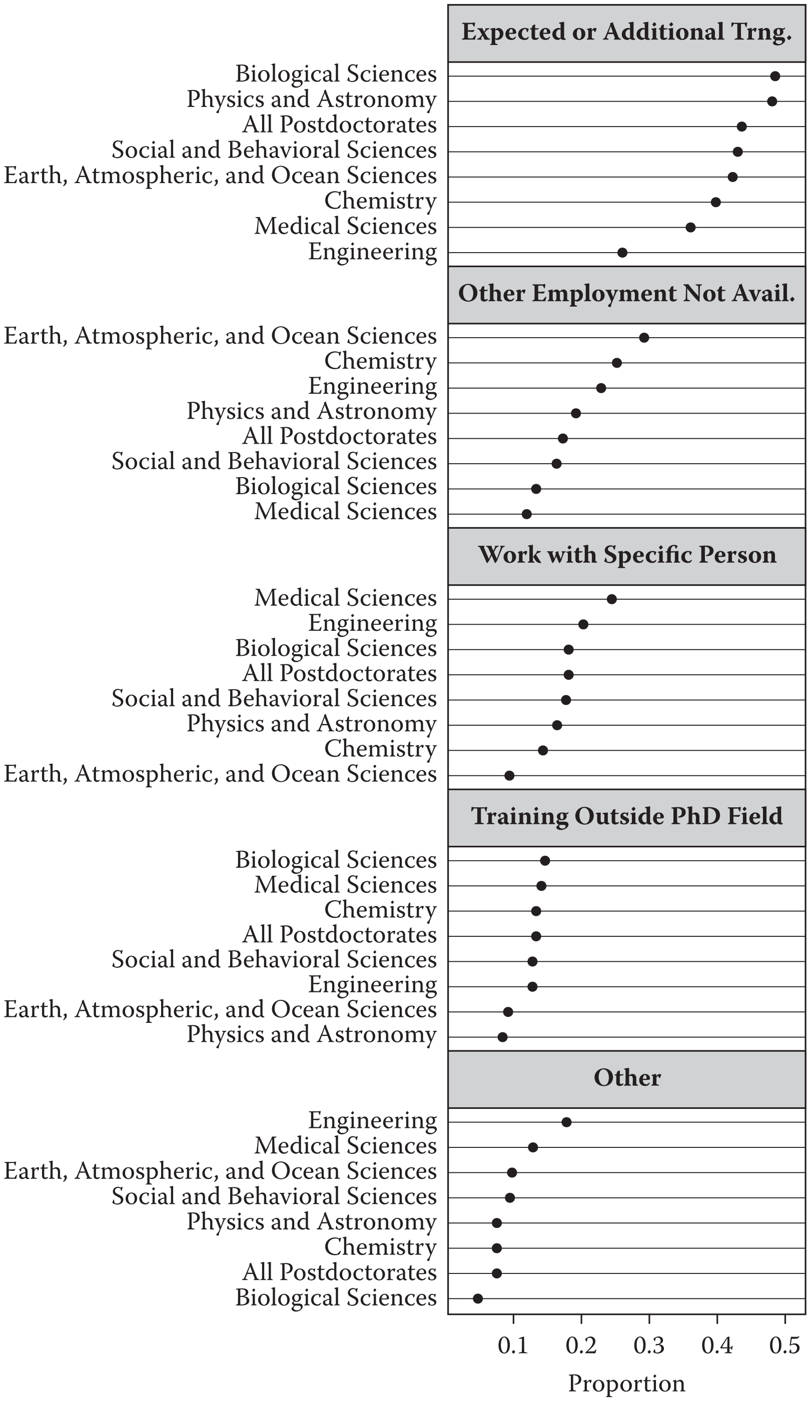


FIGURE 2.33
Reasons for choosing a postdoc position.

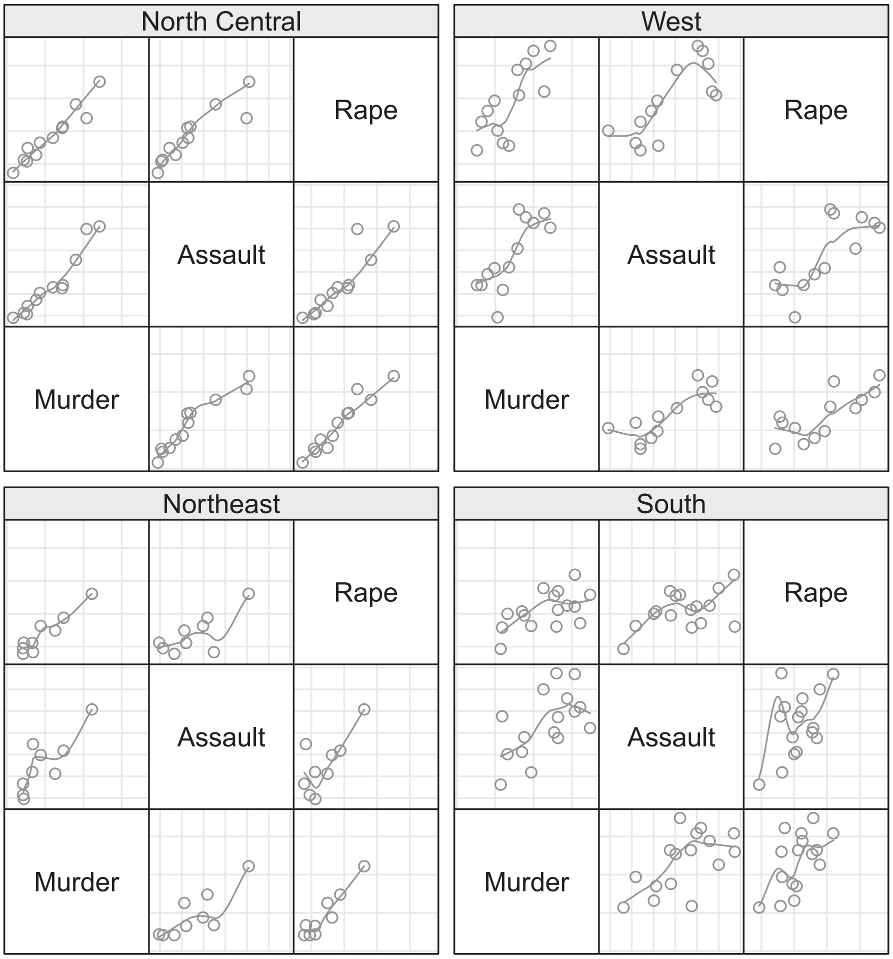


FIGURE 2.34
Scatterplot matrices of violent crime rates conditioned on geographical region.

2.6 Graphical Deception

In general, graphical displays of the kind described in previous sections are extremely useful in the examination of data; indeed, they are almost essential both in the initial phase of data exploration and in the interpretation of results from more formal statistical procedures, as will be seen in later chapters. Unfortunately, it is relatively easy to mislead the unwary with graphical material, and not all graphical displays are as honest as they should be. For example, consider the plot of the death rate per million from breast cancer for several periods over three decades, shown in Figure 2.35a. The rate appears to show a rather alarming increase. However, when the data are replotted with the vertical scale beginning at zero, as shown in Figure 2.35b, the increase in the breast cancer death rate is altogether less startling. This example illustrates that undue exaggeration or compression of the scales is best avoided when drawing graphs (unless, of course, you are actually in the business of deceiving your audience).

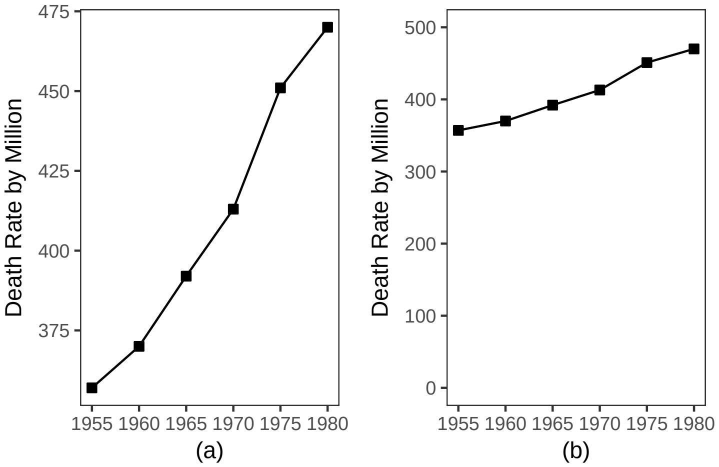


FIGURE 2.35
Death rates from breath cancer where (a) the y-axis does not include the origin and (b) the y-axis does include the origin.

A very common distortion introduced into the graphics most popular with newspapers, television, and the media in general is when both dimensions of a two-dimensional figure or icon are varied simultaneously in response to changes in a single variable. The examples shown in Figure 2.36, both taken from Tufte (1983), illustrate this point. Tufte quantifies the distortion with

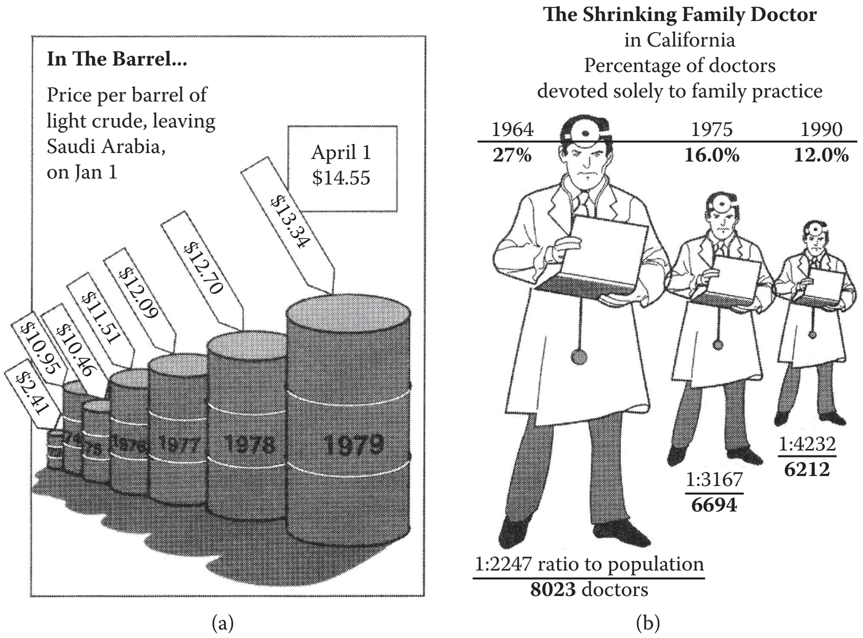


FIGURE 2.36
Graphics exhibiting lie factors of (a) 9.4 and (b) 2.8.

what he calls the *lie factor* of a graphical display, which is defined as the size of the effect shown in the graph divided by the size of the effect in the data. Lie factor values close to unity show that the graphic is probably representing the underlying numbers reasonably accurately. The lie factor for the “oil barrels” is 9.4 since a 454% increase is depicted as 4280%. The lie factor for the “shrinking doctors” is 2.8.

A further example given by Cleveland (1994) and reproduced here in Figure 2.37 demonstrates that even the manner in which a simple scatterplot is drawn can lead to misperceptions about data. The example concerns the way in which judgment about the correlation of two variables made on the basis of looking at their scatterplot can be distorted by enlarging the area in which the points are plotted. The coefficient of correlation in the diagram on the right in Figure 2.37 appears greater.

Some suggestions for avoiding graphical distortion, taken from Tufte (1983), are

- The representation of numbers, as physically measured on the surface of the graphic itself, should be directly proportional to the numerical quantities represented.

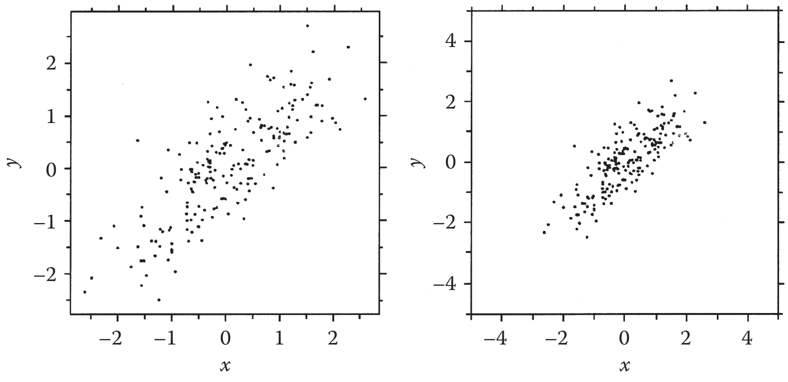


FIGURE 2.37
Misjudgment of size of correlation caused by enlarging the plot area.

- Clear, detailed, and thorough labeling should be used to defeat graphical distortion and ambiguity. Write out explanations of the data on the graphic itself. Label important events in the data.
- To be truthful and revealing, data graphics must bear on the heart of quantitative thinking: "compared to what?" Graphics must not quote data out of context.
- Above all else, show the data.

Being misled by graphical displays is usually a sobering but not a life-threatening experience. However, Cleveland (1994) gives an example, where using the wrong graph contributed to a major disaster in the American space program, namely, the explosion of the Challenger space shuttle and the deaths of the seven people on board. To assess the suggestion that low temperature might affect the performance of the O-rings that sealed the joints of the rocket motor, engineers studied the graph of the data shown in Figure 2.38. Each data point was from a shuttle flight in which the O-rings had experienced thermal distress. The horizontal axis shows the O-ring temperature, and the vertical scale shows the number of O-rings that had experienced thermal distress. On the basis of these data, Challenger was allowed to take off when the temperature was 31°F, with tragic consequences.

The data for "no failures" are not plotted in Figure 2.38 because the engineers involved believed that these data were irrelevant to the issue of dependence. They were mistaken, as shown by the plot in Figure 2.39, which includes all the data. Here a pattern does emerge, and a dependence of failure on temperature is revealed.

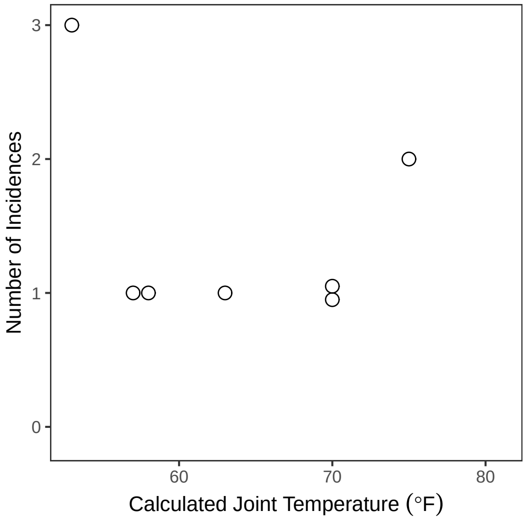


FIGURE 2.38
Data taken from Siddhartha et al. (1989) plotted by space shuttle engineers the evening before the Challenger accident to determine the dependence of O-ring failure on temperature.

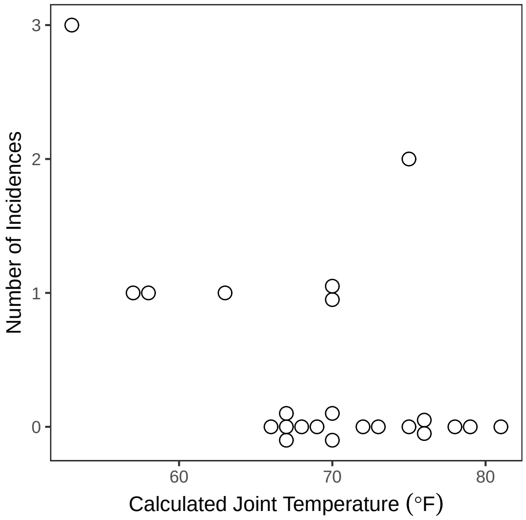


FIGURE 2.39
A plot of the complete O-ring data.

To end on a less somber note and to show that misperception and miscommunication are certainly not confined to statistical graphics, see Figure 2.40!

FIGURE 2.40
Misperception and miscommunication are sometimes a way of life! (Drawing by Charles E. Martin, ©1961, 1969, *The New Yorker Magazine.* Used with permission.)

2.7 Summary

- Graphical displays are an essential feature in the analysis of empirical data. The prime objective is to communicate to ourselves and others.
- Graphic design must do everything it can to help people understand the subject.
- In some cases, a graphical "analysis" may be all that is required (or merited) for a data set.
- Pie charts and bar plots are rarely more informative than a numerical tabulation of the data.
- Boxplots are more useful than histograms for displaying most data sets and are very useful for comparing groups. In addition, they are useful for identifying possible outliers.
- Scatterplots are the fundamental tool for examining relationships between variables. They can be enhanced in a variety of ways to provide

extra information. Scatterplots are always needed when considering numerical measures of correlation between pairs of variables.

- Scatterplot matrices are a useful first step in examining data with more than two variables.
- Trellis graphs can look very enticing and may in many, but not all, cases give greater insights into patterns in the data than simpler plots.
- Beware of graphical deception.
- Unless graphs are relatively simple, they are not likely to survive the first glance.

2.8 Exercises

(excluded from MABS for IODS)

Part II

Regression and model validation (“MABS for IODS”)

Selected excerpts of the textbook *Multivariate Analysis for the Behavioral Sciences*, Second Edition (Vehkalahti and Everitt, 2019), produced exclusively for the students of IODS (Introduction to Open Data Science, University of Helsinki), with a permission from Chapman and Hall/CRC, London, UK.

3 Simple Linear and Locally Weighted Regression

In very general terms, regression analysis involves the development and use of statistical techniques designed to reflect the way in which variation in an observed random variable changes with changing circumstances. More specifically in this chapter simple linear regression is described; here the aim is to derive an equation relating a dependent and a single explanatory variables. Estimation of the parameters in the simple linear regression model is covered and a number of examples are given. Assessing whether the assumptions behind the fitted model are valid by using regression diagnostics is described and the chapter ends with an account of scatterplot smoothers.

4 Multiple Linear Regression

This chapter builds on the one previous and examines the multiple linear regression model where there are several explanatory variables of interest and determining the effect of each on the response variable is the goal. After fitting such a model it is generally of interest to try to seek out the most parsimonious model for the data and methods for this are discussed in the chapter. The chapter ends with a description of regression diagnostics for the multiple regression model.

3

Simple Linear and Locally Weighted Regression

3.1 Introduction

Table 3.1 shows the heights (in centimeters) and the resting pulse rates (beats per minute) for 5 of a sample of 50 hospital patients (data sets with two variables are often referred to as bivariate data). Is it possible to use these data to construct a model for predicting pulse rate from height, and what type of model might be used? Such questions serve to introduce one of the most widely used statistical techniques: regression analysis. In very general terms, regression analysis involves the development and use of statistical techniques designed to reflect the way in which variation in an observed random variable changes with changing circumstances. More specifically, the aim of a regression analysis is to derive an equation relating a dependent and an explanatory variable or, more commonly, several explanatory variables. The derived equation may sometimes be used solely for prediction, but more often its primary purpose is as a way of establishing the relative importance of the explanatory variables in determining the response variable, that is, in establishing a useful model to describe the data. (Incidentally, the term regression was first introduced by Galton in the 19th century to characterize a tendency toward mediocrity, that is, more average, observed in the offspring of parents.)

In this chapter, we shall concern ourselves with regression models for a response variable that is continuous and for which there is a single explanatory variable. In Chapter 4, we will extend the model to deal with the situation in

TABLE 3.1
Pulse Rates and Heights Data

Subject	Heights (cm)	Pulse Rates (beats/min)
1	160	68
2	167	80
3	162	84
4	175	80
5	185	80

which there are several explanatory variables, and then, in Chapters 5 and 6, we shall consider various generalizations to this model, for example, to allow the response variable to be categorical.

No doubt most readers will have covered simple linear regression for a response variable and a single explanatory variable in their introductory statistics course. Despite this, it may be worthwhile reading Section 3.2 both as an aide-memoire and as an initial step in dealing with the more complex procedures needed when several explanatory variables are considered, a situation to be discussed in Chapter 4. It is less likely that readers will have been exposed to locally weighted regression, which will also be covered in this chapter and which can often serve as a useful antidote to the (frequently unthinking) acceptance of the simple linear model per se.

3.2 Simple Linear Regression

The technical details of the simple linear regression model are given in Technical Section 3.1.

Technical Section 3.1: Simple Linear Regression

Assume that y_i represents the value of what is generally known as the response variable on the ith individual and x_i represents the individual's values on what is most often called an explanatory variable; the simple linear regression model is

$$y_i = \beta_0 + \beta_1 x_i + \varepsilon_i$$

where β_0 is the intercept, and β_1 is the slope of the linear relationship assumed between the response variable y and the explanatory variable x, and ε_i is an error term measuring the amount by which the observed value of the response differs from the value predicted by the fitted model. ("Simple" here means that the model contains only a single explanatory variable; we shall deal with the situation where there are several explanatory variables in Chapter 4.) The error terms are assumed to be statistically independent random variables having a normal distribution with mean 0 and the same variance σ^2 at every value of the explanatory variable. The parameter β_1 measures the change in the response variable produced by a change of one unit in the explanatory variable.

The regression coefficients β_0 and β_1 may be estimated as $\hat{\beta}_0$ and $\hat{\beta}_1$ using least-squares estimation in which the sum of squared differences between the observed values of the response variable y_i and the values "predicted" by the regression equation $\hat{y}_i = \hat{\beta}_0 + \hat{\beta}_1 x_i$ is minimized, leading to the following estimates:

$$\hat{\beta}_0 = \bar{y} - \hat{\beta}_1 \bar{x}$$

$$\hat{\beta}_1 = \frac{\sum (y_i - \bar{y})(x_i - \bar{x})}{\sum (x_i - \bar{x})^2}$$

The predicted values of y_i from the model are

$$\hat{y}_i = \hat{\beta}_0 + \hat{\beta}_1 x_i$$

This fitted equation could be used to predict the value of the response variable for some particular value of the explanatory variable, but it is very important to note that trying to predict values of the response variable outside the observed range of the explanatory variable is a potentially dangerous business.

The variability of the response variable can be partitioned into a part that is due to regression on the explanatory variable, the regression mean square (RGMS) given by RGMS $= \sum_{i=1}^{n} (\hat{y}_i - \bar{y})^2$, and a residual mean square(RMS) given by RMS $= \sum_{i=1}^{n} (y_i - \hat{y}_i)^2/(n-2)$. The RMS gives an estimate of σ^2, and the F-statistic given by F = RGMS/RMS with 1 and $n-2$ degrees of freedom (DF) gives a test that the slope parameter β_1 is 0. (This is of course equivalent to testing that the correlation of the two variables is 0.)

The estimated variance of the slope parameter estimate is

$$\text{Var}\left(\hat{\beta}_1\right) = \frac{s^2}{\sum\limits_{i=1}^{n} (x_i - \bar{x})^2}$$

The estimated variance of a predicted value y_{pred} at a given value of x, say x_0, is

$$\text{Var}\left(y_{\text{pred}}\right) = s^2 \left[\frac{(x_0 - \bar{x})^2}{\sum\limits_{i=1}^{n} (x_i - \bar{x})^2} + \frac{1}{n} + 1 \right]$$

where s^2 is the RMS value defined earlier. (Note that the variance of the prediction increases as x_0 gets further away from $\bar{x}$.)

A confidence interval for the slope parameter can be constructed in the usual way from the estimated standard error of the parameter, and the variance of a predicted value can be used to construct confidence bounds for the fitted line.

In some applications of simple linear regression, a model without an intercept is required (when the data is such that the line must go through the origin), that is, a model of the form

$$y_i = \beta x_i + \varepsilon_i$$

In this case, application of least squares gives the following estimator for β:

$$\hat{\beta} = \sum_{i=1}^{n} x_i y_i / \sum_{i=1}^{n} x_i^2$$

3.2.1 Fitting the Simple Linear Regression Model to the Pulse Rates and Heights Data

Fitting the simple linear regression model to the data in Table 3.1 gives the results shown in Table 3.2. Figure 3.1 shows the fitted line on a scatterplot of the data and a 95% confidence interval for the predicted values calculated from the relevant variance term given in Technical Section 3.1; the diagram also contains some graphical displays giving information about the marginal distributions of each of the two variables. The results in Table 3.2 show that there is no evidence of any linear relationship between pulse rate and height. The multiple R-squared, which in this example with a single explanatory variable is simply the square of the correlation coefficient between pulse rate and height, is 0.0476, so that less than 5% of the variation in pulse rate is explained by the variation in height. Figure 3.1 shows that the fitted line is almost horizontal and that a horizontal line could easily be placed within the two dotted lines indicating the confidence interval for predicted values. Clearly, the fitted linear regression would be very poor if used to predict pulse rate from height.

Figure 3.1 also shows that pulse rate has a very skewed distribution. Because of the latter, it may be of interest to repeat the plotting and fitting process after some transformation of pulse rate (see Exercise 3.1).

TABLE 3.2
Results from Fitting a Simple Linear Regression to the Pulse and Heights Data

	Coefficients			
	Estimate	**Standard Error**	**t-Value**	**Pr(>|t|)**
Intercept	46.9069	22.8793	2.050	0.0458
Heights	0.2098	0.1354	1.549	0.1279

Note: Residual standard error: 8.811 on 48 DF; multiple R-squared: 0.04762; F-statistic: 2.4 on 1 and 48 DF; *p*-value: 0.1279.

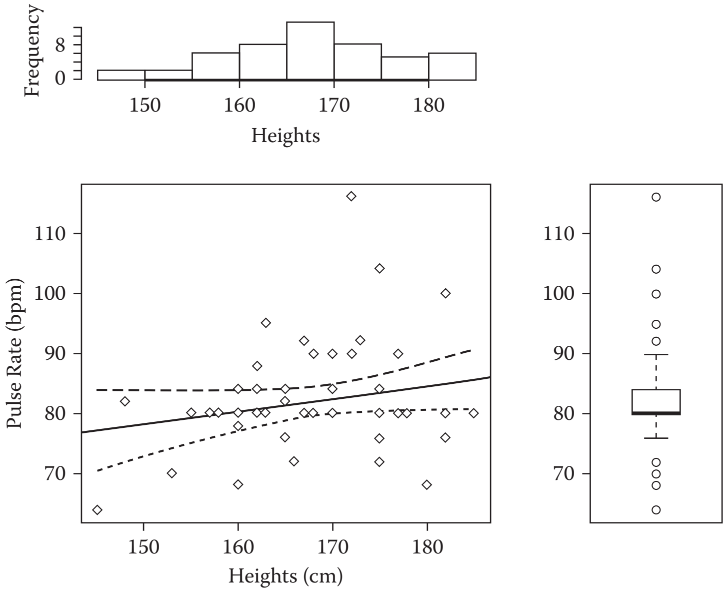


FIGURE 3.1
Scatterplot and fitted linear regression for pulse and heights data.

3.2.2 An Example from Kinesiology

For our second example of simple linear regression, we will use some data from an experiment in kinesiology, a natural care system that uses gentle muscle testing to evaluate many functions of the body in the structural, chemical, neurological, and biological realms. A subject performed a standard exercise at a gradually increasing level. Two variables were measured: (1) oxygen uptake and (2) expired ventilation, which is related to the exchange of gases in the lungs. Part of the data is shown in Table 3.3 (there are 53 subjects in the full data set), and the researcher was interested in assessing the relationship between the two variables. A scatterplot of the data along with the fitted simple linear regression is shown in Figure 3.2. The estimated regression coefficient in Table 3.4 is highly significant, but Figure 3.2 makes it very clear that

TABLE 3.3
Data on Oxygen Uptake and Expired Volume (in liters)

Subject	Oxygen Uptake	Expired Ventilation
1	574	21.9
2	592	18.6
3	664	18.6
4	667	19.1
5	718	19.2

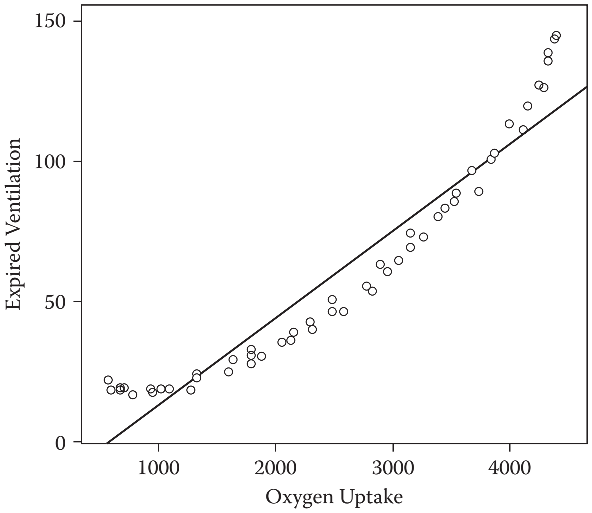


FIGURE 3.2
Scatterplot of expired ventilation against oxygen uptake with fitted simple linear regression.

the simple linear model is not appropriate for these data; we need to consider a more complicated model. The obvious choice here is to consider a model that, in addition to the linear effect of oxygen uptake, includes a quadratic term in this variable, that is, a model of the form

$$y_i = \beta_0 + \beta_1 x_i + \beta_2 x_i^2 + \varepsilon_i$$

Such a model can easily be fitted by least squares to give estimates of its three parameters. One point to note about this model that may seem confusing is that it remains, similar to the simple model outlined in Technical Section 3.1, a linear model despite the presence of the quadratic term. The reason for this

TABLE 3.4
Results from Fitting a Simple Linear Regression to the Kinesiology Data

	Coefficients			
	Estimate	**Standard Error**	**t-Value**	**Pr(>|t|)**
(Intercept)	−18.448734	3.815196	−4.836	<0.001
Oxygen	0.031141	0.001355	22.987	<0.001

Note: Residual standard error: 11.96 on 51 DF; multiple R-squared: 0.912; adjusted R-squared: 0.9103; F-statistic: 528.4 on 1 and 51 DF; *p*-value: <0.001.

is that "linear" in linear regression models refers to the parameters rather than the explanatory variables. An example of a nonlinear model would be

$$y_i = \beta_1 x_i + \exp(\beta_2 x_i) + \varepsilon_i$$

We will not deal with such models in this book. It is worth mentioning here that including polynomial terms, for example, x and x^2, in a linear regression model can sometimes lead to a problem known as collinearity, which will be discussed in Chapter 4. This can often be overcome by what is known as centering the explanatory variable, that is, using the original variable with its mean subtracted as the explanatory variable. Kleinbaum et al. (2013) provide an example of the effectiveness of such an approach for correcting collinearity.

Fitting the model containing the quadratic term in oxygen uptake gives the numerical results shown in Table 3.5 and shows that the regression coefficient for the quadratic term is highly significant. The numerical results are summarized in Figure 3.3, which shows a scatterplot of the data with the addition of the fitted quadratic curve. Clearly, the new model provides an excellent fit.

Note that the numerical results in Table 3.5 are written in scientific notation where, for example, 1.5e–3 means $1.5 \times 10^{-3} = 0.0015$. The reason for this is that values of oxygen squared are very large, so the corresponding estimated regression coefficient and its standard error are very small.

3.3 Regression Diagnostics

Having fitted a simple regression model to our data and estimated and interpreted the regression coefficients, there still remains work to be done. We need to assess the model to see whether, for example, the assumption that the variance of the response does not change with the values of the explanatory

TABLE 3.5
Results from Fitting a Linear Regression Model to the Kinesiology Data with Linear and Quadratic Terms for Oxygen Uptake

	Coefficients			
	Estimate	**Standard Error**	**t-Value**	**Pr(>|t|)**
Intercept	2.427e+01	1.940e+00	12.509	<2e–16
Oxygen	−1.344e–02	1.762e–03	−7.628	6.27e–10
Oxygen^2	8.902e–06	3.444e–07	25.850	<2e–16

Note: Residual standard error: 3.186 on 50 DF; multiple R-squared: 0.9939; F-statistic: 4055 on 2 and 50 DF; p-value: <2.2e–16.

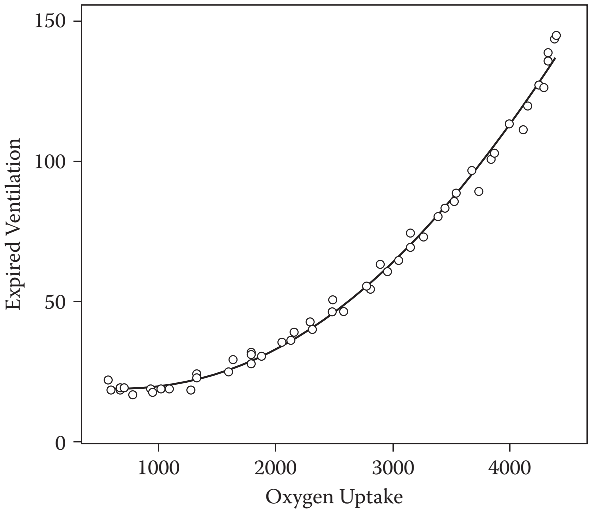
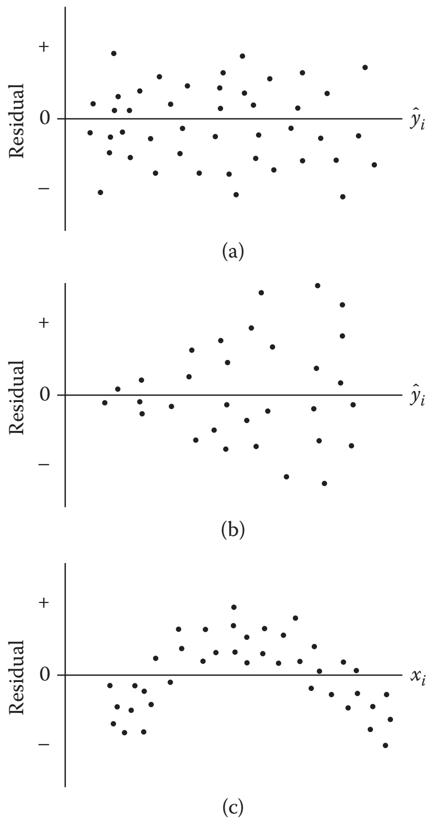


FIGURE 3.3
Kinesiology data showing a fitted linear regression model that includes both oxygen uptake and oxygen uptake squared as explanatory variables.

variable, the constant variance assumption, is reasonable. Further, we need to discover if the model we have used is sensible for the data at hand. Not checking assumptions or assessing if, say, a more complex model is needed and fitting a model that is, in one way or another, unsuitable for the data, are likely to lead to incorrect inferences and conclusions. One way of investigating both the assumptions made and the possible failings of a model is an examination of residuals, that is, the difference between an observed value of the response variable y_i and the fitted value $\hat{y}_i$. (The residuals essentially estimate the error terms in the model.)

In regression analysis, there are various ways of plotting residual values that can be helpful in assessing particular components of the regression model. The most useful plots are as follows:

- A boxplot or probability plot of the residuals can be useful in checking for symmetry and specifically the normality of the error terms in the regression model.
- Plotting the residuals against the corresponding values of the explanatory variable. Any sign of curvature in the plot might suggest that, say, a quadratic term in the explanatory variable should be included in the model.
- Plotting the residuals against the fitted values of the response variable (not the response values themselves for reasons spelt out in Rawlings et



(a)

(b)

(c)

FIGURE 3.4
Idealized residual plots.

al., 1998). If the variability of the residuals appears to increase with the size of the fitted values, a transformation of the response variable prior to fitting is indicated.

Figure 3.4 shows some idealized residual plots that indicate particular points about models:

- Figure 3.4a is what is looked for to confirm that the fitted model is appropriate.
- Figure 3.4b suggests that the assumption of constant variance is not justified so that some transformation of the response variable before fitting might be sensible.
- Figure 3.4c implies that the model needs a quadratic term in the explanatory variable.

(In practice, of course, the residual plots obtained might be somewhat more difficult to interpret than these idealized plots!)

Let us now look at some residual plots for the two examples considered earlier. For the pulse rate and heights data, Figure 3.5 shows four residual plots. The boxplot indicates two very large residuals, but the probability shows little evidence of a departure from linearity, so there is no evidence of a departure from normality. Both Figure 3.5c and 3.5d suggest that the variance of the residuals increases both with height and the fitted values of the pulse rate; the constant variance assumption seems questionable for these data, and a transformation of the response may be helpful (again, see Exercise 3.1).

Moving on to the kinesiology data, Figure 3.6 shows the same four residual plots for a simple linear regression fitted to these data as the plots in Figure 3.5. The probability plot indicates that the residuals do not have a normal distribution, and the plots of residuals against oxygen uptake and fitted expired ventilation show very clearly that a model with a quadratic term in oxygen uptake is needed. For these data, the need for a quadratic term was clear by looking at the scatterplot of expired ventilation against oxygen uptake, but this will not always be the case, and in many cases, the residual

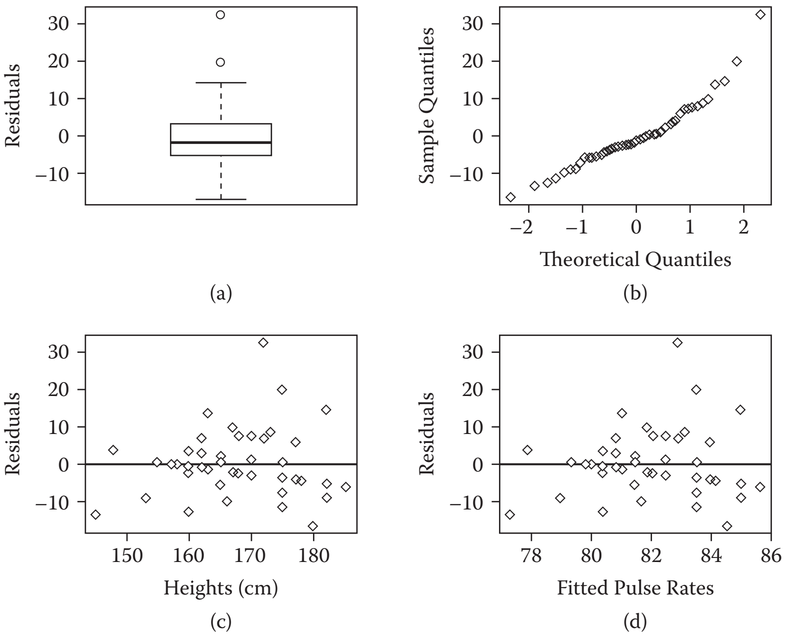
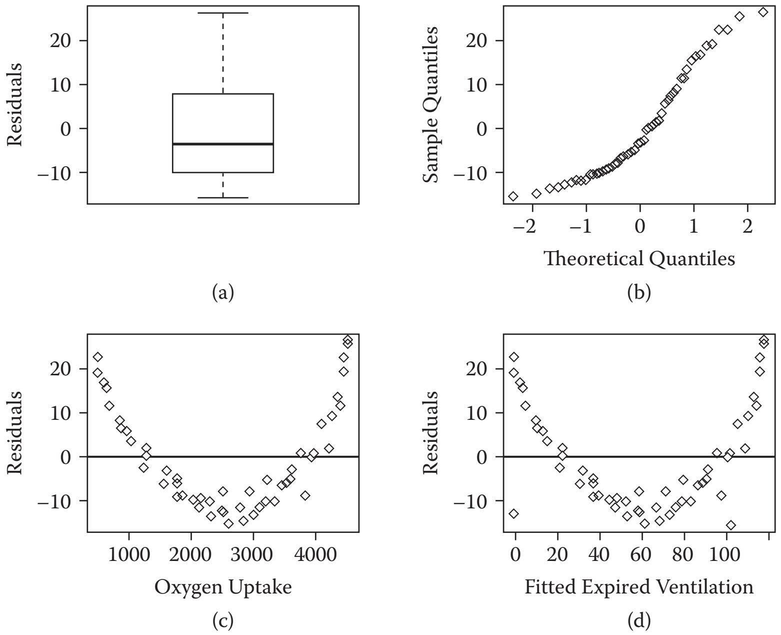


FIGURE 3.5
Residual plots for the pulse rates and heights data form fitting a simple linear regression model: (a) boxplot of residuals, (b) probability plot of residuals, (c) plot of residuals against height, and (d) plot of residuals against fitted pulse rates.



(a)

(b)

(c)

(d)

FIGURE 3.6
Residual plots for the oxygen uptake and expired ventilation data from fitting a simple linear regression model: (a) boxplot of residuals, (b) probability plot of residuals, (c) plot of residuals against oxygen uptake, and (d) plot of residuals against fitted expired ventilation.

plots will uncover problems or the need for other terms in the current model that are not apparent in the scatterplot of the data.

In Figure 3.7, the same four residual plots are given for the kinesiology data after fitting the model with both a linear and a quadratic term for oxygen uptake. We see that now the residuals are far better behaved than in Figure 3.6; clearly, this more complicated model is a far better fit than the simple linear regression model.

The "raw" residuals used here suffer from certain problems that make them less helpful in investigating fitted models than they might be with some relatively simple adjustments. These adjustments, along with a number of other diagnostic tools for regression models, will be discussed in Chapter 4.

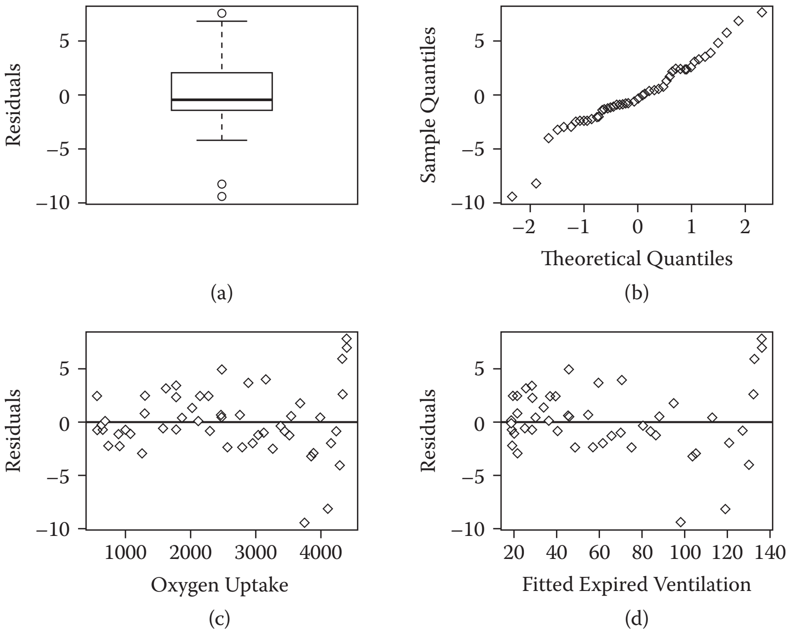


FIGURE 3.7
Residual plots for the oxygen uptake and expired ventilation data from fitting a linear regression model that includes both a linear and quadratic term for oxygen uptake: (a) boxplot of residuals, (b) probability plot of residuals, (c) plot of residuals against oxygen uptake, and (d) plot of residuals against fitted expired ventilation.

3.4 Locally Weighted Regression

(excluded from MABS for IODS)

3.5 Summary

- The scatterplot and a fit of a simple linear regression model are the first points to be considered when dealing with a set of bivariate data.
- The assumptions of the fitted model must be checked by looking at a variety of residual plots. In this way the assumptions of normality and constant variance can be assessed.
- Residual plots may also be helpful in indicating the possible need for higher-order terms in the explanatory variable to be included in the model.
- Scatterplot smoothers can be a useful additional tool in the exploration of a bivariate data set. They often provide a helpful antidote to the unthinking application of simple linear regression.

3.6 Exercises

(excluded from MABS for IODS)

4

Multiple Linear Regression

4.1 Introduction

Multiple linear regression represents a generalization, to more than a single explanatory variable, of the simple linear regression procedure described in Chapter 3. It is now that the relationship between a response variable and several explanatory variables becomes interesting. The adjective "multiple" indicates that at least two explanatory variables are involved in the modeling exercise. At the onset, it is important to note that the explanatory variables are strictly assumed to be fixed and under the control of the investigator, that is, they are not considered to be random variables; only the response variable is considered to be a random variable. In practice, of course, this assumption is unlikely to be true, in which case the results from a multiple linear regression are interpreted as being conditional on the observed values of the explanatory variables, and the inherent variation in the explanatory variables is ignored. Because there are no distributional assumptions about the explanatory variables, they may be categorical with more than two categories (such nominal variables need to be coded in an appropriate way as we shall see later), ordered categorical, or interval. The goals of a multiple regression may be to determine whether the response variable and one or more explanatory variables are associated in some systematic way or to predict values of the response variables from values of the explanatory variables, or both.

Details of the model, including the estimation of its parameters by least squares and the calculation of standard errors, are given in Technical Section 4.1.

Technical Section 4.1: Multiple Linear Regression

The multiple linear regression model for a response variable y with observed values $y_1, y_2, \dots, y_n$ and q explanatory variables $x_1, x_2, \dots, x_q$ with observed values $x_{i1}, x_{i2}, \dots, x_{iq}$ for $i = 1, 2, \dots, n$ is

$$y_i = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \cdots + \beta_q x_{iq} + \varepsilon_i$$

The regression coefficient β_i measures the change in the mean response associated with a unit change in the corresponding explanatory variable, provided the values of all the other explanatory variables do not change. This is often referred to as *partialling out* or *controlling for* other variables, although such terms are probably best avoided. The "linear" in multiple linear regression model refers to the parameters rather than to the explanatory variables, as discussed in Chapter 3.

The error terms in the model $\varepsilon_1, \varepsilon_2, \ldots, \varepsilon_n$ are assumed to have a normal distribution with zero mean and the same variance σ^2 for all values of the explanatory variables. This assumption implies that, for given values of the explanatory variables, the response variable is normally distributed with a mean that is a linear function of the explanatory variables and a variance that is not dependent on them.

The least-squares estimation process is used to estimate the parameters in the multiple linear regression model, and the resulting estimators are most conveniently described with the use of a matrix and vector notation. So we introduce a vector $\mathbf{y}' = [y_1, y_2, \ldots, y_n]$ and an $n \times (q+1)$ matrix $\mathbf{X}$ given by

$$\mathbf{X} = \begin{bmatrix} 1 & x_{11} & x_{12} & \cdots & x_{1q} \\ 1 & x_{21} & x_{22} & \cdots & x_{2q} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_{n1} & x_{n2} & \cdots & x_{nq} \end{bmatrix}$$

Now we can write the multiple linear regression model for all n observations as

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\varepsilon}$$

where $\boldsymbol{\varepsilon}' = [\varepsilon_1, \varepsilon_2, \ldots, \varepsilon_n]$ and $\boldsymbol{\beta}' = [\beta_0, \beta_1, \beta_2, \ldots, \beta_q]$. The least-squares estimators of the parameters in the multiple linear regression model are given by the set of equations

$$\hat{\boldsymbol{\beta}} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{y}$$

These matrix manipulations are easily performed on a computer, but you must ensure that there are no linear relationships between the explanatory variables, such as one variable is the sum of several others; otherwise, your regression software will complain because the inverse of the matrix $\mathbf{X}'\mathbf{X}$ will be singular. (More details of the model in matrix form and the least-squares estimation process are given in Rawlings et al., 1998.) The estimated regression coefficients have the same interpretation as given earlier for the population values of these parameters. Of course, each estimated coefficient and its interpretation are only applicable within the range of values of the corresponding explanatory variable that has been used in fitting the multiple linear regression model.

The variation in the response variable can be partitioned into a part due to regression on the explanatory variables and a residual as in the case of simple linear regression. These can be arranged in an analysis of variance table as follows:

Source	**Df**	**Sum of Squares**	**Mean Square**	**F-statistic**
Regression	q	RGSS	RGMS = RGSS$/q$	RGMS/RSMS
Residual	$n-q-1$	RSS	RSMS = RSS$/$ $(n-q-1)$	

The F-statistic gives a test of the omnibus null hypothesis that all the regression coefficients are zero, that is, none of the explanatory variables are associated with the response variable; in most practical situations, this is a relatively uninteresting hypothesis. The residual mean square s^2 is an estimator of σ^2, and the estimator of the covariance matrix (see Chapter 12) of the parameters is

$$\mathbf{S}_{\hat{\boldsymbol{\beta}}} = s^2(\mathbf{X}'\mathbf{X})^{-1}$$

The diagonal elements of this matrix give estimates of the variances of the estimated regression coefficients, and the off-diagonal elements give estimates of the estimated covariances. The estimated variances are used to assess the statistical significance of the regression coefficients and to construct confidence intervals for them.

A measure of the fit of the model is provided by the multiple correlation coefficient R, which is defined as the correlation between the observed values of the response variable y_i and the values predicted by the fitted model $\hat{y}_i$, which are given by

$$\hat{y}_i = \hat{\beta}_0 + \hat{\beta}_1 x_{i1} + \hat{\beta}_2 x_{i2} + \cdots + \hat{\beta}_q x_{iq}$$

The value of R^2 gives the proportion of variability in the response variable accounted for by the explanatory variables.

4.2 An Example of Multiple Linear Regression

As our first example of fitting a multiple linear regression model, we will return to the data introduced in Chapter 2 (see Table 2.5) concerned with how long each week people spend looking after their cars. The interest lies in investigating which of the three explanatory variables—age, a measure of extroversion, and gender—are most important in determining the amount of time people spend looking after their cars. Note that, in this example, one of the explanatory variables, gender, is a binary variable, but as explained earlier, since no distributional assumptions are made about explanatory variables, such a variable causes no problems when applying multiple linear regression.

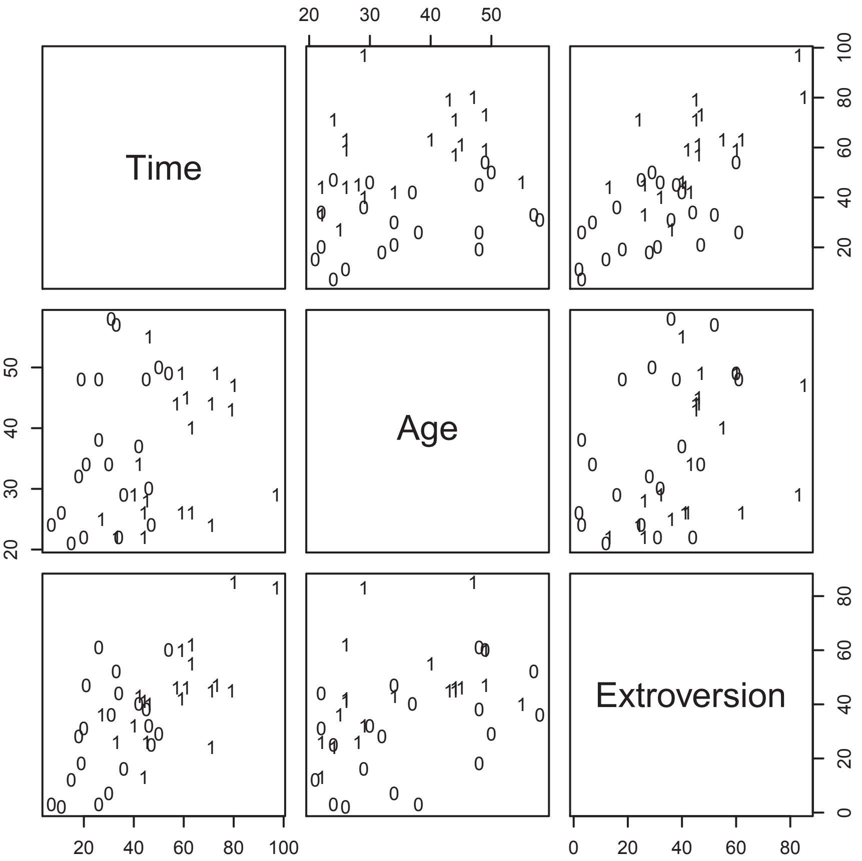


FIGURE 4.1
Scatterplot matrix for the time spent looking after car data, with gender labelled 1 = male, 0 = female.

(Categorical explanatory variables with more than two categories also cause no problems, but they have to be coded appropriately as we shall see in later examples.)

Let us begin with constructing a scatterplot matrix for the three variables—time, age, and extroversion—labeling on each panel of the plot the gender of a subject. The resulting diagram is shown in Figure 4.1. It is clear from this diagram that men spend more time looking after their cars and that time is strongly related to extroversion; perhaps it is less strongly related with age. In addition, the diagram suggests that age and extroversion scores are related, and that there may be two potentially troublesome outliers.

The results from fitting the multiple linear regression model are shown in Table 4.1. The omnibus F-test for testing the hypothesis that all three re-

TABLE 4.1
Results from Fitting Multiple Linear Regression Model to Time Spent Looking After the Car Data with Age, Extroversion Score, and Gender as Explanatory Variables

	Estimate	**Standard Error**	**t-Value**	**Pr(>|t|)**
Intercept	11.306	7.315	1.546	0.130956
Age	0.156	0.206	0.754	0.455469
Extroversion	0.464	0.130	3.564	0.001053
Gender	20.071	4.651	4.315	0.000119

Note: Residual standard error: 13.02 on 36 degrees of freedom (DF); multiple R-squared: 0.638; F-statistic: 21.13 on 3 and 36 DF; *p*-value: 4.569e-08.

gression coefficients are zero has a very low associated *p*-value; there is strong evidence that not all three coefficients are zero. The square of the multiple correlation coefficient is 0.638; the three explanatory variables together account for about 64% of the variation in time spent looking after the car.

The size of the "raw" regression coefficients in Table 4.1 should not be used to judge the relative importance of the explanatory variables in predicting the response variable, although what are known as standardized values of these coefficients can, partially at least, be used in this way. The standardized values might be obtained by applying the regression model to the values of the response variable and explanatory variables, standardized by (divided by) their respective standard deviations. In such an analysis, each regression coefficient represents the change in the standardized response variable associated with a change of one standard deviation unit in the explanatory variable, again conditional on the other explanatory variables remaining constant. The standardized regression coefficients can, however, be found without undertaking this further analysis, by simply multiplying the raw regression coefficient by the standard deviation of the appropriate explanatory variable and dividing by the standard deviation of the response variable. For the time spent looking after car data, the relevant standard deviations are time (20.79), age (11.39), extroversion (19.67), and gender (0.51); so, the required standardized regression coefficients are

$$\begin{array}{ll} \text{Age:} & 0.16 \times 11.39/20.79 = 0.09 \\ \text{Extroversion:} & 0.46 \times 19.67/20.79 = 0.44 \\ \text{Gender:} & 20.1 \times \ \ 0.51/20.79 = 0.49 \end{array}$$

In any case, it looks like extroversion and gender are more important than age in predicting the time spent looking after the car. For binary explanatory variables such as gender in this example, the unstandardized regression coefficients are more directly interpretable than the standardized versions. This is because the unstandardized coefficients for such explanatory variables simply estimate the difference in the average value of the response between the two categories defined by the variable, holding the other explanatory variables in the model constant.

The t-values associated with each explanatory variable are obtained by simply dividing the estimated regression coefficient by the standard error of the estimate, and it might be thought that the associated significance levels would indicate the importance of the explanatory variables. Here, the values of these associated p-values appear to imply that extroversion and gender are strongly associated with time spent looking after car, whereas age seems to not be associated with the response variable. But, this rather simplistic interpretation of the t-statistics is not always appropriate as we shall make clear later in the chapter.

The estimated regression coefficients give the changes in the value of the response variable when the corresponding explanatory variable changes by *one unit*; for a binary variable such as gender in this example, this statement means a change from one category to the other, so the regression coefficient gives an estimated difference between the two categories conditional on the other variables. Here, the estimated difference in time spent looking after the car between men and women, conditional on age and extroversion staying constant, is 20 min longer for men than for women, with a 95% confidence interval of $[20 - 2.04 \times 4.65,\ 20 + 2.04 \times 4.65]$, that is, $[10.5, 29.5]$ (2.04 is the value of a t-statistic with 36 degrees of freedom for a 0.05 significance level).

If here we accept, for the moment, the results from the t-statistics at face value, then we might conclude that a model that includes only the explanatory variables, extroversion score and gender, will be adequate for these data, thus providing a more parsimonious model for the data. If extroversion score and gender were both independent of age, then their regression coefficients in the new model would be the same as they are in Table 4.1. But because age is certainly related to extroversion (see Figure 4.1), the model with only extroversion and gender as explanatory variables needs to be fitted anew to get the correct regression coefficients for the gender and extroversion score explanatory variables. The results of fitting this simpler model are shown in Table 4.2. The regression coefficients for gender and extroversion have changed a little from those given in Table 4.1, but the t-statistics for both variables remain highly significant. The square of the multiple correlation is now 0.632, implying that the two explanatory variables in this model account for 63% of the variation in time spent looking after the car, only a very small reduction from the model with three explanatory variables.

The fitted model with gender and extroversion as explanatory variables is

$$\text{time} = 15.68 + 19.18 \times \text{gender} + 0.51 \times \text{extroversion}$$

So, for men (gender = 1) this becomes

$$\text{time} = 15.68 + 19.18 + 0.51 \times \text{extroversion}$$

TABLE 4.2
Results from Fitting Multiple Linear Regression Model to Time Spent Looking After Car Data, with Extroversion Score and Gender as Explanatory Variables

	Estimate	Standard Error	t-Value	Pr(>|t|)
Intercept	15.680	4.437	3.534	0.001118
Extroversion	0.509	0.115	4.423	8.24e-05
Gender	19.180	4.473	4.288	0.000124

Note: Residual standard error: 12.95 on 37 DF; multiple R-squared: 0.632; F-statistic: 31.77 on 2 and 37 DF; *p*-value: 9.284e-09.

and for women (gender = 0) the model is

$$\text{time} = 15.68 + 0.51 \times \text{extroversion}$$

The fitted model is seen to be equivalent to two simple regression fits, each with the same slope but with a different intercept for men and women. The model is conveniently summarized in Figure 4.2.

Another model we might consider is one in which an extroversion × gender interaction is allowed. The results from fitting such a model are shown in Table 4.3. The fitted model is now

$$\begin{aligned}\text{time} = 20.02 &+ 0.36 \times \text{extroversion} + 7.82 \times \text{gender}\\ &+ 0.31 \times (\text{extroversion} \times \text{gender})\end{aligned}$$

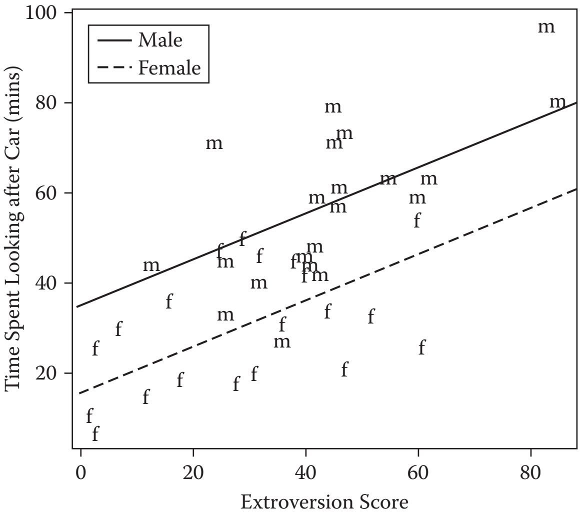


FIGURE 4.2
Plot illustrating the multiple linear regression model fitted to time spent looking after car, with extroversion and gender as the explanatory variables.

TABLE 4.3
Results from Fitting a Multiple Linear Model to the Time Spent Looking after Car Data, with Explanatory Variables, Extroversion, Gender, and Extroversion × Gender Interaction

	Estimate	**Standard Error**	**t-Value**	**Pr(>|t|)**
Intercept	20.018	5.456	3.669	0.000782
Extroversion	0.361	0.159	2.268	0.029430
Gender	7.818	9.571	0.817	0.419379
Extroversion × Gender	0.305	0.228	1.339	0.188970

Note: Residual standard error: 12.81 on 36 DF; multiple R-squared: 0.650; F-statistic: 22.23 on 3 and 36 DF; *p*-value: 2.548e-08.

So, for males (gender = 1) this becomes

$$\text{time} = 20.02 + 0.36 \times \text{extroversion} + 7.82 + 0.31 \times \text{extroversion}$$

and for females (gender = 0)

$$\text{time} = 20.02 + 0.36 \times \text{extroversion}$$

In this case, the model allows the fitted simple linear regression fits for men and women to have both different slopes and different intercepts. Figure 4.3 illustrates the results of fitting this model. Of course, Table 4.3 shows that the interaction term is not significant and so is not needed for these data; the simple model with parallel fits is to be preferred. However, the more complex model is illustrated simply as a useful teaching aid.

4.3 Choosing the Most Parsimonious Model When Applying Multiple Linear Regression

Now we introduce some data taken from Howell (2012), which arise from an evaluation of several hundred courses taught at a large university during the preceding semester. Students in each course had completed a questionnaire in which they rated a number of different aspects of the course on a five-point scale (1 = failure, very bad; . . . ; 5 = excellent, exceptional). The data we will use are the mean scores on six variables for a random sample of 50 courses; the scores for the first five chosen courses are shown in Table 4.4. The six variables are:

1. overall quality of lectures (Overall),
2. teaching skills of the instructor (Teach),

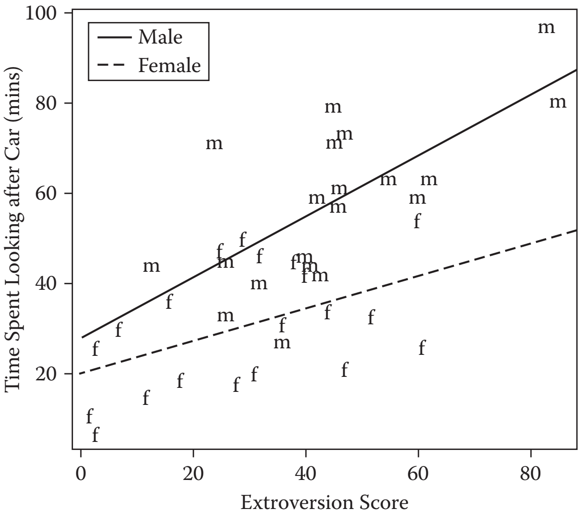


FIGURE 4.3
Diagram illustrating the results given in Table 4.3.

3. quality of the tests and exams (Exam),
4. instructor's perceived knowledge of the subject matter (Knowledge),
5. the student's expected grade in the course (Grade, where higher means better), and
6. the enrollment of the course (Enroll).

Interest lies in how variables 2 to 5 associate with or predict the Overall variable.

Before we begin the model-fitting exercise, we should examine the data graphically, and Figure 4.4 shows a scatterplot matrix of the six variables, each individual scatterplot being enhanced with both a linear and a lowess fit. The plot indicates that the overall rating is related to Teach, Exam, Knowledge, and Grade, and that these explanatory variables are also related to each other. For all the scatterplots in Figure 4.4, the fitted linear and lowess regressions are very similar, suggesting that for none of these explanatory variables is it

TABLE 4.4
Course Evaluation Data

Course	Overall	Teach	Exam	Knowledge	Grade	Enroll
1	3.4	3.8	3.8	4.5	3.5	21
2	2.9	2.8	3.2	3.8	3.2	50
3	2.6	2.2	1.9	3.9	2.8	800
4	3.8	3.5	3.5	4.1	3.3	221
5	3.0	3.2	2.8	3.5	3.2	7

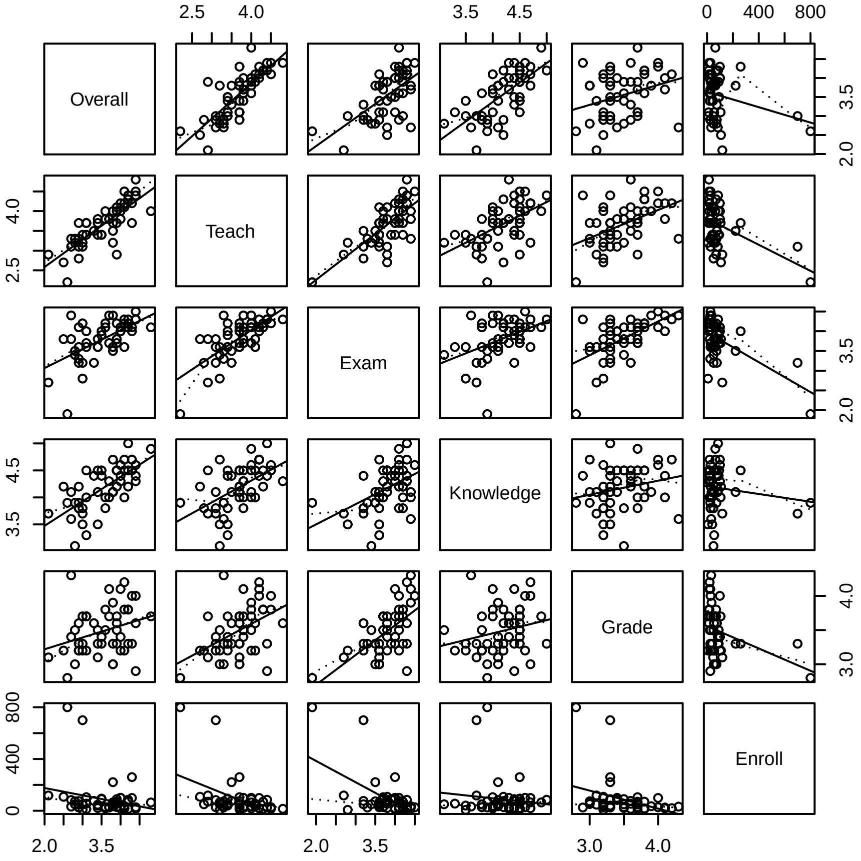


FIGURE 4.4
Scatterplot matrix of course evaluation data showing both linear regression and lowess fits for each pair of variables.

necessary to consider quadratic or higher-order terms in any model. The Enroll variable is problematic because of the presence of two very obvious outliers, one of which is course number 3 with an enroll value of 800, and the other is course 45 with an enroll value of 700. For the moment, we will not remove these two observations and will consider another problem that can occur when using multiple linear regression in practice, which we have not considered up to this point, namely, *multicollinearity.* The term is used to describe situations in which there are moderate to high correlations among some or all of the explanatory variables. Multicollinearity gives rise to a number of difficulties when multiple regression is applied:

- It severely limits the size of the multiple correlation coefficient because the explanatory variables largely attempt to explain much of the same variability in the response variable (see Dizney and Gromen, 1967, for an example).
- It makes determining the importance of a given explanatory variable difficult because the effects of explanatory variables are confounded due to their intercorrelations.
- It increases the variances of the regression coefficients, making the use of the fitted model for prediction less stable. The parameter estimates become unreliable.

Spotting multicollinearity among a set of explanatory variables may not be easy. The obvious course of action is to simply examine the correlations between these variables, but while this is often helpful, it is by no means foolproof; more subtle forms of multicollinearity may be missed. An alternative and generally far more useful approach is to examine what are known as the *variance inflation factors* of the explanatory variables. The variance inflation factor VIF_j for the jth variable is given by

$$\text{VIF}_j = \frac{1}{1 - R_j^2}$$

where R_j is the multiple correlation coefficient from the regression of the jth explanatory variable on the remaining explanatory variables. The variance inflation factor of an explanatory variable indicates the strength of the linear relationship between the variable and the remaining explanatory variables. A rough rule of thumb is that variance inflation factors greater than 10 give some cause for concern. For the course evaluation data, the required variance inflation factors are as follows:

Teach: 2.38; Exam: 3.12; Knowledge: 1.49; Grade: 1.61; Enroll: 1.54

It appears that multicollinearity is not a problem for the course evaluation data. In situations where multicollinearity may be a problem, what should be done? One possibility is to combine in some way explanatory variables that are highly correlated; an alternative approach is simply to select one of the set of correlated variables. Two more complex possibilities are regression on principal components and ridge regression, both of which are described in Chatterjee and Hadi (2012).

But here, we can now go ahead and fit the multiple linear regression model to give the results shown in Table 4.5. Together, the five explanatory variables account for about 76% of the variation in the overall rating. The omnibus F-test has a very low associated p-value, so there is very strong evidence that not all the five regression coefficients are zero. From the t-statistics, it is probably a good bet that the two most important variables for predicting the

TABLE 4.5
Results of Fitting a Multiple Linear Regression Model to the Course Evaluation Data

	Estimate	**Standard Error**	**t-Value**	**Pr(>|t|)**
Intercept	−1.195	0.6312	−1.894	0.064875
Teach	0.763	0.1329	5.742	8.06e-07
Exam	0.132	0.1628	0.811	0.421716
Knowledge	0.489	0.1365	3.581	0.000849
Grade	−0.184	0.1655	−1.113	0.271586
Enroll	0.001	0.0004	1.348	0.184555

Note: Residual standard error: 0.3202 on 44 DF; multiple R-squared: 0.756; F-statistic: 27.19 on 5 and 44 DF; *p*-value: 1.977e-12.

overall rating are the teaching skills of the instructor and the instructor's perceived knowledge of the subject matter. But as mentioned earlier, the use of *t*-statistics in this simplistic way is not really appropriate, the reason being that if say we were to drop exam from the model because its associated *t*-test has the highest *p*-value, we would need to refit the model with the remaining four explanatory variables before making any further statements about their importance because the estimated regression coefficients will now change. Of course, if the explanatory variables happened to be independent of one another, there would be no problem and the *t*-statistics could be used in selecting the most important explanatory variables. This is, however, of little consequence in most practical applications of multiple linear regression.

Before moving on, we should ponder the question of how the results in Table 4.5 are affected by removing the two outlier courses—course 3 and course 5—from the data and refitting the model. The answer is "not very much" as readers can verify by carrying out the task themselves.

So, if using the simple *t*-statistics identifying a more parsimonious model, that is, one with fewer explanatory variables but still providing an adequate fit, might be suspect in many practical applications of multiple linear regression, what are the alternatives? One approach is *all subsets regression* in which all possible models, or perhaps a subset of possible models, are compared using some suitable numerical criterion; when there are q explanatory variables, there are a total of $2^q - 1$ models (each explanatory variable can be in or out of a model, and the model in which they are all out is excluded). The course evaluation data has five explanatory variables, and so there are 31 possible models to consider. With larger numbers of explanatory variables, the number of models to consider rapidly becomes large; for example, for $q = 12$ there are 4095 models to consider. Special search algorithms are used to make this method feasible. We shall not consider this method any further.

4.3.1 Automatic Model Selection

Software packages frequently offer automatic methods of selecting variables for a final regression model from a list of candidate variables. There are three typical approaches:

- Forward selection
- Backward elimination
- Stepwise regression

The forward selection approach begins with an initial model that contains only a constant term, and successively adds explanatory variables to the model until the pool of candidate variables remaining contains no variables that, if added to the current model, would contribute information that is statistically important concerning the mean value of the response. The backward elimination method begins with an initial model that contains all the explanatory variables under investigation and successively removes variables until no variables among those remaining in the model can be eliminated without adversely affecting the predicted value of the mean response in a statistical sense. Various criteria have been suggested for assessing whether a variable should be added to an existing model in forward selection or removed in backward elimination—for example, the change in the residual sum of squares that results from the inclusion or exclusion of a variable.

The stepwise regression method of variable selection combines elements of both forward selection and backward elimination. The initial model of stepwise regression is one that contains only a constant term. Subsequent cycles of the approach involve first the possible addition of an explanatory variable to the current model, followed by the possible elimination of one of the variables included earlier if the presence of new variables has made its contribution to the model no longer important.

In the best of all possible worlds, the final model selected by applying each of the three procedures outlined here would be the same. Often this does happen, but it is in no way guaranteed. Certainly, none of the automatic procedures for selecting subsets of variables are foolproof. For example, if two explanatory variables are highly correlated with each other, it is highly unlikely that any of the usual automatic methods of model selection will produce a final model that includes both variables. In one way, this is good because it avoids the problem of collinearity discussed earlier. But the final model that automatic selection produces hides the fact that another line of modeling exists based on the second of the two highly correlated variables, and the end results of pursuing that direction might be equally satisfactory, statistically or scientifically—it may even be better (Matthews, 2005).

Automatic model selection methods must be used with care, and the researcher using them should approach the final model selected with a healthy degree of skepticism. Agresti (1996) nicely summarizes the problems:

> Computerized variable selection procedures should be used with caution. When one considers a large number of terms for potential inclusion in a model, one or two of them that are not really important may look impressive simply due to chance. For instance, when all the true effects are weak, the largest sample effect may substantially overestimate its true effect. In addition, it often makes sense to include variables of special interest in a model and report their estimated effects even if they are not statistically significant at some level.

(See McKay and Campbell, 1982a, 1982b, for some more thoughts on automatic selection methods in regression.)

4.3.2 Example of Application of the Backward Elimination

With all the caveats of the previous subsection in mind, we will illustrate how the backward elimination approach works on the course evaluation data using what is known as *Akaike's information criterion* (AIC) to decide whether a variable can be removed from the current candidate model. The AIC index takes into account both the statistical goodness of fit and the number of parameters that have to be estimated to achieve this degree of fit, by imposing a penalty for increasing the number of parameters. In a series of competing models, "lower" values of the AIC are preferable; in what follows, the judgment necessary will be made informally.

The AIC for a model is defined explicitly as minus twice the maximized log-likelihood of the model plus twice the number of parameters in the model; as the log-likelihood of the model gets larger, the AIC goes down, and as the number of parameters of the model increases, so does the value of the AIC.

The results of the backward elimination approach using the AIC are as follows:

Start: AIC $= -108.28$

Explanatory variables in the model are Teach, Exam, Knowledge, Grade, and Enroll.

Step 1: Removing one explanatory variable at a time and leaving the other four in the model

Remove Exam: AIC $= -109.54$

Remove Grade: AIC $= -108.89$

Remove Enroll: AIC $= -108.26$

Remove Knowledge: AIC $= -97.49$

Remove Teach: AIC = −82.32

Removing Exam leads to a model containing the other four explanatory variables, and this model has a lower AIC than the original five-explanatory-variable model. Consequently, we drop the Exam variable and start afresh with the model containing the explanatory variables Grade, Enroll, Knowledge, and Teach.

Current: AIC = −109.54

Explanatory variables in the model are now Teach, Knowledge, Grade, and Enroll.

Step 2: Removing one explanatory variable at a time and leaving the other three in the model

Remove Grade: AIC = −110.74

Remove Enroll: AIC = −110.14

Remove Knowledge: AIC = −97.22

Remove Teach: AIC = −76.54

Removing Grade leads to a model containing the other three explanatory variables, and this model has a lower AIC than the current four-explanatory-variable model. Consequently, we drop the Grade variable and start afresh with the model containing the explanatory variables Enroll, Knowledge, and Teach.

Current: AIC = −110.74

Explanatory variables in the model are now Enroll, Knowledge, and Teach.

Step 3: Removing one explanatory variable at a time and leaving the other two in the model

Remove Enroll: AIC = −110.98

Remove Knowledge: AIC = −98.58

Remove Teach: AIC = −77.38

Removing Enroll leads to a model containing the other two explanatory variables, and this model has a lower AIC than the current three-explanatory-variable model. Consequently, we drop the Enroll variable and start afresh with the model containing the variables Knowledge and Teach.

Current: AIC = −110.98

Explanatory variables in the model are now Teach and Knowledge.

TABLE 4.6
Results of Fitting the Multiple Linear Regression Model with the Two Explanatory Variables, Teach and Knowledge, to the Course Evaluation Data

	Estimate	Standard Error	t-Value	Pr(>|t|)
Intercept	−1.2984	0.4773	−2.720	0.009121
Teach	0.7097	0.1011	7.021	7.6e-09
Knowledge	0.5383	0.1319	4.082	0.000172

Note: Residual standard error: 0.3202 on 47 DF; multiple R-squared: 0.739; F-statistic: 66.47 on 2 and 47 DF; *p*-value: 1.991e-14.

Step 4: Removing one explanatory variable at a time and leaving the other one in the model

Remove Knowledge: AIC = −97.81

Remove Teach: AIC = −77.12

Removal of either one of the two variables, Teach and Knowledge, results in a model with a far higher value of the AIC than the model containing both these variables. Consequently, we accept this as our final model.

We now need to fit the chosen model to the data to get the relevant estimated regression coefficients, etc. The results are shown in Table 4.6. We see that an increase in one unit in Teach leads to an estimated increase of 0.71 overall, conditional on Knowledge, and an increase of one unit in Knowledge leads to an increase of 0.54 overall, conditional on Teach. The square of the multiple correlation coefficient for this model is 0.74, only a little less than its value of 0.76 in the five-variable model.

4.4 Regression Diagnostics

Having selected a more parsimonious model, there still remains one further important aspect of a regression analysis to consider, and that is to check the assumptions on which the model is based. We have already described in Chapter 3 the use of residuals for this purpose, but in this section we shall go into a little more detail and introduce several other useful regression diagnostics that are now available. These diagnostics provide ways for identifying and understanding the differences between a model and the data to which it is fitted. Some differences between the data and the model may be due to isolated observations; one, or a few, observations may be outliers, or may differ in some unexpected way from the rest of the data. Other differences may be systematic; for example, a term may be missing in a linear model. Technical Section 4.2 describes a number of regression diagnostics.

Technical Section 4.2: Regression Diagnostics

To begin, we need to introduce what is known as the hat matrix $\mathbf{H}$, defined as $\mathbf{H} = \mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'$, where $\mathbf{X}$ is the matrix introduced earlier in the chapter in Technical Section 4.1 dealing with estimation of the multiple linear regression model.

In a multiple linear regression, the predicted values of the response variable can be written in matrix form as $\hat{\mathbf{y}} = \mathbf{H}\mathbf{y}$ so that $\mathbf{H}$ "puts the hats" on $\mathbf{y}$. The diagonal elements of $\mathbf{H}$, h_{ii}, $i = 1, 2, \dots, n$, are such that $0 \leq h_{ii} \leq 1$, and have an average value of q/n. Observations with large values of h_{ii} are said to have high *leverage*, and such observations have the most effect on the estimation of the model parameters. It is often helpful to produce a plot of h_{ii} against i, an *index plot*, to identify any observations that may have undue influence on fitting the model.

The raw residuals introduced in Chapter 3 are not independent of one another, nor do they have the same variance because the variance of $r_i = y_i - \hat{y}_i$ is $\sigma^2 = (1 - h_{ii})$. Both properties make the raw residuals less useful than they might be when amended a little. Two alternative residuals are the *standardized residual* and the *deletion residual*; both are based on the raw residual r_i and are defined as follows:

$$r_i^{\text{std}} = \frac{r_i}{\sqrt{s^2(1 - h_{ii})}}$$

$$r_i^{\text{del}} = \frac{r_i}{\sqrt{s_{(i)}^2(1 - h_{ii})}}$$

where $s_{(i)}^2$ is the residual mean square estimate of σ^2 after the deletion of observation i.

The deletion residuals are often particularly helpful for the identification of outliers. A further useful regression diagnostic is *Cook's distance*, D_i, defined as

$$D_i = \frac{r_i h_{ii}}{\sqrt{q s^2(1 - h_{ii})}}$$

Cook's distance measures the influence of observation i on the estimation of all the parameters in the model. Values greater than 1 suggest that the corresponding observation has undue influence on the estimation process.

A full account of regression diagnostics is given in Cook and Weisberg (1999).

We can now take a look at these regression diagnostics using the final model chosen for the course evaluation data, namely, a model containing only the two explanatory variables: Teach and Knowledge. Figure 4.5 shows boxplots and normal probability plots for both the standardized and deletion residuals.

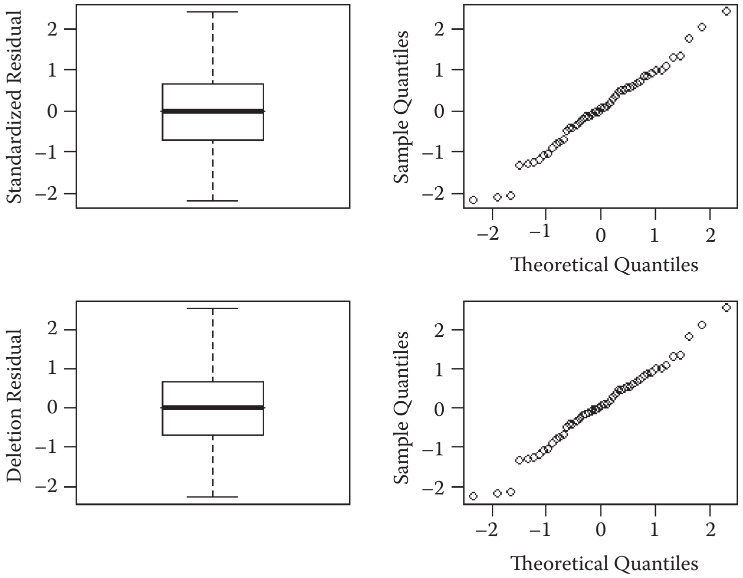


FIGURE 4.5
Boxplots and normal probability plots for both standardised and deletion residuals from the final model chosen for the course evaluation data.

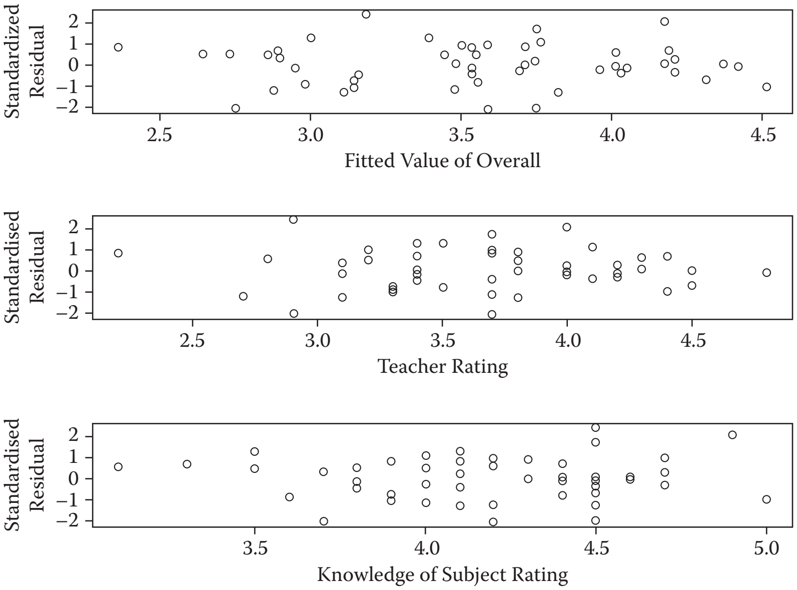


FIGURE 4.6
Plots of standardised residuals against fitted value of the overall rating—the rating of teaching ability and perceived knowledge for the course evaluation data.

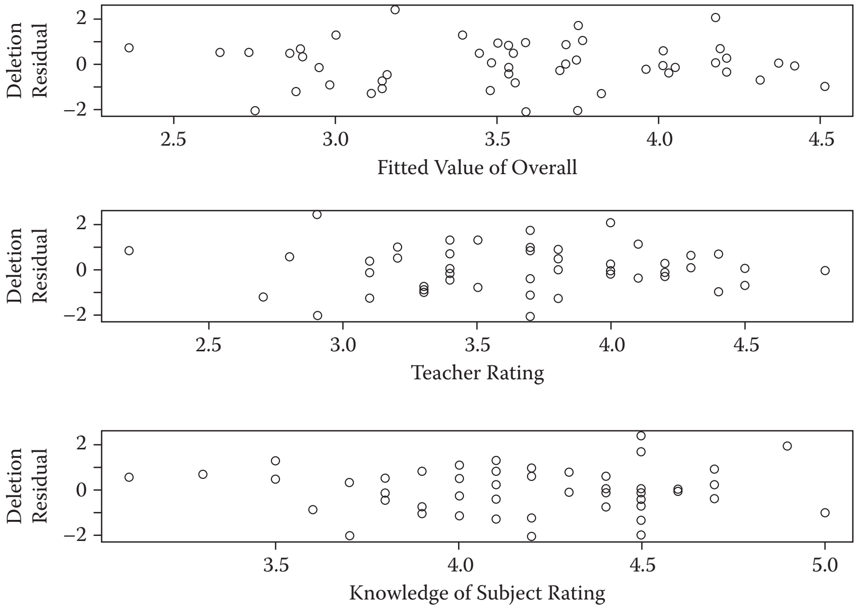


FIGURE 4.7
Plots of deletion residuals against fitted value of the overall rating—the rating of teaching ability and perceived knowledge for the course evaluation data.

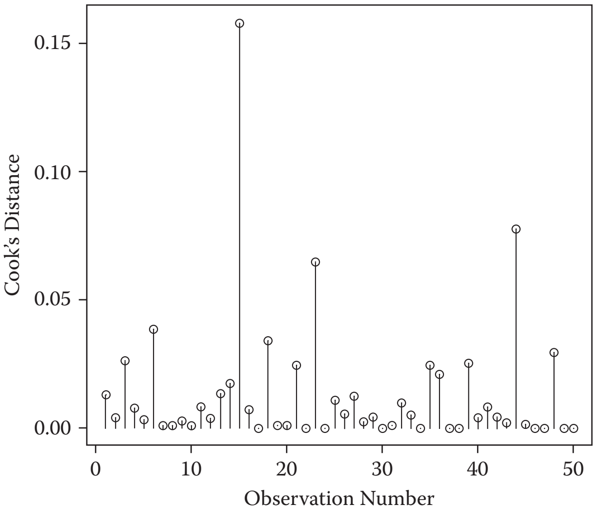


FIGURE 4.8
Index plot of Cook's distances for the final model chosen for the course evaluation data.

The corresponding plots look very similar and give no cause for concern for the model fitted. Figure 4.6 shows plots of the standardized residuals against the fitted value of the overall rating: the rating of teaching ability and perceived knowledge. Figure 4.7 shows the same three plots using deletion residuals. Again, the two sets of plots are very similar and raise no issues about the fitted model. Figure 4.8 shows an index plot of Cook's distances; none is greater than 1, and so, once again, this diagnostic, like the others, gives us some confidence that we have not violated any assumptions when fitting the chosen model.

4.5 Multiple Linear Regression and Analysis of Variance

The phrase "analysis of variance" (ANOVA) was coined by arguably the most famous statistician of the 20th century, Sir Ronald Aylmer Fisher, who defined the technique as "the separation of variance ascribable to one group of causes from the variance ascribable to other groups." ANOVA is probably the piece of statistical methodology most widely used by behavioral scientists, but there is no chapter simply entitled analysis of variance in this book. Why not? The primary reason is that the multiple linear regression model is essentially ANOVA in disguise, and so there is really no need to describe each technique separately. Instead, we will show the equivalence of ANOVA and multiple linear regression through analysis of practical examples.

4.5.1 Analyzing the Fecundity of Fruit Flies by Regression

In a study of fecundity of fruit flies, per-diem fecundity (average number of eggs laid per female per day for the first 14 days of life) for 25 females of each of three genetic lines of the fruit fly *Drosophila melanogaster* was recorded. The lines labeled RS and SS were selectively bred for resistance and susceptibility to the pesticide DDT, and the line NS as a nonselected control strain. The results for the first three fruit flies of each genetic line are shown in Table 4.7. Of interest here is whether the data give any evidence of a difference in fecundity of the three strains.

TABLE 4.7
Fecundity of Fruit Flies

Resistant (RS)	Susceptible (SS)	Nonselected (NS)
12.8	38.4	35.4
21.6	32.9	35.4
14.8	48.5	19.3

In this study, the effect of a single independent factor (genetic strain) on a response variable (per-diem fecundity) is of interest. The data arise from what is generally known as a one-way design and would usually be dealt with by analysis of variance based on the following model:

$$y_{ij} = \mu + \alpha_i + \varepsilon_{ij}$$

where y_{ij} represents the value of the jth observation in the ith genetic line, μ represents the overall mean of the response, α_i is the effect of the ith genetic line ($i = 1, 2, 3$), and ε_{ij} are random error terms assumed to have a normal distribution with mean zero and variance σ^2. The model has four parameters to describe three group means and is said to be overparameterized, which causes problems because it is impossible to find unique estimates for each parameter. This aspect of ANOVA models is discussed in detail in Maxwell and Delaney (2003), but essentially, overparameterization is overcome by imposing constraints on the parameters. In the fruit fly example, we will assume that $\alpha_1 + \alpha_2 + \alpha_3 = 0$. The usual analysis of variance table for the fruit fly data is shown in Table 4.8. The F-test is highly significant, and there is strong evidence that the average number of eggs laid per day differs among the three lines.

How can this analysis be undertaken using multiple linear regression? First, we introduce two dummy variables x_1 and x_2 defined below, which are used to label the three genetic lines:

	Genetic line		
	RS	**SS**	**NS**
x_1	1	0	−1
x_2	0	1	−1

The usual one-way ANOVA model for this situation is the one described earlier:

$$y_{ij} = \mu + \alpha_i + \varepsilon_{ij} \quad \text{with} \quad \alpha_1 + \alpha_2 + \alpha_3 = 0$$

This can be rewritten in terms of the variables x_1 and x_2 as

$$y_{ij} = \mu + \alpha_1 x_1 + \alpha_2 x_2 + \varepsilon_{ij}$$

and this is exactly the same form as a multiple linear regression model with two

TABLE 4.8
Analysis of Variance (ANOVA) Table for Fruit Fly Data

Source	**Sum of Squares**	**Df**	**Mean Square**	**F**	***p*-Value**
Between lines	1362.21	2	681.11	8.67	< 0.001
Within lines (error)	5659.02	72	78.60	–	–

explanatory variables. So, applying multiple regression and regressing average number of eggs laid per day on x_1 and x_2, what do we get? The regression sum of squares is 1362.21 with 2 degrees of freedom, and the residual sum of squares is 5659.02 with 72 degrees of freedom. The results are identical to those from ANOVA, and the estimates of the regression coefficients from the regression analysis are

$$\hat{\mu} = 27.42, \quad \hat{\alpha_1} = -2.16, \quad \hat{\alpha_2} = -3.79$$

The estimates of α_1 and α_2 are simply the differences between each genetic line mean and the grand mean.

4.5.2 Multiple Linear Regression for Experimental Designs

Now let us consider a 2 × 2 factorial design with factors A and B both at two levels: A1 and A2, and B1 and B2. The usual ANOVA model for such a design is

$$y_{ijk} = \mu + \alpha_i + \beta_j + \gamma_{ij} + \varepsilon_{ijk}$$

where y_{ijk} represents the kth observation in the ijth cell of the design; α_i represents the effect of the ith level of factor A; β_j represents the effect of the jth level of factor B; γ_{ij} represents the interaction of A and B; and, as always, ε_{ijk} represents random error terms with the usual distributional assumptions. The usual constraints on the parameters to deal with overparameterization in this case are

$$\sum_{i=1}^{2} \alpha_i = 0, \quad \sum_{j=1}^{2} \beta_j = 0, \quad \sum_{i=1}^{2} \gamma_{ij} = \sum_{j=1}^{2} \gamma_{ij} = 0$$

These constraints imply that the parameters in the model are such that

$$\alpha_1 = -\alpha_2, \quad \beta_1 = -\beta_2, \quad \gamma_{1j} = -\gamma_{2j}, \quad \gamma_{i1} = -\gamma_{i2}$$

The last two equations imply that

$$\gamma_{12} = -\gamma_{11}, \quad \gamma_{21} = -\gamma_{11}, \quad \gamma_{22} = \gamma_{11}$$

showing that there is only a single interaction parameter, namely γ_{11}. The model for the observations in each of the four cells of the design can now be written explicitly as follows:

	A1	**A2**
B1	$\mu + \alpha_1 + \beta_1 + \gamma_{11}$	$\mu - \alpha_1 + \beta_1 - \gamma_{11}$
B2	$\mu + \alpha_1 - \beta_1 - \gamma_{11}$	$\mu - \alpha_1 - \beta_1 + \gamma_{11}$

We define two variables as follows:

$x_1 = 1$ if first level of A, $x_1 = -1$ if second level of A.

$x_2 = 1$ if first level of B, $x_2 = -1$ if second level of B.

The original ANOVA model for the design can now be written as

$$y_{ijk} = \mu + \alpha_1 x_1 + \beta_1 x_2 + \gamma_{11} x_3 + \varepsilon_{ijk}, \text{ where } x_3 = x_1 \times x_2$$

We can recognize this as a multiple linear regression model with three explanatory variables, and we can fit it in the usual way.

4.5.3 Analyzing a Balanced Design

Here, the fitting process can be used to illustrate the difference in analyzing a balanced 2 × 2 design (equal number of observations per cell) and an unbalanced design (unequal number of observations per cell). To begin, we will apply the multiple regression model to the balanced data in Table 4.9.

TABLE 4.9
A Balanced 2 × 2 Data Set

	A1	**A2**
B1	23	22
	25	23
	27	21
	29	21
B2	26	37
	32	38
	30	40
	31	35

So, for fitting the multiple regression model, all observations in cell A1,B1 have $x_1 = 1$ and $x_2 = 1$; all observations in cell A1,B2 have $x_1 = 1$, $x_2 = -1$; and so on for the remaining observations in Table 4.9. To begin, we will fit the model with the single explanatory variable x_1 to give the following results:

Source	**Sum of Squares**	**Df**	**Mean Square**
Regression	12.25	1	12.25
Residual	580.75	14	41.48

together with $\hat{\mu} = 28.75$ and $\hat{\alpha_1} = -0.875$.

The regression sum of squares 12.25 is what would be the between levels of A sum of squares in an ANOVA table.

Now, fit the regression with x_1 and x_2 as explanatory variables to give the following results:

Source	**Sum of Squares**	**Df**	**Mean Square**
Regression	392.50	2	196.25
Residual	200.50	13	15.42

together with $\hat{\mu} = 28.75$, $\hat{\alpha_1} = -0.875$, and $\hat{\beta_1} = -4.875$.

The difference between the regression sums of squares for the two-variable and one-variable models gives the sum of squares for factor B that would be obtained in an ANOVA.

Finally, we can fit a model with three explanatory variables to give the following:

Source	**Sum of Squares**	**Df**	**Mean Square**
Regression	536.50	3	178.83
Residual	56.50	12	4.71

together with $\hat{\mu} = 28.75$, $\hat{\alpha_1} = -0.875$, $\hat{\beta_1} = -4.875$, and $\hat{\gamma_{11}} = 3.0$.

The difference between the regression sums of squares for the three-variable and two-variable models gives the sum of squares for the A × B interaction that would be obtained in an analysis of variance. The residual sum of squares in the final step corresponds to the error sum of squares in the usual ANOVA table. (Readers might like to confirm these results by running an analysis of variance on the data.)

Note that, unlike the estimated regression coefficients in the examples considered in earlier sections, the estimated regression coefficients for the balanced 2 × 2 design do not change as extra explanatory variables are introduced into the regression model. The factors in a balanced design are independent; a more technical term is that they are orthogonal.

4.5.4 Analyzing an Unbalanced Design

Above we saw that when the explanatory variables are orthogonal, adding variables to the regression model in a different order than the one used earlier will alter nothing; the corresponding sums of squares and regression coefficient estimates will be the same. Is the same true of an unbalanced design? To answer this question, we shall use the data in Table 4.10.

Again, we will fit regression models first with only x_1, then with x_1 and x_2, and finally with x_1, x_2, and x_3.

TABLE 4.10
Unbalanced 2 × 2 Data Set

	A1	**A2**
B1	23	22
	25	23
	27	21
	29	21
	30	19
	27	23
	23	17
	25	—
B2	26	37
	32	38
	30	40
	31	35
	—	39
	—	35
	—	38
	—	41
	—	32
	—	36
	—	40
	—	41
	—	38

Results for x_1 model:

Source	**Sum of Squares**	**Df**	**Mean Square**
Regression	149.63	1	149.63
Residual	1505.87	30	50.19

with $\hat{\mu} = 29.567$ and $\hat{\alpha_1} = -2.233$.
The regression sum of squares gives the sum of squares for factor A.
Results for x_1 and x_2 model:

Source	**Sum of Squares**	**Df**	**Mean Square**
Regression	1180.86	2	590.42
Residual	476.55	29	16.37

with $\hat{\mu} = 29.667$, $\hat{\alpha_1} = -0.341$, and $\hat{\beta_1} = -5.997$.

The difference in the regression sums of squares for the two-variable and one-variable models gives the sum of squares due to factor B, conditional on A already being in the model.

Results for x_1, x_2, and x_3 model:

Source	**Sum of Squares**	**Df**	**Mean Square**
Regression	1474.25	3	491.42
Residual	181.25	28	6.47

with $\hat{\mu} = 28.606$, $\hat{\alpha_1} = -0.667$, $\hat{\beta_1} = -5.115$, and $\hat{\gamma_{11}} = 3.302$.

The difference in the regression sums of squares for the three-variable and two-variable models gives the sum of squares due to the A × B interaction, conditional on A and B being in the model.

For an unbalanced design the factors are no longer orthogonal, and so the estimated regression parameters change as further variables are added to the model, and the sums of squares for each term in the model are now conditional on what has entered the model before them. If variable x_2 was entered before x_1, then the results would differ from those given earlier, as readers should confirm by repeating the fitting process as an exercise.

So, using the regression approach clearly demonstrates why there is a difference between analyzing a balanced design (not just a 2 × 2 design as in the example) and an unbalanced design. In the latter, the order of entering effects is important. From the need to consider order, a great deal of confusion has arisen. For example, some authors have suggested that, in a two-way unbalanced design with factors A and B, the main effects of A and B can be entered after the A × B interaction to give what are called type III sums of squares; indeed, this is the default in many software packages. However, this approach is heavily criticized by Nelder (1977) and Aitkin (1978). The arguments are relatively subtle, but they go something like this:

- When fitting models to data, the principle of parsimony is of critical importance. In choosing among possible models, we do not want to adopt complex models for which there is no empirical evidence.

- Thus, if there is no convincing evidence of an A × B interaction, we do not retain this term in the model. Thus, additivity of A and B is assumed unless there is convincing evidence to the contrary.

- So, the argument proceeds that type III sum of squares for, say, A, in which it is adjusted for the A × B interaction, makes no sense.

- First, if the interaction term is necessary in the model, then the experimenter will usually want to consider simple effects of A at each level of B separately. A test of the hypothesis of no A main effect would not usually be carried out if the A × B interaction is significant.

- If the A × B interaction is not significant, then adjusting for it is of no interest and causes a substantial loss of power in testing A and B main effects.

The arguments of Nelder and Aitkin against the use of type III sums of squares are persuasive and powerful. Their recommendation to use what are generally known as type I sums of squares in which interaction terms are considered after the main effects of the factors in the interaction term, perhaps considering main effects in a number of orders, as the most suitable way in which to identify a suitable model for a data set is also convincing and strongly endorsed.

Note that, although ANOVA models can be expressed as multiple linear regression models (as seen in a series of examples), we are not suggesting that behavioral researchers should stop using the ANOVA module in whatever software they use, because that module will conveniently take care of the conversion to a multiple linear regression model and print out the usual analysis of variance table that is required by the researcher.

In the next chapter, we will look at a general framework for linear models, which will allow the appropriate models to be fitted to response variables that do not satisfy the assumptions required by ANOVA and multiple linear regression models.

4.6 Summary

- Multiple linear regression is used to assess the relationship between a set of explanatory variables and a continuous-response variable.
- The response variable is assumed to be normally distributed with a mean that is a linear function of the explanatory variables, and a variance that is independent of them.
- The explanatory variables are strictly assumed to be fixed. In practice, where this is almost never the case, the results of multiple regression are to be interpreted conditional on the observed values of these variables.
- It may be possible to find a more parsimonious model for the data, that is, one with fewer explanatory variables using all subsets of regression or one of the “stepping” methods. Care is required when using the latter.
- An extremely important aspect of a regression analysis is the inspection of a number of regression diagnostics in a bid to identify any departures from assumptions, outliers, etc.
- The models used in ANOVA are equivalent to those used in multiple linear regression.
- By using dummy variables to appropriately code the levels of the factors in an ANOVA design, the model for the design can be put in the form of a multiple linear regression model.

- ANOVA software essentially transforms the required analysis into a regression format and then gives results in the form of an ANOVA table. Consequently, such software remains useful for undertaking the required analysis.

4.7 Exercises

(excluded from MABS for IODS)

Part III

Logistic regression (“MABS for IODS”)

Selected excerpts of the textbook *Multivariate Analysis for the Behavioral Sciences*, Second Edition (Vehkalahti and Everitt, 2019), produced exclusively for the students of IODS (Introduction to Open Data Science, University of Helsinki), with a permission from Chapman and Hall/CRC, London, UK.

5 Generalized Linear Models

This chapter describes how a wide range of seemingly disparate problems of statistical modelling and inference can be set in a unifying framework of great power and flexibility. In this way regression models suitable for, for example, categorical, in particular binary response and count response variables can be developed. The approach involves some transformation of the mean response modelled by a linear function of the explanatory variables.

6 Applying Logistic Regression

In many areas of the behavioral sciences response variables of interest are binary, for example a rating of “improved” or “not improved” for subjects being treated with some therapeutic regime. The appropriate regression model for such data is known as logistic regression and in this chapter several examples are given of its use after definition of some necessary terms such as odds and odds ratios.

5

Generalized Linear Models

5.1 Introduction

In the previous chapter we showed that analysis of variance (ANOVA) models and the multiple linear regression model are essentially completely equivalent. Both involve a linear combination of a set of explanatory variables (dummy variables coding factor levels in the case of ANOVA) as a model for the observed response variable. And both include residual terms assumed to have a normal distribution. Also analysis of covariance (ANCOVA) is the same model, with a mixture of continuous and categorical explanatory variables.

But situations often arise when a response variable of interest cannot be assumed to have the conditional normal distribution required by the models described in Chapter 4. For example, a response such as improved/not improved as a rating of a patient's condition is clearly not normally distributed—it is not even continuous. Such a variable may be coded, say, one for improvement and zero for not improved and is generally known as a *binary variable*. A further type of non-normal response is when it is a count and so takes only positive (or non-negative) integer values, for example, the number of correct scores in a testing situation. The question then arises as to how the effects of explanatory variables on such non-normal responses can be modelled? This question was largely answered in a landmark paper by Nelder and Wedderburn (1972) who introduced what is known as the *generalized linear model* (GLM), which enables a wide range of seemingly disparate problems of statistical modeling and inference to be set in an elegant unifying framework of great power and flexibility. A comprehensive account of GLMs is given in McCullagh and Nelder (1989) and a more concise description in Dobson and Barnett (2018). Here a brief description is given in Technical Section 5.1.

Technical Section 5.1: Generalized Linear Models

Essentially GLMs consist of three main features:

1. An *error distribution* giving the distribution of the response around the mean. For ANOVA and multiple linear regression this will be the normal distribution. For binary responses (see Section 5.2) it is the binomial distribution, and for responses

that are counts (see Section 5.3) it is the Poisson distribution. Each of these (and others used in other situations) come from the same, *exponential family* of probability distributions, and it is this family that is used in generalized linear modeling (see Everitt and Pickles, 2004).

2. A *link function*, g, that shows how the linear function of the explanatory variables is related to the expected value of the response:

$$g(\mu) = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \cdots + \beta_q x_q$$

For ANOVA and multiple linear regression the link function is simply the identity function, that is, the explanatory variables are then directly related to the expected value of the response. A suitable link function for binary variables is described in the next section and one for count variables is introduced in Section 5.3.

3. The *variance function* $V(\mu)$ that captures how the variance of the response variable depends on the mean. We will return to this aspect of GLMs later in this chapter.

Estimation of the parameters in a GLM is usually achieved through a maximum likelihood approach—see McCullagh and Nelder (1989) for details. Having estimated a GLM for a data set the question of the quality of its fit arises. Clearly the investigator needs to be satisfied that the chosen model describes the data adequately, before drawing conclusions about the parameter estimates themselves. In practice, most interest will lie in comparing the fit of competing models, particularly in the context of selecting subsets of explanatory variables that describe the data in a parsimonious manner. In GLMs a measure of fit is provided by a quantity known as the *deviance* which measures how closely the model-based fitted values of the response approximate the observed value. Comparing the deviance values for two models gives a likelihood ratio test of the two models that can be compared by using a statistic having a chi-squared distribution with degrees of freedom equal to the difference in the number of parameters estimated under each model. More details are given in Cook (2005).

In the next two sections, we will go through two important special cases of the GLM. The first one, introduced in Section 5.2, is widely used for modeling binary response variables and is known as *logistic regression*. The second example of a GLM is applicable to count data and is known as *Poisson regression*; this is described in Section 5.3.

5.2 Binary Response Variables

The case of a binary response variable is essential in a huge number of applications in behavioral sciences, but also in medicine, social sciences, and many other areas.

In any regression problem, the key quantity is the population mean (or expected value) of the response variable given the values of the explanatory variables. As we have learned in Chapter 4, in multiple linear regression, the mean of the response variable is modeled directly as a linear function of the explanatory variables, that is, using the E operator to denote expected value

$$E(y|x_1, x_2, \ldots, x_q) = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \cdots + \beta_q x_q$$

where $E(y|x_1, x_2, \ldots, x_q)$ represents the expected value (population mean) of the response variable given the values of the explanatory variables. However, we now want to consider how to model appropriately a binary response variable with its two categories labeled 0 and 1. The first question we need to ask is: what is the expected value of such a variable? It is easy to show that the mean (expected value) in this case is simply the probability that the response variable takes the value 1. (We shall denote this probability by π.) So, to investigate the effects of a set of explanatory variables on a binary response, why not simply continue to use the multiple linear regression approach and consider a model of the form

$$\pi = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \cdots + \beta_q x_q$$

There are two problems with this model:

- The predicted value of the probability π must satisfy $0 \leq \pi < 1$, whereas a linear predictor can yield any values from minus infinity to plus infinity.
- The observed values of the response variable y, conditional on the values of the explanatory variables, will not now follow a normal distribution with mean π but rather what is known as a Bernoulli distribution.

Details of how these problems are overcome by a type of GLM known as logistic regression are described in Technical Section 5.2.

Technical Section 5.2: Logistic Regression

We have a binary response variable y, coded 0 or 1, and a set of explanatory variables $x_1, x_2, \ldots, x_q$. The mean of the response variable given the values of the explanatory variables is the probability that it takes the value 1; we represent this probability as π. Because of the problems identified earlier, π cannot be modeled directly as a linear function of the explanatory variables; instead, some suitable transformation of π must be modeled. In the GLM context, this transformation is called the *link function*. For logistic regression, the link function most often used is the *logit function* of the probability, which is simply the logarithm of the odds, that is, $\log(\frac{\pi}{1-\pi})$, and this leads to the logistic regression model having the form

$$\text{logit}\,(\pi) = \log \frac{\pi}{1-\pi} = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \cdots + \beta_q x_q$$

The logit link is chosen because, from a mathematical point of view, it is extremely flexible and, from a practical point of view, it leads to meaningful and convenient interpretation, as we will discuss in Chapter 6 when looking at examples of the application of logistic regression. The logit transformation of π can take any values ranging from minus infinity to plus infinity and thus overcome the first problem associated with modeling π directly.

In a logistic regression model, the parameter β_i associated with the explanatory variable x_i represents the expected change in the log odds when x_i is increased by one unit, conditional on the other explanatory variables remaining the same. Interpretation is simpler using $\exp(\beta_i)$, which corresponds to an *odds ratio*, as we will see later when discussing some examples in Chapter 6.

The preceding logistic regression model can be rearranged to give the following model for π:

$$\pi = \frac{\exp\,(\beta_0 + \beta_1 x_1 + \beta_2 x_2 + \cdots + \beta_q x_q)}{1 + \exp\,(\beta_0 + \beta_1 x_1 + \beta_2 x_2 + \cdots + \beta_q x_q)}$$

This equation can be used to predict the probability that the response variable takes the value 1 for any values of the explanatory variables, but it would, of course, only make sense for values in the observed range of the explanatory variables in the data set being modeled.

In linear regression, the observed value of the outcome variable is expressed as its expected value, given the explanatory variables plus an error term. The error terms are assumed to have a normal distribution with mean 0 and a variance that is constant across levels of the explanatory variables. With a binary response, we can express an observed value y in the same way as

$$y = \pi(x_1, x_2, \ldots, x_q) + \varepsilon$$

but here ε can only assume one of two possible values (note that here we have introduced a slight change in the nomenclature to remind us that the expected value of the response is dependent on the explanatory variables). If $y = 1$ then $\varepsilon = 1 - \pi(x_1, x_2, \ldots, x_q)$ with probability $\pi(x_1, x_2, \ldots, x_q)$, and if $y = 0$, then $\varepsilon = \pi(x_1, x_2, \ldots, x_q)$ with probability $1 - \pi(x_1, x_2, \ldots, x_q)$. Consequently, ε has a distribution with mean

0 and variance equal to $\pi(x_1, x_2, \ldots, x_q)\,(1 - \pi(x_1, x_2, \ldots, x_q))$. So, the distribution of the response variable conditional on the explanatory variables follows what is known as a Bernoulli distribution (which is simply a binomial distribution for a single trial) with probability $\pi(x_1, x_2, \ldots, x_q)$.

The importance of the logistic regression model, and its connection with the concept of the *odds ratio*, merits discussion of its application in a separate chapter—see Chapter 6.

5.3 Response Variables That Are Counts

(excluded from MABS for IODS)

5.4 Summary

- The generalized linear model (GLM) allows a suitable transform of the mean of the response variable to be modeled as a linear function of the explanatory variables, and to have an error distribution appropriate for the type of response involved.
- Two important cases of the GLM are logistic regression for the binary response variables and Poisson regression for responses that are counts.
- Logistic regression is a GLM with a binomial error distribution, and typically used with the logit link function.
- Poisson regression is a GLM with a Poisson error distribution, and typically used with the log link function.
- Overdispersion is common with both the above models, as their variance functions are completely determined by the mean. The problem can usually be dealt with the quasi-likelihood procedure, which allows the dispersion or scale parameter ϕ to be estimated from the data.
- Applications of the logistic regression model are considered in Chapter 6.

5.5 Exercises

(excluded from MABS for IODS)

6

Applying Logistic Regression

6.1 Introduction

In the previous chapter, the basic theory behind a regression model for dealing with a binary response variable, logistic regression, was covered. In this chapter, a number of examples of the application of this type of regression will be described. But before this we need to digress for a short account of *odds* and *odds ratios* both of which are central to interpreting the results of fitting logistic regression models.

6.2 Odds and Odds Ratios

Table 6.1 shows part of a data set collected in a study of a psychiatric screening questionnaire known as the GHQ (General Health Questionnaire; see Goldberg, 1972 for details). Each person in the study was given a score on the GHQ and also categorized as being a psychiatric case or not. Here, the question of interest to the researcher is how being judged to be a "case" is related to gender and GHQ score. In Table 6.1, the binary responses (case/not case) of individuals with the same values of the two explanatory variables, GHQ score and gender, have been grouped together.

If we collapse these data over the GHQ score, we get the following 2×2 contingency table of caseness against gender:

	Case	**Noncase**
Male	25	79
Female	43	131

Such a table would usually be analyzed to assess the independence or otherwise of gender and caseness using a chi-squared test. However, here we will use the table to explain the meanings of the terms odds and odds ratios.

First odds, which is defined for an event with probability p as $p/(1-p)$. For women in the 2×2 table in the preceding text, the probability of being judged

TABLE 6.1
Psychiatric Caseness Data

GHQ Score	Gender		Number of Cases	Number of Noncases
0	F		4	80
1	F		4	29
2	F		8	15
		...		
		...		
10	F		1	0
0	M		1	36
1	M		2	25
2	M		2	8
		...		
		...		
10	M		2	0

a case is estimated to be $43/174 = 0.247$, and so, for women, the odds of being judged a case versus being judged a noncase is $0.247/(1-0.247) = 0.328$. The same calculations for men show that the probability of being judged a case is 0.240, and the corresponding value for the odds is 0.316. It is easy to see that the odds for women can be calculated directly from the frequencies in the 2×2 table as $43/131$; similarly, for men, the odds are $25/79$.

Further, having found the odds for caseness versus noncaseness for women and for men, the odds ratio is simply what it says—the ratio of the two odds, that is, $0.316/0.328 = 0.963$. When the two variables forming the contingency table are independent, the odds ratio in the population will be 1. So, is it possible to use the estimated odds ratio to test the hypothesis that the population value is 1 and, more importantly, is it possible to construct a confidence interval (CI) for the odds ratio? Technical Section 6.1 shows how to do the latter.

Technical Section 6.1: CI for the Odds Ratio

Consider the general 2×2 table given by

	Variable 1	
Variable 2	**Category 1**	**Category 2**
Category 1	a	b
Category 2	c	d

The odds ratio in the population will be denoted by ψ, and it can be estimated from the observed frequencies in the table as

$$\hat{\psi} = \frac{a/b}{c/d} = \frac{ad}{bc}$$

A CI for ψ can be constructed relatively simply by using the following estimator of the variance of $\log(\psi)$:

$$\widehat{\text{var}}(\log \psi) = 1/a + 1/b + 1/c + 1/d$$

So, an approximate 95% confidence interval for $\log(\psi)$ is given by

$$\log(\hat{\psi}) \pm 1.96 \times \sqrt{\widehat{\text{var}}(\log \hat{\psi})}$$

If the limits of the CI for $\log(\psi)$ obtained in this way are ψ_L, ψ_U, then the corresponding confidence interval for ψ is $[\exp(\psi_L), \exp(\psi_U)]$.

We can illustrate the construction of the CI for the odds ratio using the data from the 2×2 table of gender and caseness given earlier in the chapter. First, the odds ratio is estimated to be

$$\hat{\psi} = \frac{25 \times 131}{43 \times 79} = 0.964$$

and so $\log(\hat{\psi}) = -0.037$ and the estimated variance of $\log(\psi)$ is

$$1/25 + 1/43 + 1/79 + 1/131 = 0.084,$$

leading to a 95% CI for $\log(\psi)$ of

$$[-0.037 - 1.96 \times 0.290, -0.037 + 1.96 \times 0.290], \quad \text{that is,} \quad [-0.604, 0.531]$$

Finally, the CI for ψ is found as $[\exp(-0.604), \exp(0.531)]$, that is, [0.546, 1.701]. As this interval contains the value 1, we can conclude that there is no evidence of an association between caseness and gender.

6.3 Applying Logistic Regression to the GHQ Data

To begin, we will fit both a logistic regression and a linear regression to the data using the GHQ score as the single explanatory variable. So, for the linear model, the probability of being a case is modeled as a linear function of the GHQ score, whereas in the logistic model, the logit transformation of the probability of being a case is modeled as a linear function of the GHQ score. The results from fitting both models are shown in Table 6.2.

TABLE 6.2
Results of Fitting a Linear and a Logistic Regression Model to the GHQ Data with Only a Single Explanatory Variable, the GHQ Score

	Logistic Model[a]			
	Estimate	**Standard Error**	**z-Value**	**Pr(>|z|)**
Intercept	−2.71073	0.27245	−9.950	<2e-16
GHQ	0.73604	0.09457	7.783	7.1e-15
	Linear Model[b]			
	Estimate	**Standard Error**	**z-Value**	**Pr(>|z|)**
Intercept	0.11434	0.05923	1.931	0.0678
GHQ	0.10024	0.01001	10.012	3.1e-09

[a] Null deviance: 130.306 on 21 DF; residual deviance: 16.237 on 20 DF; AIC: 56.211; number of Fisher scoring iterations: 5.

[b] Residual standard error: 0.1485 on 20 DF; multiple R-squared: 0.8337; F-statistic: 100.2 on 1 and 20 DF; *p*-value: 3.099e-09

The results from both models show that the GHQ score is a highly significant predictor of the probability of being judged a case. In the linear model, the estimated regression coefficient is 0.10; the estimated increase in the probability of being a case is 0.10 for each increase of 1 in the GHQ score. For an individual with a GHQ score of, say, 10, the linear model would predict that the probability of the individual being judged a case is $0.114 + 0.100 \times 10 = 1.114$; with this model, fitted values of the probabilities are not constrained to lie in the interval (0,1). Now consider the fitted logistic regression model, that is,

$$\log \frac{\Pr(\text{case})}{\Pr(\text{not case})} = -2.71 + 0.74 \times \text{GHQ score}$$

This equation can be rearranged to give the predicted probabilities for the fitted logistic regression model as

$$\Pr(\text{case}) = \frac{\exp(-2.71 + 0.84 \times \text{GHQ score})}{1 + \exp(-2.71 + 0.84 \times \text{GHQ score})}$$

For the individual with a GHQ score of 10, this model predicts the probability of the individual being judged a case as 0.99.

Now, let us consider the fitted logistic regression model for individuals with GHQ scores of, say, S and S + 1; the corresponding models for the logits can be written as

$$\log \frac{\Pr(\text{case})}{[\Pr(\text{not case}) \mid \text{GHQ} = \text{S}]} = -2.71 + 0.74 \times \text{S}$$

$$\log \frac{\Pr(\text{case})}{[\Pr(\text{not case}) \mid \text{GHQ} = \text{S} + 1]} = -2.71 + 0.74 \times (\text{S} + 1)$$

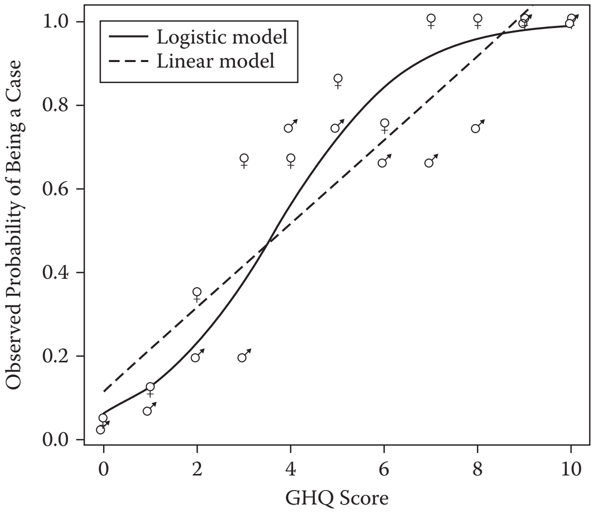


FIGURE 6.1
Plot of predicted probabilities of caseness from both linear and logistic regression models with GHQ score as the single explanatory variable and observed probabilities labelled by gender.

So, subtracting the first equation from the second, we get

$$\log \frac{\Pr(\text{case})}{[\Pr(\text{not case}) \mid \text{GHQ} = \text{S}+1]} - \log \frac{\Pr(\text{case})}{[\Pr(\text{not case}) \mid \text{GHQ} = \text{S}]} = 0.74$$

This can be rewritten as

$$\log \left\{ \frac{\Pr(\text{case})}{[\Pr(\text{not case}) \mid \text{GHQ} = \text{S}+1]} \Big/ \frac{\Pr(\text{case})}{[\Pr(\text{not case}) \mid \text{GHQ} = \text{S}]} \right\} = 0.74$$

and thus, by exponentiating, we get

$$\frac{\Pr(\text{case})}{[\Pr(\text{not case}) \mid \text{GHQ} = \text{S}+1]} \Big/ \frac{\Pr(\text{case})}{[\Pr(\text{not case}) \mid \text{GHQ} = \text{S}]} = \exp(0.74)$$

The left-hand side is simply the odds ratio for being rated a case for a subject with a GHQ score 1 higher than another subject, and this is estimated to be exp(0.74) = 2.10. The corresponding approximate 95% CI is calculated as [exp(0.74 − 1.96 × 0.09), exp(0.74 + 1.96 × 0.09)] to give [1.76, 2.50]. The increase in the odds of being judged a case associated with a 1 unit increase in the GHQ is estimated to be between 76% and 150%.

The null deviance given in Table 6.2 is for a model with no explanatory variables, and the residual deviance is that for a model with GHQ as the single explanatory variable; the reduction in deviance is considerable, and could be tested as a chi-squared with 1 DF. The value of Akaike's fit criterion AIC (see Chapter 4) is also given, and this might be useful when comparing competing models as we shall see later.

In Figure 6.1, we plot the predicted probabilities of being a case from each model against GHQ, along with the observed probabilities labeled by gender. (The observed probabilities are found from the data by dividing number of cases by number of cases plus number of noncases.) The plot again demonstrates that the linear regression model leads to predicted probabilities greater than 1 for some values of GHQ.

Next, we will fit a logistic regression model that includes only gender as an explanatory variable. The results are shown in Table 6.3. The estimated regression coefficient of −0.037 is the odds ratio calculated earlier in the chapter for the gender × case/not case cross-classification, and the estimated standard error of the estimated regression coefficient is also the same as we calculated earlier.

The next logistic model we will consider for the GHQ data is one where the gender and GHQ scores are both included as explanatory variables. The results are shown in Table 6.4. In this model, both GHQ and gender are significant. The regression coefficient for gender shows that, conditional on GHQ score, the log odds of caseness for men is −0.94 lower than for women, which gives an estimated odds ratio of $\exp(-0.94) = 0.39$ with 95% CI of [0.167, 0.918]. For a given GHQ score, the odds of a man being diagnosed as a case is between about 0.17 and 0.92 of the corresponding odds for a woman, although we know from previous analyses that the overall odds ratio, ignoring the GHQ score, does not differ significantly from 1. We might ask: why the difference? The reason is that the overall odds ratio is dominated by the large number of cases for the lower GHQ scores.

The estimated regression coefficient for GHQ conditional on gender is 0.779. This is very similar to the value for the model having only the GHQ score, and so the interpretation of the conditional coefficient is very similar to that given previously.

TABLE 6.3
Results from Fitting a Logistic Regression Model to the GHQ Data with Only a Single Explanatory Variable, Gender

	Estimate	**Standard Error**	**z-Value**	**Pr(>|z|)**
Intercept	−1.11400	0.17575	−6.338	2.32e-10
Gender	−0.03657	0.28905	−0.127	0.9

Note: Null deviance: 130.31 on 21 DF; residual deviance: 130.29 on 20 DF; AIC: 170.26

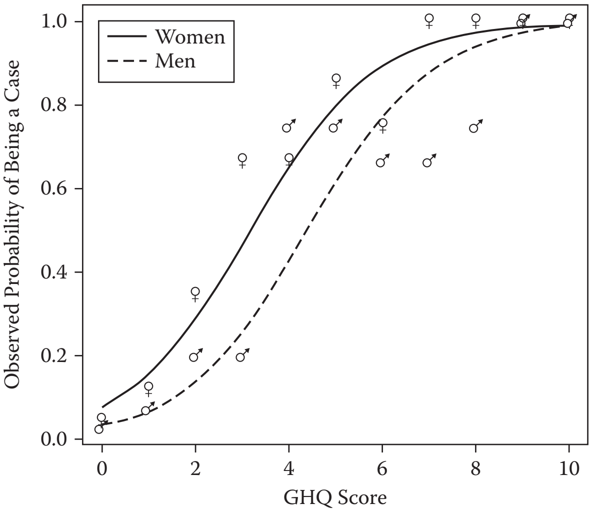


FIGURE 6.2
Plot of predicted probabilities of caseness from logistic regression model with gender and GHQ score as explanatory variables and observed probabilities labelled by gender

The AIC value of 53.1 is lower than that for the models with only the GHQ score or gender, so the model with both is considered a better model. The fitted model is displayed graphically in Figure 6.2.

Finally, for the GHQ data we will fit a model with gender, GHQ score, and gender × GHQ score interaction. The result is shown in Table 6.5. The model is illustrated graphically in Figure 6.3. Although the AIC value is a little lower than for the previously fitted model with no interaction term, the regression coefficient for the interaction term in Table 6.5 is not significant, and a reasonable conclusion is that the model with only gender and GHQ score provides the best description of these data.

TABLE 6.4
Results from Fitting a Logistic Regression Model to the GHQ Data with Gender and GHQ Scores as Explanatory Variables

	Estimate	**Standard Error**	**z-Value**	**Pr(>|z|)**
Intercept	−2.49351	0.28164	−8.854	<2e-16
Gender	−0.93609	0.43435	−2.155	0.0311
GHQ	0.77910	0.09903	7.867	3.63e-15

Note: Null deviance: 130.306 on 21 DF; residual deviance: 11.113 on 19 DF; AIC: 53.087.

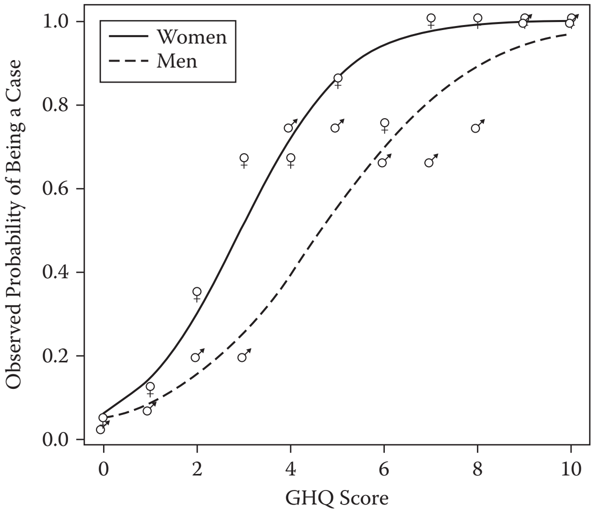


FIGURE 6.3
Plot of predicted probabilities of caseness from logistic regression model with gender, GHQ score, gender × GHQ as explanatory variables, and observed probabilities labeled by gender.

TABLE 6.5
Results from Fitting a Logistic Regression Model to the GHQ Data with Gender, GHQ Score, and the Interaction of Gender and GHQ Score as Explanatory Variables

	Estimate	**Standard Error**	**z-Value**	**Pr(>|z|)**
Intercept	−2.7732	0.3586	−7.732	1.06e-14
Gender	−0.2253	0.6093	−0.370	0.712
GHQ	0.9412	0.1569	6.000	1.97e-09
Gender×GHQ	−0.3020	0.1990	−1.517	0.129

Note: Null deviance: 130.306 on 21 DF; residual deviance: 8.767 on 18 DF; AIC: 52.741.

6.4 Selecting the Most Parsimonious Logistic Regression Model

As with the fitting of multiple linear regression models, the aim when fitting logistic regression models is to select the most parsimonious model that gives an adequate description of the data. We can use exactly the same approach as given in Chapter 4, as we shall illustrate on data collected from a survey of employed men aged between 18 and 67 years who were asked whether in the preceding year they had carried out work on their home for which they would

TABLE 6.6
Do-It-Yourself Data

			Accommodation					
			Apartment Age			**House Age**		
Work	**Tenure**	**Response**	**<30**	**31–45**	**46+**	**<30**	**31–45**	**46+**
Skilled	Rent	Yes	18	15	6	34	10	2
		No	15	13	9	28	4	6
	Own	Yes	5	3	1	56	56	35
		No	1	1	1	12	21	8

have employed a craftsman previously. The response variable is their answer, yes/no, to this question. In addition to age, the respondents' accommodation type, apartment or house; whether this accommodation was rented or owned; and their type of work, skilled, unskilled, or office were recorded. Part of the data is shown in Table 6.6.

The first point to consider about these data is how to deal with the categorical variables, work and age, that have more than two categories. We could simply label the categories for work one, two, three, and likewise the age categories, and use these numerical values in the model-fitting process. But this would be a mistake, particularly for the work variable; such coding would imply that changing, say, from work category one to work category two, and from work category two to work category three, has an equal effect on the probability of responding yes in the survey, which is not necessarily the case. The appropriate method is to use dummy variable coding for both work and age. So, for the work variables, we define two dummy variables D1 and D2 to label the three categories such that

Work	**D1**	**D2**
Skilled	0	0
Unskilled	1	0
Office	0	1

So, in the fitted logistic regression model, the estimated regression coefficient for D1 will quantify the difference between unskilled and skilled workers, and D2 will quantify the difference between office and skilled workers. A similar coding will be used for the age variable. We will now fit a logistic model for the probability of responding yes in the survey with work, tenure, accommodation type, and age as explanatory variables. The results are shown in Table 6.7. We will wait to interpret the estimated regression coefficients until we have explored whether a simpler model might be adequate for these data. This we will do by using a backward search procedure using the AIC

TABLE 6.7
Results from Fitting a Logistic Regression Model to the Do-It-Yourself Data with Explanatory Variables Work, Tenure, Type, and Age

	Estimate	**Standard Error**	**z-Value**	**Pr(>|z|)**
Intercept	0.30606	0.15428	1.984	0.0473
Work(D1)	−0.76267	0.15197	−5.018	5.21e-07
Work(D2)	−0.30535	0.14088	−2.167	0.0302
Type	−0.00249	0.14717	−0.017	0.9865
Tenure	1.01570	0.13787	7.367	1.74e-13
Age(D1)	−0.11304	0.13697	−0.825	0.4092
Age(D2)	−0.43661	0.14059	−3.106	0.0019

Note: Null deviance: 158.884 on 35 DF; residual deviance: 29.671 on 29 DF; AIC: 167.87.

criterion to guide the search, that is, the same method was used in Chapter 4 for multiple linear regression models.

The results of the backward search are as follows:

Start: AIC = 167.87

Explanatory variables in the model are Work, Tenure, Type, and Age.

Step 1: Removing one explanatory variable at a time and leaving the other three in the model

Remove Type: AIC = 165.87

Remove Age: AIC = 174.76

Remove Work: AIC = 191.72

Remove Tenure: AIC = 221.80

The variable Type can be removed because the model without Type but with the other three explanatory variables has a lower AIC value than the four-variable model.

Current: AIC = 165.87

Explanatory variables in the model are now Work, Tenure, and Age.

Step 2: Removing one explanatory variable at a time and leaving the other two in the model

Remove Age: AIC = 172.81

Remove Work: AIC = 189.19

Remove Tenure: AIC = 244.98

TABLE 6.8
Results from Fitting the Model with Work, Age, and Tenure as Explanatory Variables

	Estimate	**Standard Error**	**z-Value**	**Pr(>|z|)**
Intercept	0.3048	0.1347	2.262	0.02370
Work(D1)	−0.7627	0.1520	−5.019	5.21e-07
Work(D2)	−0.3053	0.1408	−2.168	0.03012
Tenure	1.0144	0.1144	8.866	<2e-16
Age(D1)	−0.1129	0.1367	−0.826	0.40877
Age(D2)	−0.4364	0.1401	−3.116	0.00183

Note: Null deviance: 158.884 on 35 DF; residual deviance: 29.671 on 30 DF; AIC: 165.87.

TABLE 6.9
Estimated Odds Ratios and CIs of Each Explanatory Variable in the Final Model Chosen for the Do-It-Yourself Data

Variable	**Estimated Odds Ratio**	**95% CI**
Work(D1)	0.466	[0.346, 0.628]
Work(D2)	0.737	[0.559, 0.972]
Tenure	2.757	[2.205, 3.447]
Age(D1)	0.893	[0.683, 1.168]
Age(D2)	0.647	[0.491, 0.851]

Removing any of the three explanatory variables currently in the model leads to an AIC value greater than that for the current model and so we accept the current model that has Work, Age, and Tenure as explanatory variables. Fitting this model gives the results shown in Table 6.8. In Table 6.9 we list the estimated odds ratios and 95% CIs for each variable. The results show the following:

- The odds of unskilled workers responding yes to the questions asked are between about 35% and 63% of the odds of skilled workers.
- The odds of office workers responding yes to the question asked are between about 56% and 97% of the odds of skilled workers.
- The odds of home owners responding yes to the question asked are between about twice to three-and-a-half times the odds of non-home owners.
- The odds of respondents in the age range 31–45 responding yes to the question asked does not differ from the odds of those respondents less than 30.

- The odds of respondents aged over 46 responding yes to the question asked are between about 50% and 85% of the odds of respondents less than 30.

6.5 Driving and Back Pain: A Matched Case–Control Study

(excluded from MABS for IODS)

6.6 Summary

- The logistic regression model is a GLM that can be used to assess the effects of a set of explanatory variables on a binary response variable (see details in Chapter 5).
- The estimated parameters in the logistic regression model can be interpreted in terms of odds and odds ratios.
- Parsimonious models can be selected by the same approach as for the multiple linear regression model.
- There are a number of diagnostics available for logistic regression that can be used to assess various aspects of the model. Details are available in Collett (2003), however, the binary nature of the response variable often makes the use of these diagnostics somewhat difficult to interpret.
- Logistic regression is also very useful in the analysis of matched case–control studies.

6.7 Exercises

(excluded from MABS for IODS)

Part IV

Clustering and classification (“MABS for IODS”)

Selected excerpts of the textbook *Multivariate Analysis for the Behavioral Sciences*, Second Edition (Vehkalahti and Everitt, 2019), produced exclusively for the students of IODS (Introduction to Open Data Science, University of Helsinki), with a permission from Chapman and Hall/CRC, London, UK.

12 Multivariate Data and Multivariate Analysis

Multivariate data, as the term is most widely used, arise when several measurements or observations are made on each sampling unit, commonly an individual, and where all these variables need to be considered simultaneously, in order to uncover whatever message the data may hold. Here there is no division into response and explanatory variables. Multivariate analysis is essentially a collection of techniques that are designed to help in this aim; most such methods are descriptive rather than inferential.

17 Cluster Analysis

Classification of similar objects, similar people, similar countries etc. is an important component of virtually all scientific research. The investigator is usually interested in finding a classification in which the objects/people etc., are sorted into a small number of homogeneous groups or clusters. At the very least, any derived classification scheme should provide a convenient method of organizing a large, complex set of multivariate data but it may also serve a more fundamental purpose; for example, the classification of psychiatric patients might help in the search for causes of different psychiatric illnesses. In this chapter a number of methods of cluster analysis are described and their use illustrated on a number of data sets.

18 Grouped Multivariate Data

Multivariate data are often collected from a number of a priori defined groups of the sampling units. For example, a researcher may collect observations of a number of symptoms for patients from different diagnostic categories. In this chapter methods for assessing whether the groups differ on the observed variables are described along with how to construct a classification rule that may allow other, as yet ungrouped sampling units, to be allocated to a group in such a way that misclassifications are minimized.

12

Multivariate Data and Multivariate Analysis

12.1 Introduction

In this chapter and the following five longer chapters (Chapters 13 to 17) we will be concerned with what is most often termed *multivariate data.* Such data arise when researchers measure several variables on each individual in their study, and where all variables need to be examined simultaneously in order both to uncover whatever "patterns" or "structure" the data may contain and understand the key features of the data. All the variables in this type of 'multivariate data' are considered random unlike in the type of 'multivariate data' discussed in Chapters 3 to 11 where only the response variable is considered random and where the regression models described seek to uncover the relationship between the response and the remaining variables.

The techniques described in this and the remaining chapters of the book are those that generally fall under the umbrella of *multivariate analysis* and they are largely, although not exclusively, descriptive rather than inferential, that have in common the aim to display or extract any "signal" in the data in the presence of noise and, in a very general sense, to discover what the data may be trying to tell us.

The starting point of most multivariate analysis methods is the data matrix **X** introduced in the Preface, that is

$$\mathbf{X} = \begin{bmatrix} x_{11} & x_{12} & \cdots & x_{1q} \\ x_{21} & x_{22} & \cdots & x_{2q} \\ \vdots & \vdots & \ddots & \vdots \\ x_{n1} & x_{n2} & \cdots & x_{nq} \end{bmatrix}$$

where n is the number of units in the sample, q is the number of variables measured on each unit, and x_{ij} denotes the value of the jth variable for the ith individual; an individual in this context may be something other than a human being. The variables will often be at different levels in the measurement hierarchy described in Chapter 1, for example, some categorical, some interval, and some ratio measurements. Further, often some variable values will be missing, and so, the problems associated with missing data mentioned in Chapter 1 and again in Chapter 11 may assume importance.

12.2 The Initial Analysis of Multivariate Data

The main techniques for analyzing multivariate data are those to be described in the subsequent chapters, but an initial graphical and numerical description can often be very helpful in gaining some insight into the data and in interpreting the results from later analyses. We will illustrate what can be done with an initial analysis using first the very simple multivariate data set shown in Table 12.1. The data consists of chest, hip, and waist measurements (in inches) of 20 individuals.

12.2.1 Summary Statistics for Multivariate Data

In order to provide a numerical summary for a multivariate data set, we need to produce summary statistics for each of the variables separately and also calculate appropriate statistics that summarize the relationships between the variables. For the former, we generally use means and variances (assuming that we are dealing with continuous variables), and for the latter, we usually take pairs of variables at a time and look at their covariances or correlations. Population and sample versions of all these quantities are defined in Technical Section 12.1.

TABLE 12.1
Chest, Waist, and Hip Measurements of 20 Individuals

Individual	Chest	Waist	Hips
1	34	30	32
2	37	32	37
3	38	30	36
4	36	33	39
5	38	29	33
6	43	32	38
7	40	33	42
8	38	30	40
9	40	30	37
10	41	32	39
11	36	24	35
12	36	25	37
13	34	24	37
14	33	22	34
15	36	26	38
16	37	26	37
17	34	25	38
18	36	26	37
19	38	28	40
20	35	23	35

Technical Section 12.1: Numerical Summary Statistics for Multivariate Data

For q variables, the population mean vector is usually represented as $\boldsymbol{\mu}' = [\mu_1, \mu_2, \ldots, \mu_q]$, where $\mu_i = E(x_i)$ is the population mean (or expected value as denoted by the E operator) of the ith variable. An estimate of $\boldsymbol{\mu}'$ based on n q-dimensional observations is $\bar{x}' = [\bar{x}_1, \bar{x}_2, \ldots, \bar{x}_q]$, where $\bar{x}_i$ is the sample mean of the variable x_i.

The vector of population variances can be represented by $\boldsymbol{\sigma}' = \left[\sigma_1^2, \sigma_2^2, \ldots, \sigma_q^2\right]$, where $\sigma_i^2 = E(x_i - \mu_i)^2$. An estimate of $\boldsymbol{\sigma}'$ based on n q-dimensional observations is $\mathbf{s}' = \left[s_1^2, s_2^2, \ldots, s_q^2\right]$, where s_i^2 is the sample variance of x_i.

The population covariance of two variables x_i and x_j is defined by

$$\operatorname{Cov}(x_i, x_j) = E\left(x_i - \mu_i\right)\left(x_j - \mu_j\right)$$

If $i = j$, we note that the covariance of the variable with itself is simply its variance, and therefore, there is no real need to define variances and covariances independently in the multivariate case. The covariance of x_i and x_j is usually denoted by σ_{ij} (so, the variance of the variable x_i is often denoted by σ_{ii} rather than σ_i^2).

With q variables, $x_1, x_2, \ldots, x_q$, there are q variances and $q(q-1)/2$ covariances. In general, these quantities are arranged in a $q \times q$ symmetric matrix $\mathbf{\Sigma}$ where

$$\mathbf{\Sigma} = \begin{bmatrix} \sigma_{11} & \sigma_{12} & \cdots & \sigma_{1q} \\ \sigma_{21} & \sigma_{22} & \cdots & \sigma_{2q} \\ \vdots & \vdots & \ddots & \vdots \\ \sigma_{q1} & \sigma_{q2} & \cdots & \sigma_{qq} \end{bmatrix}$$

Note that $\sigma_{ij} = \sigma_{ji}$. This matrix is generally known as the *variance-covariance matrix* or simply the *covariance matrix*. The matrix $\mathbf{\Sigma}$ is estimated by the matrix $\mathbf{S}$, given by

$$\mathbf{S} = \frac{\sum_{i=1}^{n}\left(\mathbf{x}_i - \bar{\mathbf{x}}\right)\left(\mathbf{x}_i - \bar{\mathbf{x}}\right)'}{(n-1)}$$

where $\mathbf{x}_i' = [\mathbf{x}_{i1}, \mathbf{x}_{i2}, \ldots, \mathbf{x}_{iq}]$ is the vector of observations for the ith individual. The diagonal of $\mathbf{S}$ contains the variances of each variable. The covariance is often difficult to interpret because it depends on the units in which the two variables are measured; consequently, it is often standardized by dividing by the product of the standard deviations of the two variables to give a quantity called the correlation coefficient, ρ_{ij}, where

$$\rho_{ij} = \frac{\sigma_{ij}}{\sqrt{\sigma_{ii}\sigma_{jj}}}$$

The correlation coefficient lies between -1 and $+1$ and gives a measure of the linear relationship between the variables x_i and x_j. It is positive if high values of x_i are associated with high values of x_j, and negative if high values of x_i are associated with low values of x_j. With q variables, there are $q(q-1)/2$ distinct correlations, which may be arranged in a $q \times q$ matrix whose diagonal elements are unity.

For sample data, the correlation matrix contains the usual estimates of the ρ values, namely, Pearson's correlation coefficient, and is generally denoted by **R**. The matrix may be written in terms of the sample covariance matrix **S** as follows:

$$\mathbf{R} = \mathbf{D}^{-1/2}\mathbf{S}\mathbf{D}^{-1/2}$$

where $\mathbf{D}^{-1/2} = \mathrm{diag}\,(1/\mathrm{s_i})$.

In most situations, we will be dealing with covariance and correlation matrices of full rank q, so that both matrices will be nonsingular (i.e., invertible).

For the body measurements data, the numerical summary statistics described earlier are as follows:

Means:

Chest	**Waist**	**Hips**
37.00	28.00	37.05

Variances:

Chest	**Waist**	**Hips**
6.63	12.53	5.94

Covariance matrix:

	Chest	**Waist**	**Hips**
Chest	6.63	6.37	3.00
Waist	6.37	12.53	3.58
Hips	3.00	3.58	5.94

Correlation matrix:

	Chest	**Waist**	**Hips**
Chest	1.00	0.70	0.48
Waist	0.70	1.00	0.41
Hips	0.48	0.41	1.00

We see that the waist measurements have the largest variance, with chest and hip measurements having very similar variances. Waist and hip measurements have the largest correlation with a value of 0.70.

12.2.2 Graphical Descriptions of the Body Measurement Data

As always, numerical summaries need to be interpreted alongside appropriate graphics, and so, in Figure 12.1, we give the boxplots of each of the three body measurements, and then, in Figure 12.2, a scatterplot matrix of the three variables is shown with a histogram of each measurement placed on the diagonal. The boxplot for chest measurements shows a mild degree of skewness and one potential outlier. The scatterplot matrix is more interesting, with the panel showing the scatterplot of waist and hip measurements suggesting the possibility that the data may consist of two separate groups of observations, a possibility underlined by the bimodality of the histogram for waist measurements. The two-group possibility could be investigated further by applying cluster analysis (see Chapter 17) to the data, but here, it is not too taxing to come up with an explanation for the possible two-group structure, which is that there are men and women in the sample. (If there really are distinct groups of observations in the data, the previously calculated summary statistics for the whole sample may not give an accurate description of the separate groups.)

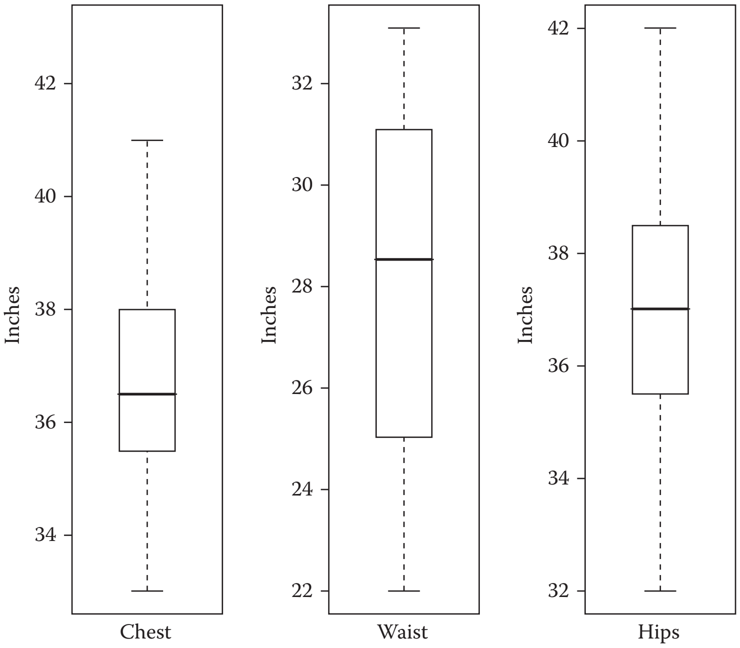


FIGURE 12.1
Boxplots of body measurements.

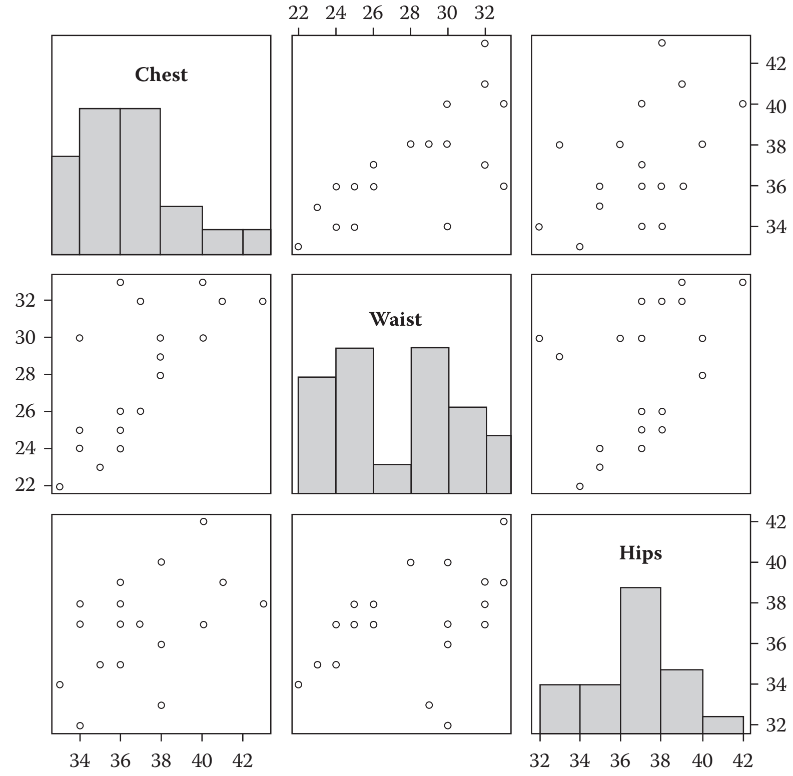


FIGURE 12.2
Scatterplot matrix of body measurements.

12.3 The Multivariate Normal Probability Density Function

As we have seen in earlier chapters, the normal probability density function is the basis of the inferences derived from most multivariable techniques. In multivariate analysis, it is the multivariate normal density function that has a similar role, although many multivariate analyses are carried out in the spirit of data exploration, where questions of statistical significance are of minor or no importance. Nevertheless, researchers in behavioral sciences dealing with the complexities of multivariate data may on occasion need to know a little about the multivariate density function and, in particular, how to assess whether or not a set of multivariate data can be assumed to have this probability density function. So, in Technical Section 12.2, we define the multivariate normal density and describe some of its properties.

Technical Section 12.2: Multivariate Normal Density Function

For a vector of q random variables $\mathbf{x}' = [x_1, x_2, \ldots, x_q]$, the multivariate normal density function takes the form

$$f(\mathbf{x}) = (2\pi)^{-q/2}|\mathbf{\Sigma}|^{-1/2}\text{exp}\left\{-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})'\mathbf{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu})\right\}, -\infty < x_i < \infty$$

where $\mathbf{\Sigma}$ is the population covariance matrix of the variables, and $\boldsymbol{\mu}$ is the vector of population mean values of the variables. The simplest example of the multivariate normal density function is the bivariate normal density with $q = 2$; this can be written explicitly as

$$f(x_1, x_2) = \frac{1}{2\pi\sigma_1\sigma_2\sqrt{(1-\rho^2)}} \quad \times$$

$$\text{exp}\left\{\frac{-1}{2(1-\rho^2)}\left[\left(\frac{x_1-\mu_1}{\sigma_1}\right)^2 - 2\rho\left(\frac{x_1-\mu_1}{\sigma_1}\right)\left(\frac{x_2-\mu_2}{\sigma_2}\right)+\left(\frac{x_2-\mu_2}{\sigma_2}\right)^2\right]\right\}$$

where μ_1 and μ_2 are the population means of the two variables, σ_1^2 and σ_2^2 are the population variances, and ρ is the population correlation between the two variables. Figure 12.3 shows an example of a bivariate normal density function with both means equal to 0, both variances equal to 1, and correlation equal to 0.5.

The population mean vector and the population covariance matrix of a multivariate density function are estimated from a sample of multivariate observations as described in Technical Section 12.1.

One property of a multivariate normal density function that is worth mentioning here is that linear combinations of the variables, that is,

$$y = a_1x_1 + a_2x_2 + \cdots + a_qx_q$$

where $a_1, a_2, \ldots, a_q$ is a set of scalars, are themselves normally distributed with mean $\mathbf{a}'\boldsymbol{\mu}$ and variance $\mathbf{a}'\mathbf{\Sigma}\mathbf{a}$ where $\mathbf{a}' = [a_1, a_2, \ldots, a_q]$. Linear combinations of variables will be of importance in later chapters.

For many multivariate methods to be described in later chapters, the assumption of multivariate normality is often not critical to the results of the analysis. But there may be occasions when testing for multivariate normality may be of interest. A start can be made perhaps by testing each separate variable for univariate normality using, say, a probability plot, as described in Chapter 2. Such plots can be helpful, but unfortunately, marginal multivariate normality does not necessarily imply multivariate normality. An alternative (additional)

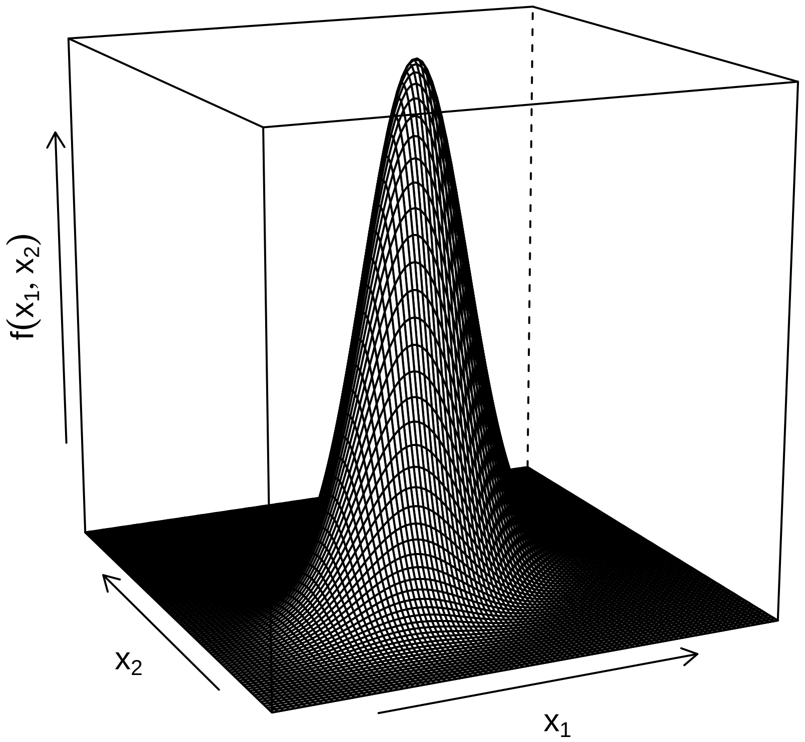


FIGURE 12.3
Bivariate normal density function with means equal to 0, variances equal to 1, and correlation equal to 0.5.

approach is to convert the multivariate observations $\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n$ into a set of generalized distances d_i^2, giving a measure of the distance of each particular observation from the mean vector of the complete sample $\bar{\mathbf{x}}$. The generalized distances (also called Mahalanobis distances) d_i^2 are calculated as

$$d_i^2 = (\mathbf{x}_i - \bar{\mathbf{x}})' \, \mathbf{S}^{-1} \, (\mathbf{x}_i - \bar{\mathbf{x}})$$

where $\mathbf{S}$ is the sample covariance matrix. This distance measure takes into account the different variances of the variables and the covariances of pairs of variables. If the observations do arise from a multivariate normal distribution, then the generalized distances have, approximately, a chi-squared distribution with q degrees of freedom. So, plotting the ordered distances against the corresponding quantiles of the appropriate chi-squared distribution should lead to a straight line through the origin.

12.3.1 Assessing Multivariate Data for Normality

We will now assess the body measurements data for normality, although, because there are only 20 observations in the sample, there is really too little information to come to any convincing conclusion. Figure 12.4 shows separate probability plots for each measurement; in the plots, there appears to be no evidence of any departures from linearity.

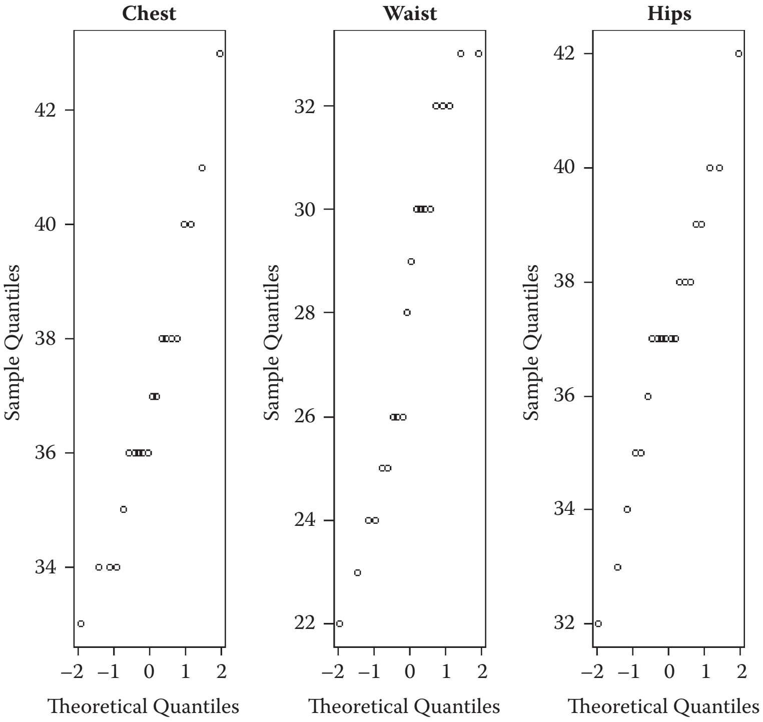


FIGURE 12.4
Normal probability plots of chest, waist, and hip measurements.

The chi-square plot of the 20 generalized distances in Figure 12.5 does seem to deviate a little from linearity, but with so few observations, it is hard to be certain.

Now let us look at a larger example of a multivariate data set collected in

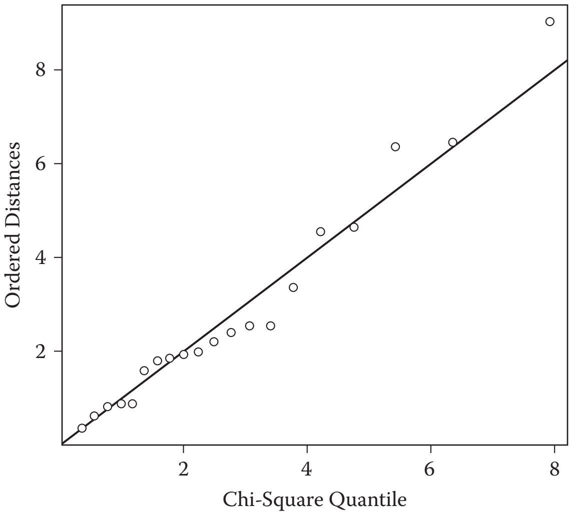


FIGURE 12.5
Chi-square plot of generalized distances for the body measurements data.

a health survey of 103 paint sprayers in a car assembly plant. Six variables were recorded on each individual:

Hemo:	Hemoglobin concentration
PCV:	Packed cell volume
WBC:	White blood cell count
Lympho:	Lymphocyte count
Neutro:	Neutrophil count
Lead:	Serum lead concentration

Data for the first five paint sprayers are shown in Table 12.2. We begin by looking at separate normal probability plots of each of the six variables; the plots are given in Figure 12.6. The plots for WBC, Lympho, and Lead show some deviation for linearity that would suggest that the six variables do not have a multivariate normal density. The chi-square plot of generalized

TABLE 12.2
Part of the Data on Paint Sprayers

Case	Hemo	PCV	WBC	Lympho	Neutro	Lead
1	13.4	39	4100	14	25	17
2	14.6	46	5000	15	30	20
3	13.5	42	4500	19	21	18
4	15.0	46	4600	23	16	18
5	14.6	44	5100	17	31	19

distances in Figure 12.7 appears to confirm this because there is considerable departure from linearity in this plot although this is primarily due to a relatively few observations. Here, it is of interest to see what happens when we take a log transformation of all the variables and then look at the chi-square plot of the transformed data, given in Figure 12.8. In this plot, it looks like just six observations deviate from the linearity required to give the data a multivariate normal density seal of approval. Identifying these outliers and creating a chi-square plot for the remaining log-transformed observations might be useful (see Exercise 12.2).

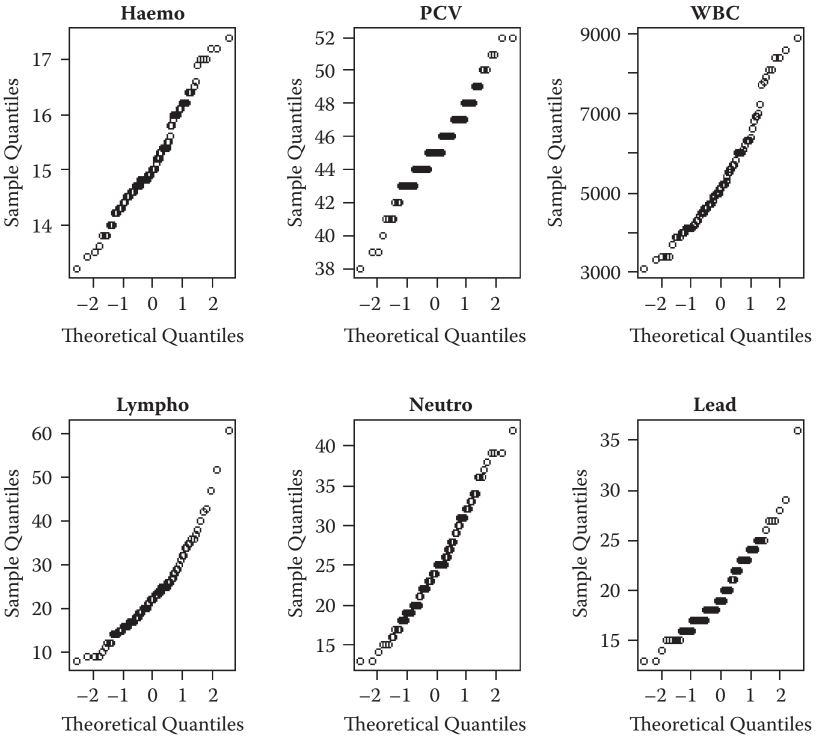


FIGURE 12.6
Normal probability plots for the six variables in the data on paint sprayers.

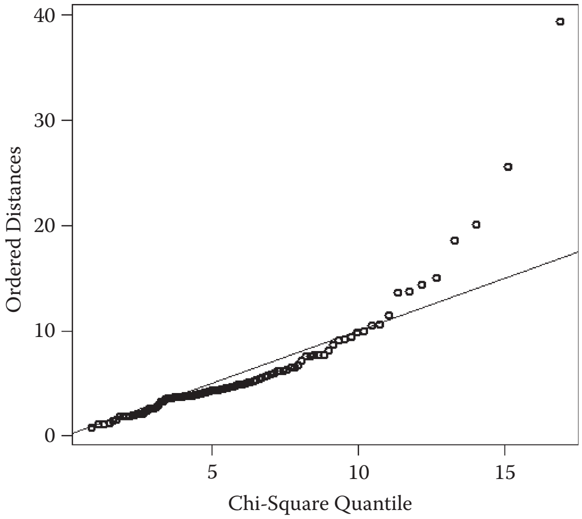


FIGURE 12.7
Chi-square plot of generalized distances for paint-sprayer data.

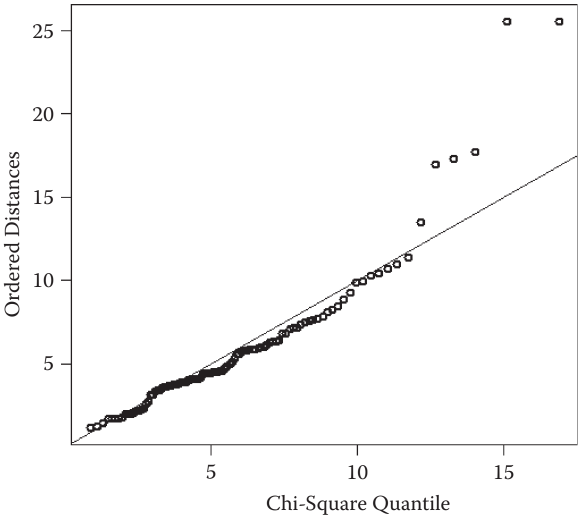


FIGURE 12.8
Chi-square plot of paint sprayers data after a log transformation of all the six variables.

12.4 Summary

- Multivariate data arise when researchers measure several variables on each individual in their sample and there is no response variable.

- Although in some cases it may make sense to isolate each variable and study it separately, in the main it does not. In most instances the variables are related in such a way that, when analyzed in isolation, they may often fail to reveal the full structure of the data. With the great majority of multivariate data sets, all the variables need to be examined simultaneously in order to uncover the patterns and key features in the data.

- Several multivariate techniques are largely “exploratory” in nature and, in many cases, a set of multivariate data may not arise as a sample from some populations. Consequently, questions of inference become less important.

- Where inference for multivariate data is an issue, it is usually based on the assumption that the sample data arise from a population in which the variables have a multivariate normal density function. In such cases, it may be worth assessing the assumption.

12.5 Exercises

(excluded from MABS for IODS)

17

Cluster Analysis

17.1 Introduction

> An intelligent being cannot treat every object it sees as a unique entity unlike anything else in the universe. It has to put objects in categories so that it may apply its hard-won knowledge about similar objects encountered in the past, to the object at hand.
>
> **Steven Pinker, *How the Mind Works*, 1997**

One of the most basic abilities of living creatures involves the grouping of similar objects to produce a *classification.* The idea of sorting similar objects into categories is clearly a primitive one because early humans, for example, must have been able to realize that many individual objects shared certain properties such as being edible, or poisonous, or ferocious, and so on. Further, classification in its widest sense is needed for the development of language, which consists of words that help us recognize and discuss the different types of events, objects, and people we encounter. Each noun in a language, for example, is essentially a label used to describe a class of objects that have striking features in common; thus, animals are called cats, dogs, horses, etc., and each name collects individuals into groups. Naming and classifying are essentially synonymous.

As well as being a basic human conceptual activity, classification of the phenomena being studied is an important component of virtually all scientific research. In the behavioral sciences, for example, these "phenomena" may be individuals or societies, or even patterns of behavior or perception. The investigator is usually interested in finding a classification in which the items of interest are sorted into a small number of *homogeneous groups* or *clusters*, the terms being synonymous. Most commonly, the required classification is one in which the groups are *mutually exclusive* (an item belongs to a single group) rather than overlapping (items can be members of more than one group). At the very least, any derived classification scheme should provide a convenient method of organizing a large, complex set of multivariate data with the class labels providing a parsimonious way of describing the patterns of similarities and differences in the data. In market research, for example, it might be useful to group a large number of potential customers according to their needs in a particular product area. Advertising campaigns might then be tailored to the different types of consumers as represented by the different groups.

But often, a classification may seek to serve a more fundamental purpose. In psychiatry, for example, the classification of psychiatric patients with different symptom profiles into clusters might help in the search for the causes of mental illnesses and even perhaps to improved therapeutic methods. These twin aims of prediction (separating diseases that require different treatments) and etiology (searching for the causes of disease) for classifications will be the same in other branches of medicine.

Clearly, a variety of classifications will always be possible for whatever is being classified. Human beings could, for example, be classified with respect to economic status into groups labeled lower class, middle class, and upper class, or they might be classified by the annual consumption of alcohol into low, medium, and high. Clearly, different classifications may not collect the same set of individuals into groups, but some classifications will be more useful than others—a point made clearly by the following extract from Needham (1967), in which he considers the classification of human beings into men and women:

> The usefulness of this classification does not begin and end with all that can, in one sense, be strictly inferred from it, namely, a statement about sexual organs. It is a very useful classification because classifying a person as man or woman conveys a great deal more information about probable relative size, strength, certain types of dexterity, and so on. When we say that persons in class man are more suitable than persons in class woman for certain tasks, and conversely, we are only incidentally making a remark about sex, our primary concern being strength, endurance, etc. The point is that we have been able to use a classification of persons that conveys information on many properties. On the contrary, a classification of persons into those with hairs on their forearms between $^3/_{16}$ and $^1/_4$ in. long and those without, though it may serve some particular use, is certainly of no general use, for imputing membership in the former class to a person conveys information on this property alone. Put another way, there are no known properties that divide up a set of people in a similar way.

In a similar vein, a classification of books based on subject matter into classes such as dictionaries, novels, biographies, and so on is likely to be far more useful than one based on, say, the color of the book's binding. Such examples illustrate that any classification of a set of multivariate data is likely to be judged on its usefulness.

It should be noted here that this chapter is concerned only with the problems of classifying previously unclassified material, and so begins with both the number of groups and their composition as unknowns. The situation when groups are known a priori, and the aims are to assess whether these groups differ on a set of variables or to derive a rule for classifying new individuals on the basis of their scores on these variables, is taken up in Chapter 18.

17.2 Cluster Analysis

Cluster analysis is a generic term for a wide range of numerical methods with the common goal of uncovering or discovering groups or clusters of observations that are homogeneous and separated from other groups. Clustering techniques essentially try to formalize what human observers do so well in two or three dimensions. Consider, for example, the scatterplot shown in Figure 17.1. The conclusion that there are three natural groups or clusters of dots is reached with no conscious effort or thought. Clusters are identified by the assessment of the relative distances between points, and, in this example, the relative homogeneity of each cluster and the degree of separation between the clusters makes the task very simple. The examination of scatterplots based either on the original data or perhaps on the first few principal component scores of the data is often a very helpful initial phase when intending to apply some form of cluster analysis to a set of multivariate data.

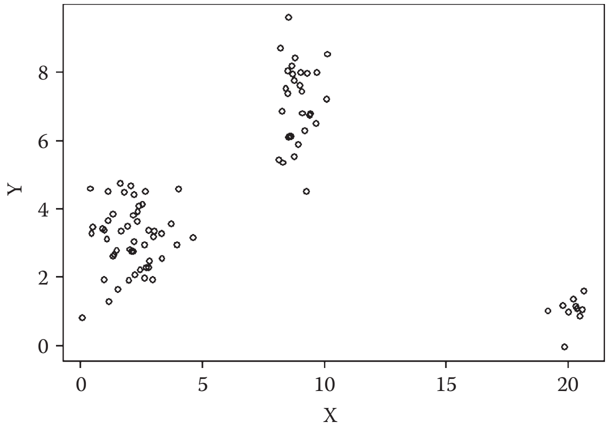


FIGURE 17.1
Bivariate data clearly showing the presence of three clusters.

Cluster analysis techniques are described in detail in Gordon (1987, 1999) and Everitt et al. (2011). In this chapter, we give a relatively brief account of three types of clustering methods: agglomerative hierarchical techniques, k-means clustering, and model-based clustering.

17.3 Agglomerative Hierarchical Clustering

In a *hierarchical classification*, the data are not partitioned into a particular number of classes or groups at a single step. Instead, the classification consists of a series of partitions that may run from a single "cluster" containing all individuals, to n clusters, each containing a single individual. *Agglomerative hierarchical clustering* techniques produce partitions by a series of successive fusions of the n individuals into groups. With such methods, fusions, once made, are irreversible, so that when an agglomerative algorithm has placed two individuals in the same group, they cannot subsequently appear in different groups. Since all agglomerative hierarchical techniques ultimately reduce the data to a single cluster containing all the individuals, the investigator seeking the solution with the "best" fitting number of clusters will need to decide which division to choose. The problem of deciding on the "correct" number of clusters will be taken up later.

An agglomerative hierarchical clustering procedure produces a series of partitions of the data, $P_n, P_{n-1}, \ldots, P_1$. The first, P_n, consists of n single-member clusters, and the last, P_1, consists of a single group containing all n individuals. The basic operation of all methods is similar:

Start: Clusters $C_1, C_2, \ldots, C_n$, each containing a single individual.

Step 1: Find the nearest pair of distinct clusters, say, C_i and C_j, merge C_i and C_j, delete C_j, and decrease the number of clusters by one.

Step 2: If number of clusters equals one, then stop; else return to Step 1.

However, before the process can begin, an interindividual *distance matrix* or *similarity matrix* needs to be calculated (similarly as in multidimensional scaling, see Chapter 14). There are many ways to calculate distances or similarities between pairs of individuals, but here we only deal with a commonly used distance measure, namely, Euclidean distance, defined as follows:

$$d_{ij} = \sqrt{\sum_{k=1}^{q} (x_{ik} - x_{jk})^2}$$

where d_{ij} is the Euclidean distance between individual i with variable values $x_{i1}, x_{i2}, \ldots, x_{iq}$, and individual j with variable values $x_{j1}, x_{j2}, \ldots, x_{jq}$. (Details of other possible distance measures and similarity measures are given in Everitt et al., 2011.) The Euclidean distances between each pair of individuals can be arranged in a matrix that is symmetric because $d_{ij} = d_{ji}$ and has zeros on the main diagonal. Such a matrix is the starting point of many clustering examples, although the calculation of Euclidean distances from the raw data may not be sensible when the variables are on very different scales. In such cases, the variables can be standardized in the usual way before calculating the distance matrix, although this can be unsatisfactory in some cases (see Everitt et al., 2011, for details).

Given an interindividual distance matrix, the hierarchical clustering can begin and, at each stage in the process, the methods fuse individuals or groups of individuals formed earlier who are closest (or most similar). So, as groups are formed, the distance between an individual and a group containing several individuals, and the distance between two groups of individuals will need to be calculated. How such distances are defined leads to a variety of different techniques. Two simple intergroup measures are

$$d_{\min}(A,B) = \min_{i \in A, j \in B} d_{ij} \quad \text{and} \quad d_{\max}(A,B) = \max_{i \in A, j \in B} d_{ij}$$

where $d(A,B)$ is the distance between two clusters A and B, and d_{ij} is the distance between individuals i and j found from the initial interindividual distance matrix.

The intergroup distance measure $d_{\min}(A,B)$ is the basis of *single linkage clustering*, $d_{\max}(A,B)$ that of *complete linkage clustering*. Both these techniques have the desirable property that they are invariant under monotone transformations of the original interindividual distances, that is, they only depend on the ranking on these distances, not their actual values.

A further possibility for measuring intercluster distance or dissimilarity is

$$d_{\text{mean}}(A,B) = \frac{1}{n_A n_B} \sum_{i \in A} \sum_{j \in B} d_{ij}$$

where n_A and n_B are the number of individuals in clusters A and B. The measure $d_{\text{mean}}(A,B)$ is the basis of a commonly used procedure known as *average linkage clustering*. All three intergroup measures described here are illustrated in Figure 17.2.

Hierarchic classifications may be represented by a two-dimensional diagram known as a *dendrogram*, which illustrates the fusions made at each stage of the analysis. An example of such a diagram is given in Figure 17.3. The structure of Figure 17.3 resembles an evolutionary tree, a concept introduced by Darwin under the term "Tree of Life" in his book *On the Origin of Species by Natural Selection* in 1859 (see Figure 17.4), and it is in biological applications that hierarchical classifications are most relevant and most justified (although this type of clustering has also been used in many other areas).

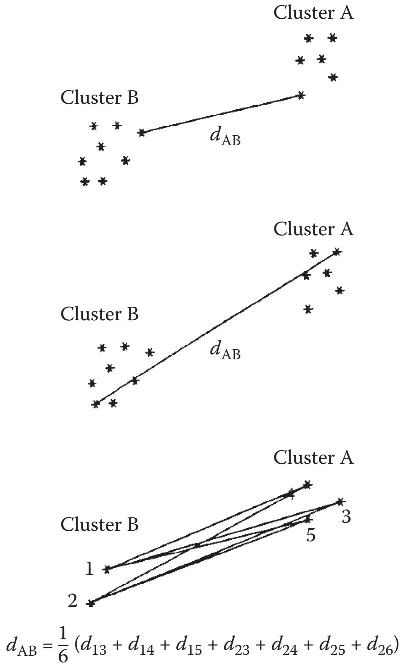

Cluster A
Cluster B
d_{AB}
Cluster A
Cluster B
d_{AB}
Cluster A
Cluster B
3
5
1
2
$d_{AB} = \frac{1}{6}(d_{13} + d_{14} + d_{15} + d_{23} + d_{24} + d_{25} + d_{26})$

FIGURE 17.2
Intercluster distance measures based on minimum, maximum, and mean of distances between clusters A and B.

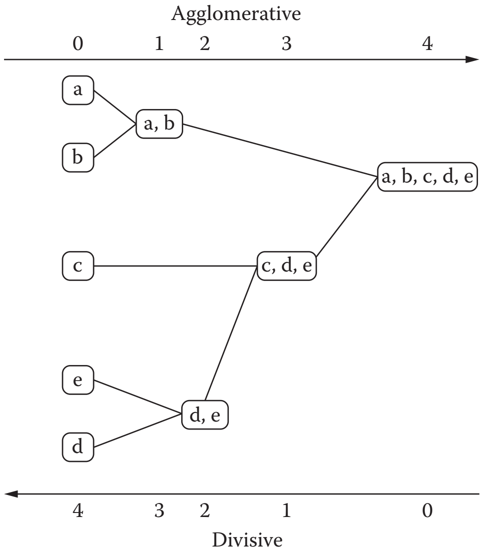


FIGURE 17.3
Example of a dendrogram.

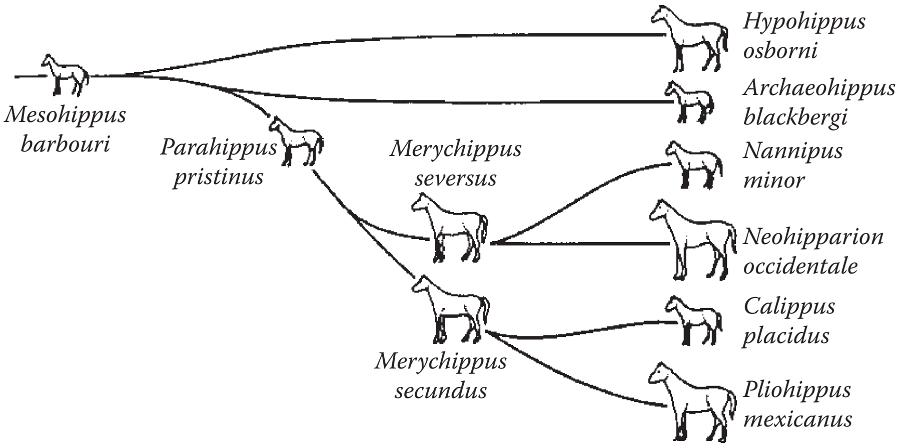


FIGURE 17.4
Evolutionary tree. (From Kaufman, L. and Rousseeuw, P. J. (1990). *Finding Groups in Data: An Introduction to Cluster Analysis*, Wiley, New York. Used with permission of John Wiley & Sons.)

17.3.1 Clustering Individuals Based on Body Measurements

As a first example of the application of the three clustering methods (single linkage, complete linkage, and average linkage), each will be applied to the chest, waist, and hip measurements of 20 individuals given in Chapter 12, Table 12.1.

First Euclidean distances are calculated on the unstandardized measurements; application of each of the three methods to this distance matrix gives the three dendrograms shown in Figure 17.5. How do we select specific partitions of the data from the complete dendrogams? The answer is that we "cut" the dendrogram at some height, and this will give a partition with a particular number of groups. How do we choose where to cut or, in other words, how do we decide on a particular number of groups that is, in some sense, optimal for the data? One informal approach is to examine the sizes of the changes in height in the dendrogram and take a "large" change to indicate the appropriate number of clusters for the data. (More formal approaches are described in Everitt et al., 2011.)

Even using this informal approach on the dendrograms in Figure 17.5, it is not easy to decide where to "cut." So, instead, because we know that these data consist of measurements on 10 men and 10 women, we will look at the two-group solutions from each method that are obtained by cutting the dendrograms at suitable heights. We can display and compare the three solutions graphically by plotting the first two principal component scores of the data, labeling the points to identify the cluster solution of one of the methods. Such plots are also shown in Figure 17.5. The plot associated with the single linkage

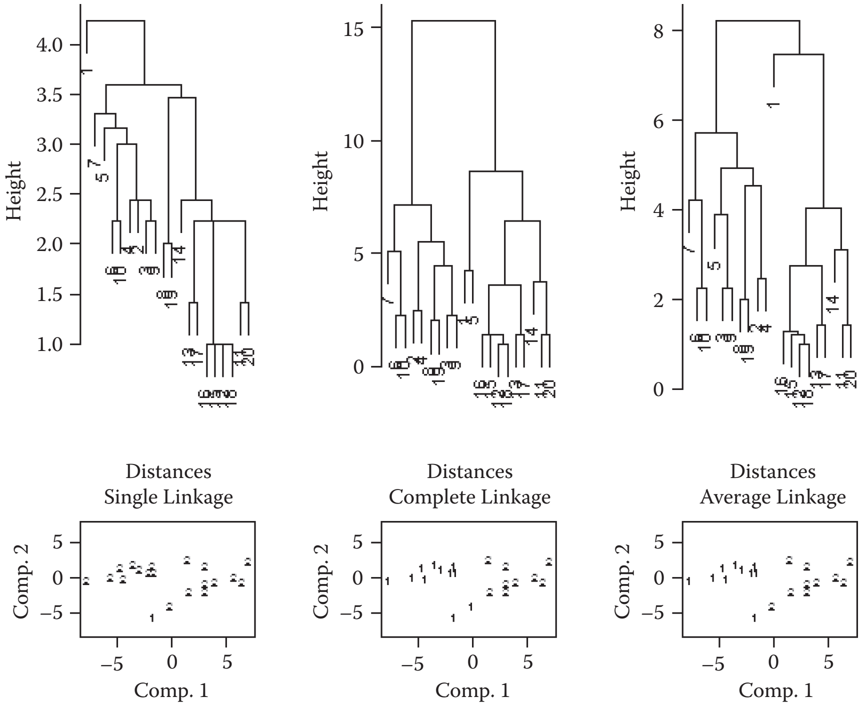


FIGURE 17.5
Dendrograms for single linkage, complete linkage, and average linkage applied to body measurements data.

solution immediately demonstrates one of the problems with using this method in practice, and that is a phenomenon known as *chaining*, which refers to the tendency to incorporate intermediate points between clusters into an existing cluster rather than initiating a new one. As a result, single linkage solutions often contain long "straggly" clusters that do not give a useful description of the data. The two-group solutions from complete linkage and average linkage, also shown in Figure 17.5, are similar and, in essence, place the men (observations 1 to 10) together in one cluster and women (observations 11 to 20) in the other.

17.3.2 Clustering Countries on the Basis of Life Expectancy

The yearbook of United Nations (2016) is full of population statistics related to all countries and special regions of the world. To be more specific about the countries, we refer to *sovereign states*. Updating (or even compiling) a list of such entities around the world is far from trivial, as some areas might have a *de facto* status of a sovereign state, although they might not be official states etc.

TABLE 17.1
Life Expectancies at Different Ages for Men in Seven Countries

	Birth	**Aged 25**	**Aged 50**	**Aged 75**	**Aged 100**
Japan	80.8	56.3	32.4	12.0	2.2
Italy	80.3	55.9	31.9	11.6	1.8
Spain	80.0	55.5	31.5	11.7	3.4
United Kingdom	79.0	54.7	31.1	11.2	2.2
Finland	78.5	54.1	30.5	11.1	1.7
Cuba	76.5	52.5	29.2	11.0	2.0
United States	76.4	52.6	29.8	11.2	2.1

Ignoring however such complications, the data to be used in this subsection have been extracted from the UN databases listing 46 variable values related to life expectancy by age and gender in six regions: Africa, America (North), America (South), Asia, Europe, and Oceania. From the 134 sovereign states in these data here we shall concentrate on the analysis of a subset relating to men in 50 countries where life expectancy data are available for ages from birth to 100 years, the latter being an ever increasing possibility for many 'lucky' people! (Repeating the analysis described here for the corresponding data for women is left as an exercise for readers—see Exercise 17.6).

Table 17.1 shows life expectancies for seven countries that are precisely those whose birth and death rates were shown based on their Euclidean distance matrix in Chapter 14. Here, we shall have a somewhat broader view, although we focus on the life expectancies, and select just five crucial ages (0, 25, 50, 75, 100) to represent the potential lifespan of a human-being. We quickly check the variances of the life expectancy of men at those ages in the 50 countries:

Birth variance = 21.6
Aged 25 variance = 18.5
Aged 50 variance = 11.5
Aged 75 variance = 2.11
Aged 100 variance = 0.41

As might have been predicted, the variances are quite different, so calculating the initial intercountry Euclidean distance matrix on the life expectancies as they are in Table 17.1 would not necessarily appear to be very sensible, and thus we could standardize each of the five life expectancies to have the variance of one and then calculate the required Euclidean distances on the standardized data. However, we shall first work with the raw data.

Here, we shall apply only complete linkage to the data, and the resulting dendrogram is shown in Figure 17.6. Again, there is no completely "best" place to cut the dendrogram, but the four-group cluster solution produced by cutting at a height of 10 is shown in Table 17.2. The countries grouped together in each cluster are perhaps different from what might have been expected from intuition. The 17 countries in group 1 have the highest life expectancies at each age, while the 16 countries in group 2 have the second highest figures. Group 3 (10 countries) and group 4 (seven countries) follow this trend with their patterns for mean profiles. The only exception is that the life expentancy at age 100 is somewhat higher in group 4 than in group 3.

We can illustrate the cluster solution graphically in a number of ways. Here, we shall first plot the four-group cluster solution on the scatterplot matrix of the five life expectancies to give Figure 17.7. Most of the plots in this scatterpot matrix are not very interesting, as they merely show the order of the groups based on their mean profiles. The most interesting lots in

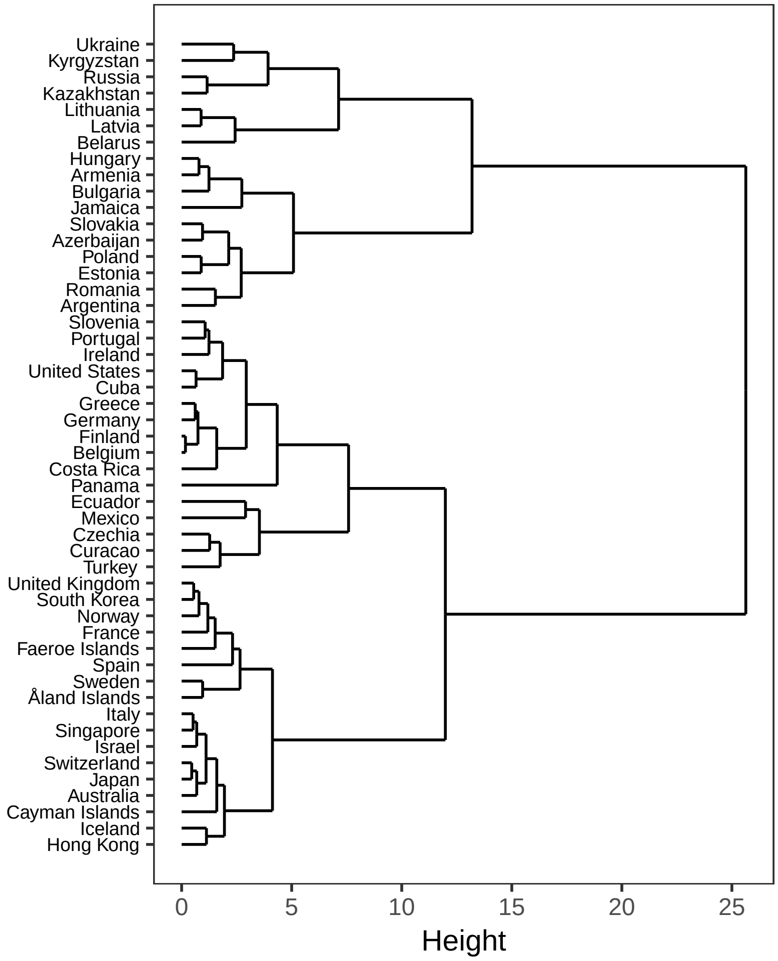


FIGURE 17.6
Complete-linkage dendrogram for life expectancy data.

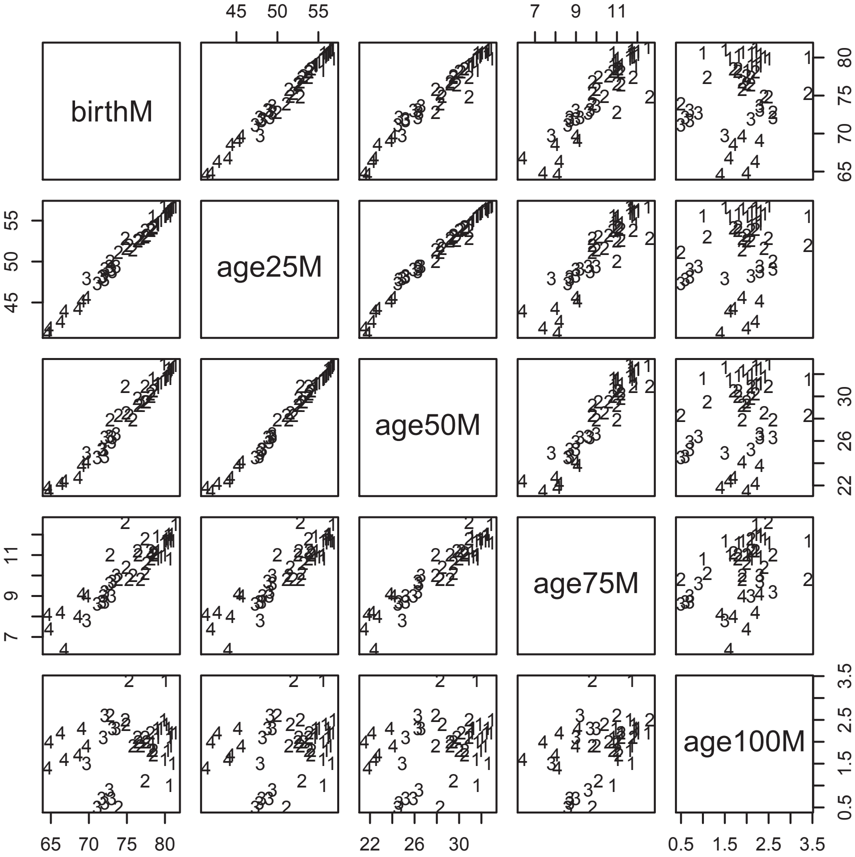


FIGURE 17.7
Scatterplot matrix of life expectancy data showing the four-cluster solution from complete linkage.

this figure are those with age 100 as the other axis, as they all display the spread of the data. The groups seem to have more variance related to the life expectancies of the countries at age 100.

A further graphic of the cluster solution is shown in Figure 17.8, where the data are plotted in the space of the first two principal components and labeled by cluster membership and the country in question. Now, the data have been standardized, as the principal components have been calculated on the basis of correlations. The first component is essentially the average of the five life expectancies, reflecting the same order and trend that was visible from the mean profiles given in Table 17.2. The second component is mostly displaying the spread of the life expectancy at 100 years of age across the countries in all groups. The longest life expectancies at 100 are in Spain and Turkey while

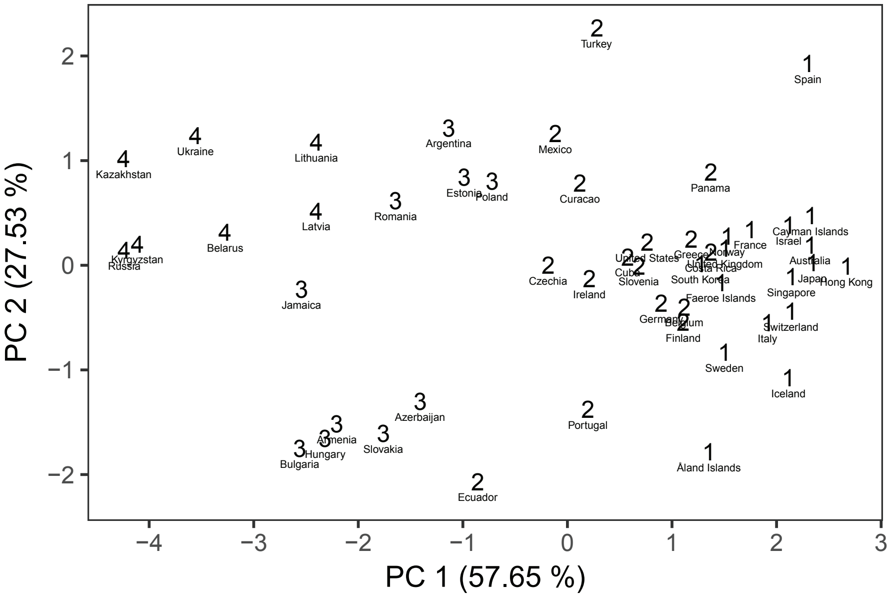


FIGURE 17.8
Four-cluster solution from complete linkage applied to life expectancy data plotted in the space of the first two principal components.

the shortest is in Ecuador. The first two components account for 85% of the variance of the five life expectancies. Figure 17.8 demonstrates that the four clusters differ largely on their average life expectancy over the five ages.

(As an aside, there are many questions of interest that relate to population dynamics, for example, "Why the world's population is increasing?", or "How many young women go to school?", or "How many of us live in poverty?" Answering such questions is not simple and Rosling et al. (2018) in their quite brilliant book, *Factfulness*, demonstrate that a chimpanzee choosing answers at random will consistently outguess 'informed' answers by journalists, Nobel laureates and investment bankers—no surprise about the latter!)

17.4 *k*-Means Clustering

The k-means clustering technique seeks to partition the n individuals in a set of multivariate data into k groups or clusters, $(G_1, G_2, \ldots, G_k)$, where G_i denotes the set of n_i individuals in the ith group, and k is given (or a possible range is specified by the researcher; the problem of choosing the "true" value of k will be taken up later) by minimizing some numerical criterion, low values of

TABLE 17.2
Four Group Solution Produced by Complete Linkage Clustering Applied to the Life Expectancy Data

Countries and Mean Life Expectancies of Males in Each Group				
Group 1				
Australia, Åland Islands, Cayman Islands, Faeroe Islands, France, Hong Kong, Iceland, Israel, Italy, Japan, Norway, Singapore, South Korea, Spain, Sweden, Switzerland, United Kingdom				
		Mean		
birthM	**age25M**	**age50M**	**age75M**	**age100M**
80.0	55.7	31.9	11.5	2.1
Group 2				
Belgium, Costa Rica, Cuba, Curaçao, Czechia, Ecuador, Finland, Germany, Greece, Ireland, Mexico, Panama, Portugal, Slovenia, Turkey, United States				
		Mean		
birthM	**age25M**	**age50M**	**age75M**	**age100M**
76.4	52.7	29.4	10.8	2.0
Group 3				
Argentina, Armenia, Azerbaijan, Bulgaria, Estonia, Hungary, Jamaica, Poland, Romania, Slovakia				
		Mean		
birthM	**age25M**	**age50M**	**age75M**	**age100M**
72.1	48.5	25.6	9.0	1.4
Group 4				
Belarus, Kazakhstan, Kyrgyzstan, Latvia, Lithuania, Russia, Ukraine				
		Mean		
birthM	**age25M**	**age50M**	**age75M**	**age100M**
67.1	43.6	22.6	8.0	1.9

which are considered indicative of a “good” solution. The most commonly used implementation of k-means clustering is one that tries to find the partition of the n individuals into k groups that minimizes the within-group sum of squares (WGSS) over all variables; explicitly this criterion is

$$\text{WGSS} = \sum_{j=1}^{q} \sum_{l=1}^{k} \sum_{i \in G_l} \left(x_{ij} - \bar{x}_j^{(l)} \right)^2$$

where

$$\bar{x}_j^{(l)} = \frac{1}{n_l} \sum_{i \in G_l} x_{ij}$$

is the mean of the individuals in group G_l on variable j.

The problem then appears relatively simple; consider every possible partition of the n individuals into k groups, and select the one with the lowest within-group sum of squares. Unfortunately, the problem in practice is not so straightforward. The numbers involved are so vast that complete enumeration of every possible partition remains impossible even with the fastest computer. The scale of the problem is illustrated in the following table:

n	**k**	**Number of Possible Partitions**
15	3	$2,375,101$
20	4	$45,232,115,901$
25	8	$690,223,721,118,368,580$
100	5	10^{68}

The impracticability of examining every possible partition has led to the development of algorithms designed to search for the minimum values of the clustering criterion by rearranging existing partitions and keeping the new one only if it provides an improvement. Such algorithms do not, of course, guarantee finding the global minimum of the criterion. The essential steps in these algorithms are as follows:

1. Find some initial partition of the individuals into the required number of groups. Such an initial partition could be provided by a solution from one of the hierarchical clustering techniques described in the previous section.
2. Calculate the change in the clustering criterion produced by "moving" each individual from its own to another cluster.
3. Make the change that leads to the greatest improvement in the value of the clustering criterion.
4. Repeat steps 2 and 3 until no move of an individual causes the clustering criterion to improve.

For a more detailed account of the k-means algorithm, see Steinley (2008).

The k-means approach to clustering using the minimization of the WGSS over all the variables is widely used, but it suffers from two problems:

1. k-means is not scale invariant, that is, different solutions may result from clustering the raw data and the data standardized in some way.
2. k-means imposes a spherical structure on the data, that is, k-means will find clusters shaped like hyper-footballs even if the "true" clusters in the data are of some other shape (see Everitt et al., 2011, for some examples of this phenomenon).

Nevertheless, the k-means method remains very popular. With k-means clustering, the investigator can choose to partition the data into a specified number of groups. In practice, solutions for a range of values for number of groups are found and, in some way, the optimal or "true" number of groups for the data must be chosen. Several suggestions have been made as to how to answer the number of groups question, but none is completely satisfactory. The method we shall use in the forthcoming example is to plot the WGSS associated with the k-means solution for each number of groups. As the number of groups increases, the sum of squares will necessarily decrease, but an obvious "elbow" in the plot may be indicative of the most useful solution for the investigator to look at in detail. (Compare the scree plot described in Chapter 13.)

17.4.1 Clustering Crime Rates

We shall illustrate the application of k-means clustering using the crime rate data introduced in Chapter 13 after removing the outlier, DC, identified in Chapter 13. If we first calculate the variances of the crime rates for the different types of crime we find the following:

	Murder	**Rape**	**Robbery**	**Assault**	**Burglary**	**Theft**
Variance	11.93	209.76	1889.53	19373.54	175895.00	565276.59

The variances are very different, and using k-means on the raw data would not be sensible; we must standardize the data in some way. Here, we standardize each variable by its range. After the standardization, the variances become:

	Murder	**Rape**	**Robbery**	**Assault**	**Burglary**	**Theft**	**Vehicle**
Variance	0.076	0.056	0.046	0.059	0.052	0.062	0.068

The variances of the standardized data are very similar, and we can now progress with clustering the data. First, we plot the WGSS for one- to six-group solutions to see if we can get any indication of number of groups. The plot is shown in Figure 17.9. The only "elbow" in the plot occurs for two groups, and so we will now look at the two-group solution. In Table 17.3, the group membership and means are given. Everything is worse in group 1! A plot of the two-group solution in the space of the first two principal components of the correlation matrix of the data is shown in Figure 17.10. The two groups are created essentially on the basis of the first principal component score, which is, as we have seen in Chapter 13, a weighted average of the crime rates. Perhaps all that cluster analysis is doing here is dividing into two parts a homogenous set of data? This is always a possibility as discussed in some detail in Everitt et al. (2011).

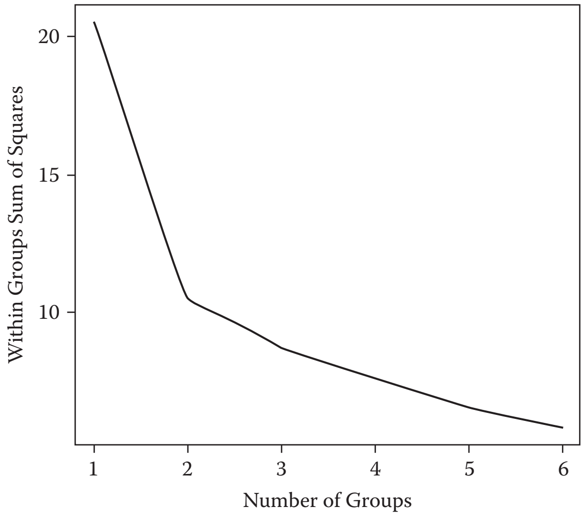


FIGURE 17.9
Plot of within-groups sum of squares against number of clusters.

17.5 Model-Based Clustering

(excluded from MABS for IODS)

TABLE 17.3
Group Membership and Means for the Two-Group Solution from *k*-Means Applied to Crime Rate Data

Group 1						
MA, NY, NJ, IL, MI, MO, MD, NC, SC, GA, KY, AR, LA, OK, WY, CO, NM, UT, NV, WA, OR, CA						
			Mean Crime Rates			
Murder	**Rape**	**Robbery**	**Assault**	**Burglary**	**Theft**	**Vehicle**
9.37	45.37	229.00	394.77	1543.41	3368.05	554.27
Group 2						
ME, NH, VT, RI, CT, PA, OH, IN, WI, MN, IA, ND, SD, NE, KS, DE, DC, VA, WV, FL, TN, AL, MS, TX, MT, ID, AZ, AK, HI						
			Mean Crime Rates			
Murder	**Rape**	**Robbery**	**Assault**	**Burglary**	**Theft**	**Vehicle**
4.74	24.80	73.82	182.07	924.21	2564.71	247.04

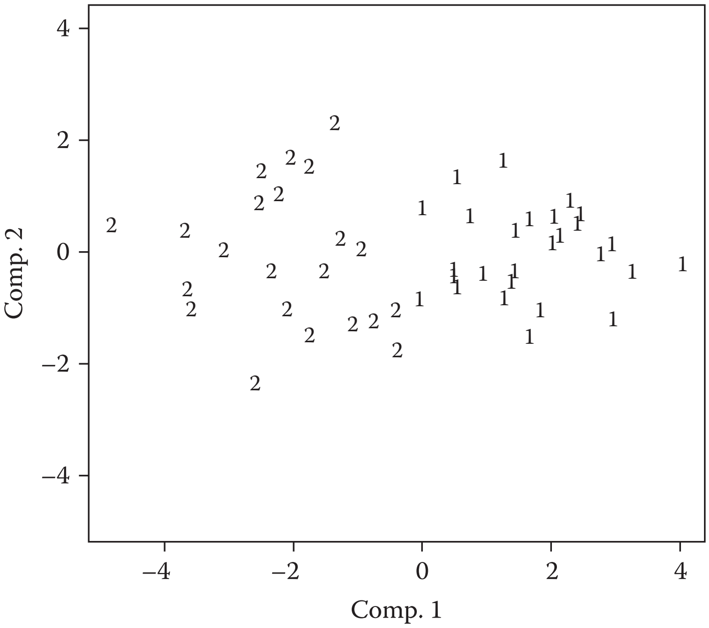


FIGURE 17.10
Plot of k-means two-group solution for standardized crime rate data.

17.6 Summary

- Cluster analysis techniques are used to search for clusters/groups in a priori unclassified multivariate data.
- Although clustering techniques are potentially very useful for the exploration of multivariate data, they require care in their application if misleading solutions are to be avoided.
- Many methods of cluster analysis have been developed, and most studies have shown that no one method is best for all types of data. However, the more statistical techniques covered briefly in Section 17.5 and in more detail in Everitt et al. (2011) have definite statistical advantages because the clustering is based on sensible models for the data.
- Cluster analysis is a large area and has been covered only briefly in this chapter. The many problems that need to be considered when using clustering in practice have barely been touched upon. For a detailed discussion of these problems, see Everitt et al. (2011).

17.7 Exercises

(excluded from MABS for IODS)

18

Grouped Multivariate Data

18.1 Introduction

The importance of classification in science in general and behavioral science in particular has already been remarked upon in Chapter 17, in which techniques were described for examining multivariate data to discover whether the data consisted of a number of relatively distinct groups or clusters of observations. In this chapter, a further aspect of classification will be discussed, namely that when the groups are known a priori. Such data arises when investigators collect samples of multivariate observations from several different populations, for example, observations on a number of symptoms for patients from different diagnostic categories.

A variety of questions might be asked about grouped multivariate data, and so, there are a variety of (overlapping) approaches to their analysis. In some cases, the investigator will simply be interested in testing whether the groups differ on the variables that have been recorded. When there are two groups, the multivariate analog of Student's t-test, Hotelling's T^2 test, can be used, and when there are more than two groups, *multivariate analysis of variance* (MANOVA) is available. Both methods will be described later in the chapter.

A further question that is often of interest for grouped multivariate data is whether or not it is possible to use the measurements made to construct a classification rule derived from the original observations (the training set) that will allow new individuals having the same set of measurements (the test sample), but no group label, to be allocated to a group in such a way that misclassifications are minimized. The relevant technique is now some form of *discriminant function analysis*, which is the subject of Section 18.2.2. A question that might be posed about constructing such an allocation rule is, "if group labels can be allocated a priori in some definitive fashion, why would we want to use the recorded variables for classification?" The answer might simply be "convenience" if definitive group labeling is costly or lengthy, or it might be "necessity," for example, in medicine if definitive group labeling can only be made by postmortem examination.

We begin by looking at the simplest case of grouped multivariate data, namely, when there are only two groups.

18.2 Two-Group Multivariate Data

18.2.1 Hotelling's T^2 Test

Willerman et al. (1991) collected data on 20 male and 20 female right-handed Anglo psychology students at a large university in the United States. The subjects took three subtests of the Wechsler Adult Intelligence Scale-Revised test. The scores recorded were full-scale IQ (FSIQ), verbal IQ (VIQ), and performance IQ (PIQ). The data for the first five men and the first five women are given in Table 18.1.

TABLE 18.1
Wechsler Adult Intelligence IQ Scores for Five Men and Five Women

Subject	FSIQ	VIQ	PIQ
1	140	150	124
2	139	123	150
3	133	129	128
4	89	93	84
5	133	114	147
6	133	132	124
7	137	132	134
8	99	90	110
9	138	136	131
10	92	90	98

Note: FSIQ = Full-scale IQ; VIQ = verbal IQ; PIQ = performance IQ.

In this case interest lies in testing the hypothesis that the three-dimensional mean vectors of IQ scores are the same for men and women. The appropriate test is Hotelling's T^2 test, the multivariate analog of the independent samples t-test. The test and the assumptions on which it is based are described in Technical Section 18.1.

Technical Section 18.1: Hotelling's T^2

If there are q variables, the null hypothesis is that the means of the variables in the first population equal the means of the variables in the second population.

If $\boldsymbol{\mu}_1$ and $\boldsymbol{\mu}_2$ are the mean vectors of the two populations, the null hypothesis can be written as

$$H_0 : \boldsymbol{\mu}_1 = \boldsymbol{\mu}_2$$

The test statistic T^2 is defined as

$$T^2 = \frac{n_1 n_2}{n_1 + n_2} D^2$$

where n_1 and n_2 are the sample sizes in each group, and D^2 is the generalized distance introduced in Chapter 12, namely,

$$D^2 = (\bar{\mathbf{x}}_1 - \bar{\mathbf{x}}_2)' \mathbf{S}^{-1} (\bar{\mathbf{x}}_1 - \bar{\mathbf{x}}_2)$$

where $\bar{\mathbf{x}}_1$ and $\bar{\mathbf{x}}_2$ are the two sample mean vectors, and $\mathbf{S}$ is the estimate of the assumed common covariance matrix of the two populations, calculated from the two sample covariance matrices $\mathbf{S}_1$ and $\mathbf{S}_2$ as

$$\mathbf{S} = \frac{(n_1 - 1)\mathbf{S}_1 + (n_2 - 1)\mathbf{S}_2}{n_1 + n_2 - 2}$$

Note that the form of the test statistic in the multivariate case is very similar to that for the univariate independent samples t-test, involving a difference between "means" (here, mean vectors), and an assumed common "variance" (here, a covariance matrix). Under H_0 (and when the assumptions given below hold), the statistic F given by

$$F = \frac{(n_1 + n_2 - q - 1)T^2}{(n_1 + n_2 - 2)q}$$

has a Fisher's F-distribution with q and $n_1 + n_2 - q - 1$ degrees of freedom.

The T^2 test is based on the following assumptions:

- In each population, the variables have a multivariate normal distribution.
- The two populations have the same covariance matrix.
- The observations are independent.

Here, Hotelling's T^2 takes the value 0.27, with the corresponding F-statistic being 0.09, having 3 and 36 degrees of freedom; the associated p-value is 0.97. There is no evidence of a gender difference on the three measures of IQ.

It might be thought that the results of Hotelling's T^2 test would simply reflect those that would be obtained using a series of univariate t-tests, in the sense that if no significant differences are found by the separate t-tests, then the T^2 test will inevitably lead to acceptance of the null hypothesis that the population mean vectors are equal. On the other hand, if any significant difference is found when using the t-tests on the individual variables, then the T^2 statistic must also lead to a significant result. But, these speculations are not correct (if they were, the whole T^2 test would be a waste of time). It is entirely possible to find no significant difference for each separate t-test but a significant result for the T^2 test, and vice versa. An explanation of how this can happen in the case of two variables is provided in Technical Section 18.2.

Technical Section 18.2: Univariate and Multivariate Tests for Equality of Means of Two Variables

Suppose we have a sample of n observations on two variables x_1 and x_2, and we wish to test whether the population means of the two variables μ_1 and μ_2 are both 0. Assume that the mean and standard deviation of the x_1 observations are $\bar{x}_1$ and s_1, respectively, and of the x_2 observations, $\bar{x}_2$ and s_2. If we test separately whether each mean takes the value 0, then we would use two t-tests. For example, to test $\mu_1 = 0$ against $\mu_1 \neq 0$, the appropriate test statistic is

$$t = \frac{\bar{x}_1 - 0}{s_1/\sqrt{n}}$$

The hypothesis $\mu_1 = 0$ would be rejected at the α percent level of significance, if

$$t < -t_{100(1-\alpha/2)} \quad \text{or} \quad t > t_{100(1-\alpha/2)}$$

that is, if $\bar{x}_1$ fell outside the interval

$$\left[-\frac{s_1 t_{100(1-\alpha/2)}}{\sqrt{n}}, +\frac{s_1 t_{100(1-\alpha/2)}}{\sqrt{n}}\right]$$

where $t_{100(1-\alpha/2)}$ is the $100(1-\alpha/2)$ percent point of the t distribution with $n-1$ degrees of freedom. Thus, the hypothesis would not be rejected if $\bar{x}_1$ fell within this interval. Similarly, the hypothesis $\mu_2 = 0$ for the variable x_2 would not be rejected if the mean $\bar{x}_2$ of the x_2 observations fell within a corresponding interval with s_2 substituted for s_1.

The multivariate hypothesis $[\mu_1, \mu_2] = [0, 0]$ would therefore not be rejected if both these conditions were satisfied. If we were to plot the point $(\bar{x}_1, \bar{x}_2)$ against rectangular axes, the area within which the point could lie and the multivariate hypothesis not rejected is given by the rectangle ABCD of Figure 18.1, where AB and DC are of length $2s_1 t_{100(1-\alpha/2)}/\sqrt{n}$, while AD and BC are of length $2s_2 t_{100(1-\alpha/2)}/\sqrt{n}$.

Thus, a sample that gave the means $(\bar{x}_1, \bar{x}_2)$ represented by the point P (see Figure 18.1) would lead to acceptance of the multivariate hypothesis. Suppose, however, that the variables x_1 and x_2 are moderately highly correlated. Then all points (x_1, x_2), and hence, $(\bar{x}_1, \bar{x}_2)$ should lie reasonably close to the straight line MN through the origin marked on the diagram. Therefore, samples consistent with the multivariate hypothesis should be represented by points $(\bar{x}_1, \bar{x}_2)$ that lie within a region encompassing the line MN. When we take account of the nature of the variation of bivariate normal samples that include correlation, this region can be

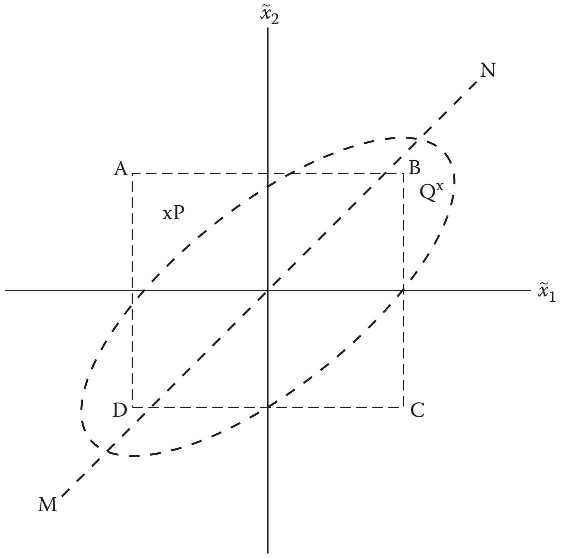


FIGURE 18.1
Why the results of univariate and multivariate tests can differ.

shown to be an ellipse such as that marked on the diagram. The point P is not consistent with this region and, in fact, *should be rejected* for this sample. Thus, the inference drawn from the two separate univariate tests conflicts with the one drawn from a single multivariate test, and it is the wrong inference.

A sample giving the $(\bar{x}_1, \bar{x}_2)$ values represented by point Q (again, see Figure 18.1) would give the other type of mistake, where the application of two separate univariate tests leads to the rejection of the null hypothesis, but the correct multivariate inference is that the hypothesis *should not be rejected*. This explanation is taken with permission from Krzanowski (2000).

18.2.2 Fisher's Linear Discriminant Function

Spicer et al. (1987), in an investigation of sudden infant death (SID) syndrome, recorded four variables for each of 16 babies who were victims of SID and for 49 control babies. The babies who died and the control babies all had a gestational age of 37 weeks or more. Part of the data is shown in Table 18.2. The factor 68 variable arises from a particular aspect of 24h recordings or electrocardiograms and respiratory movements made for each child; the SID victims and the controls were matched for age at which these recordings were made. Here, interest lies in deriving a classification rule that could use measurements of

TABLE 18.2
Part of the SIDs Data

Group	HR	BW	F68	GA
1	108.2	3000	0.321	37
1	131.1	4310	0.450	40
1	129.7	3975	0.244	40
1	142.0	3000	0.173	40
1	145.5	3940	0.304	41
2	139.7	3740	0.409	40
2	121.3	3005	0.626	38
2	131.4	4790	0.383	40
2	152.8	1890	0.432	38
2	125.6	2920	0.347	40

Note: Group = 1 for controls and 2 for SID victims; HR = heart rate (bpm); BW = birth weight (g); F68 = factor 68; GA = gestational age (weeks).

the four variables on babies to be able to identify children at risk of SID and, if possible, take appropriate action to prevent the death of the baby.

The required classification rule can be constructed using Fisher's *linear discriminant function*, and this is described in Technical Section 18.3.

Technical Section 18.3: Fisher's Linear Discriminant Function

The aim is to find a way of classifying observations into one of two known groups using a set of variables, $x_1, x_2, \dots, x_q$. Fisher's idea was to find a linear function of the variables $z = a_1x_1 + a_2x_2 + \cdots + a_qx_q$ such that the ratio of the between-group variance of z to its within-group variance is maximized. Therefore, the coefficients $\mathbf{a}' = [a_1, a_2, \dots, a_q]$ have to be chosen so that V, given by

$$V = \frac{\mathbf{a}'\mathbf{B}\mathbf{a}}{\mathbf{a}'\mathbf{S}\mathbf{a}}$$

is maximized, where **S** is the pooled within-group covariance matrix and **B** the covariance matrix of group means defined as follows:

$$\mathbf{S} = \frac{1}{n-2}\sum_{i=1}^{2}\sum_{j=1}^{n_i}\left(\mathbf{x}_{ij} - \bar{\mathbf{x}}_j\right)\left(\mathbf{x}_{ij} - \bar{\mathbf{x}}_j\right)'$$

$$\mathbf{B} = \sum_{i=1}^{2} n_i\left(\bar{\mathbf{x}}_i - \bar{\mathbf{x}}\right)\left(\bar{\mathbf{x}}_i - \bar{\mathbf{x}}\right)'$$

where $\mathbf{x}'_{ij} = [x_{ij1}, x_{ij2}, \ldots, x_{ijq}]$ represents the set of q variable values for the jth individual in group i, $\bar{x}_j$ is the mean vector of the jth group, and $\bar{\mathbf{x}}$ is the mean vector of all observations. The number of observations in group 1 is n_1, and in group 2 is n_2, with $n = n_1 + n_2$. The vector $\mathbf{a}$ that maximizes V is given by the solution of the following equation:

$$(\mathbf{B} - \lambda\mathbf{S})\mathbf{a} = \mathbf{0}$$

In the two-group situation, the single solution can be shown to be

$$\mathbf{a} = \mathbf{S}^{-1}(\bar{\mathbf{x}}_1 - \bar{\mathbf{x}}_2)$$

The allocation rule is now to allocate an individual with discriminate score z to group 1 if

$$z > \frac{\bar{z}_1 + \bar{z}_2}{2}$$

where $\bar{z}_1$ and $\bar{z}_2$ are the mean discriminant scores in each group. (We are assuming that the groups are labeled such that $\bar{z}_1 > \bar{z}_2$.)

Fisher's discriminant function also arises from assuming that, in the population, the observations in group 1 have a multivariate normal distribution with mean vector $\boldsymbol{\mu}_1$ and covariance matrix $\boldsymbol{\Sigma}$, and those in group 2 have a multivariate normal distribution with mean vector $\boldsymbol{\mu}_2$ and, again, covariance matrix $\boldsymbol{\Sigma}$. Misclassifications are minimized if an individual with vector of scores $\mathbf{x}$ is allocated to group 1 if

$$MVN(\mathbf{x}, \boldsymbol{\mu}_1, \boldsymbol{\Sigma}) > MVN(\mathbf{x}, \boldsymbol{\mu}_2, \boldsymbol{\Sigma})$$

where MVN is shorthand for the multivariate normal density function. Substituting sample mean vectors for $\boldsymbol{\mu}_1$ and $\boldsymbol{\mu}_2$ and the matrix $\mathbf{S}$ defined earlier for $\boldsymbol{\Sigma}$, we are led to the same allocation rule as that given previously. But, the derived classification rule is only valid if the prior probabilities of being in each group are assumed to be the same. If the prior probability of group 1 is π_1 and that of group 2 is π_2, then the new allocation rule becomes allocated to group 1 if

$$z > \frac{\bar{z}_1 + \bar{z}_2}{2} + \log\frac{\pi_2}{\pi_1}$$

To begin, we will use only the factor 68 variable and birth weight in applying Fisher's linear discriminant function to the SID data. We can first construct a scatterplot of the data (see Figure 18.2). The numerical details of the calculations involved are shown in Table 18.3. The discriminant function is

$$z = 0.00195 \times \text{birth weight } - 16.077 \times \text{factor 68}$$

Assuming equal prior probabilities (unrealistic, but a point we shall return to

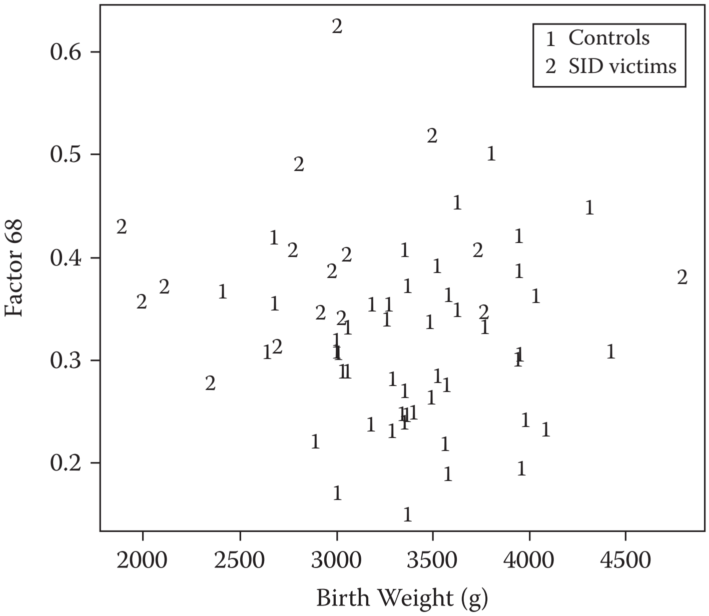


FIGURE 18.2
Scatterplot of the variables birth weight and factor 68 from the SID data.

later), the allocation rule for a new infant becomes "allocate to group 1 (little SID risk) if $z > 0.506$ (the 'cutoff' value halfway between the discriminant function means of each group), otherwise allocate to group 2 (SID risk)." The discriminant function can be shown on the scatterplot of the birth weight and factor 68 variables simply by plotting the line $z - 0.506 = 0$, that is, a line with intercept given by $0.506/a_2$ and a slope of $-a_1/a_2$, where a_1 and a_2 are the discriminant function coefficients, to give Figure 18.3. In terms of this plot, a new infant with values of the two variables leading to a position on the plot above the line would be allocated to the SID risk group, and an infant with a position below the line to the little SID risk group.

A deficiency of the derived allocation rule is that it takes no account of the prior probabilities of class membership in the population under study. Therefore, if used as a screening device for babies at risk of SID in the simple form suggested here many more infants would be considered at risk than is genuinely merited because, fortunately, SID is known to be a relatively rare condition.

A question of some importance about a discriminant function allocation rule is "how well does it perform?" One way this question could be answered is to see how many of the original sample of observations (the training set) it misclassifies. In the case of the discriminant function for the SID data derived

TABLE 18.3
Calculating Fisher's Linear Discriminant Function on SID Data Using Birth Weight and Factor 68 Variables

Group		**Controls**		**SID**	
Means		BW	F68	BW	F68
		3437.88	0.31	2964.69	0.41
Covariance		BW	F68	BW	F68
Matrix	BW	1.95e+05	3.24	5.45e+05	7.76
	F68	3.24	0.006	7.76	0.007

Pooled Covariance Matrix

	BW	F68
BW	278612.28	4.32
F68	4.32	0.006

Coefficients of Discriminant Function

BW	0.00195
F68	−16.07705

Discriminant function mean in controls: 1.6984
Discriminant function mean in SID victims: −0.6860, Cutoff value: 0.5062

Note: BW = Birth weight; F68 = factor 68.

here based on birth weight and factor 68, the results of applying it to the data from which it was calculated are

Actual Group	**Allocation Rule Group**	
	Controls	**SID**
Controls	41	8
SID	3	13

So, the percentage of misclassifications is 16.9. This method of estimating the misclassification rate is known to be optimistic in many cases. Other more realistic methods for estimating the misclassification rate are described in Everitt and Dunn (2001). (Finding Fisher's linear discriminant function based on all four variables recorded in the SID data is left as an exercise for the reader.)

Fisher's linear discriminant function is optimal when the data arise from populations having multivariate normal distributions with the same covariance matrices. When the distributions are clearly nonnormal, an alternative approach is *logistic discrimination* (see, for example, Anderson, 1972), although the results of both this and Fisher's method are likely to be very similar in most cases. When the two covariance matrices are thought to be unequal, then the linear discriminant function is no longer optimal, and a quadratic version

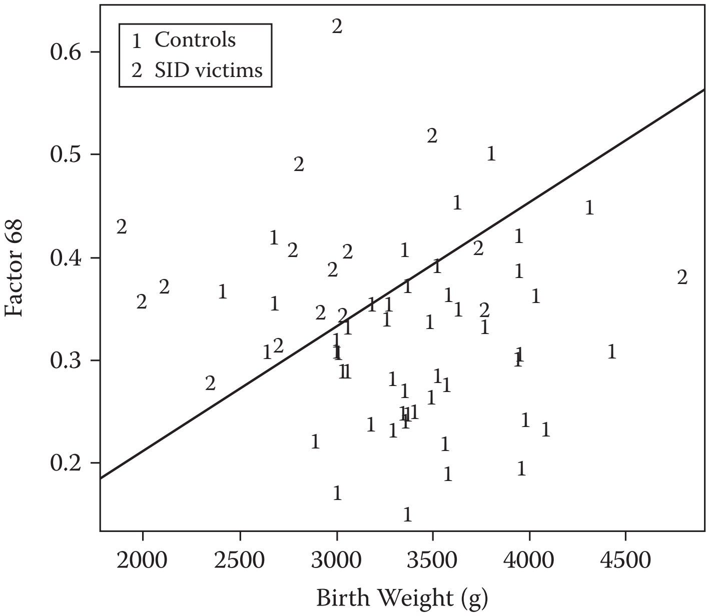


FIGURE 18.3
Scatterplot of factor 68 against birth weight for SID data, showing Fisher's linear discriminant function based on the two variables.

may be needed. Details are given in Everitt and Dunn (2001). The quadratic discriminant function has the advantage of increased flexibility compared to the linear version. There is, however, a penalty involved in the form of potential overfitting, making the derived function poor at classifying new observations. Friedman (1989) attempts to find a compromise between the data variability of quadratic discrimination and the possible bias of linear discrimination by adopting a weighted sum of the two, called regularized discriminant analysis.

18.3 More Than Two Groups

18.3.1 Multivariate Analysis of Variance (MANOVA)

Timm (2002) reports the data collected in a large study by Dr. Stanley Jacobs and Mr. Ronald Hritz at the University of Pittsburgh to investigate risk-taking behavior. Students were randomly assigned to three different direction treatments known as Arnold and Arnold (AA), Coombs (C), and Coombs with no penalty (NC) in the direction. Using the three treatment conditions, students were administered two parallel forms of a test given under low and high penalty. Part of the data is shown in Table 18.4. The question of interest here is whether the two-dimensional population mean vectors for the three groups

TABLE 18.4
Part of Data from Investigation of Risk Taking

AA		C		NC	
Low	**High**	**Low**	**High**	**Low**	**High**
8	28	46	13	50	55
18	28	26	10	57	51
8	23	47	22	62	52

Note: AA = Arnold and Arnold; C = Coombs; NC = Coombs with no penalty.

are the same. The technique to be used is MANOVA, which is an extension of univariate analysis of variance to multivariate observations. A short account of one-way MANOVA is given in Technical Section 18.4, but MANOVA can, of course, be used with more complex designs when the response is multidimensional.

Technical Section 18.4: One-Way MANOVA

We assume that we have multivariate observations of a sample of individuals from m different populations, where $m \geq 2$, and there are n_i observations sampled from population i. The linear model for observation x_{ijk}, the jth observation on variable k in group i ($k = 1, \ldots, q,\ j = 1, \ldots, n_i,\ i = 1, \ldots, m$) is

$$x_{ijk} = \mu_k + \alpha_{ik} + \varepsilon_{ijk}$$

where μ_k is a general effect for the kth variable, α_{ik} is the effect of group i on the kth variable, and ε_{ijk} is a random disturbance term. The vector $\boldsymbol{\varepsilon}'_{ij} = [\varepsilon_{ij1}, \ldots, \varepsilon_{ijq}]$ is assumed to have a multivariate normal distribution with null mean vector and covariance matrix $\mathbf{\Sigma}$, assumed to be the same in all m populations. The error terms of different individuals are assumed independent of one another.

The hypothesis of equal mean vectors in the m populations can be written as

$$H_0 : \alpha_{ik} = 0, \quad i = 1, \ldots, m,\ k = 1, \ldots, q$$

MANOVA is based on two matrices $\mathbf{H}$ and $\mathbf{E}$, the elements of which are defined as follows:

$$h_{rs} = \sum_{i=1}^{k} n_i(\bar{x}_{ir} - \bar{x}_r)(\bar{x}_{is} - \bar{x}_s), \quad r, s = 1, \ldots, q$$

$$e_{rs} = \sum_{i=1}^{k} \sum_{j=1}^{n_i} (\bar{x}_{ijr} - \bar{x}_{ir})(\bar{x}_{ijs} - \bar{x}_{is}), \quad r, s = 1, \ldots, q$$

where $\bar{x}_{ir}$ is the mean of variable r in group i, and $\bar{x}_r$ is the grand mean of variable r. The diagonal elements of $\mathbf{H}$ and $\mathbf{E}$ are, respectively, the between-groups sum of squares for each variable and the within-group sum of squares for the variable. The off-diagonal elements of $\mathbf{H}$ and $\mathbf{E}$ are the corresponding sums of cross products for pairs of variables. In the multivariate situation when $m > 2$, there is no single test statistic that is always the most powerful one for detecting all types of departures from the null hypothesis of the mean vectors of the populations. A number of different test statistics have been proposed that may lead to different conclusions when used in the same data set, although on most occasions they will not. The following are the principal test statistics for MANOVA:

a. Wilks' determinantal ratio $\Lambda = \dfrac{|\mathbf{E}|}{|\mathbf{H} + \mathbf{E}|}$
b. Roy's greatest root; the criterion is the largest eigenvalue of $\mathbf{E}^{-1}\mathbf{H}$
c. Lawley–Hotelling trace $t = \text{trace}\left(\mathbf{E}^{-1}\mathbf{H}\right)$
d. Pillai trace $v = \text{trace}[\mathbf{H}\left(\mathbf{H} + \mathbf{E}\right)^{-1}]$

Each test statistic can be converted into an approximate F-statistic that allows associated p-values to be calculated. For details, see Morrison (2005).

When there are only two groups, all four test criteria are equivalent and lead to the same F-value as Hotelling's T^2 described in Technical Section 18.1.

Prior to any formal analysis of the data from the risk-taking investigation, it is useful to look at some boxplots, and these are given in Figure 18.4. The 'Low'

TABLE 18.5
MANOVA on Data from the Risk-Taking Investigation

	Df	Pillai	approx. F	num DF	den Df	Pr(>F)
Group	1	0.866	268.323	2	83	<2.2e-16
		Wilks				
Group	1	0.134	268.323	2	83	<2.2e-16
		Hotelling-Lawley				
Group	1	6.466	268.323	2	83	<2.2e-16
		Roy				
Group	1	6.466	268.323	2	83	<2.2e-16

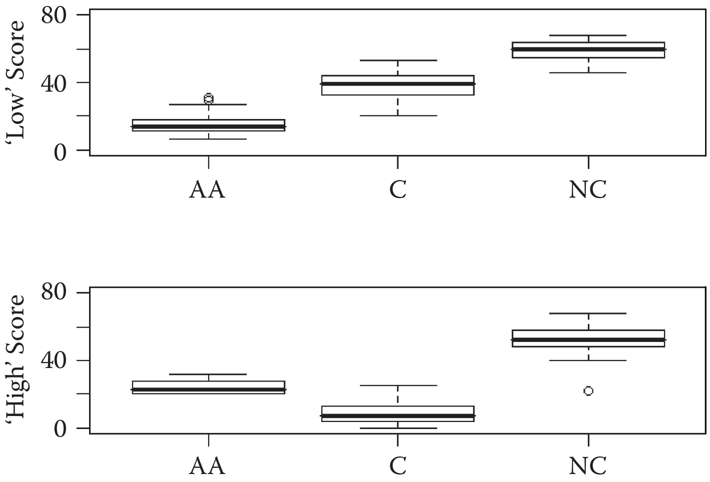


FIGURE 18.4
Boxplots for data from risk-taking experiment.

scores appear to increase across the three groups, with the group differences on the 'High' score being rather smaller. Applying MANOVA to the data from the investigation of risk taking, we get the results shown in Table 18.5. Clearly, the two-dimensional mean vectors of low and high scores differ in the three groups.

The tests applied in MANOVA assume multivariate normality for the error terms in the corresponding model. An informal assessment of this assumption can be made using the chi-square plot described in Chapter 12, applied to the residuals from fitting the one-way MANOVA model; note that the residuals in this case are each two-dimensional vectors. The plot is shown in Figure 18.5. There is some evidence of departure from the multivariate normal, but the p-values in Table 18.5 are so small that minor departures from the distributional assumption are unlikely to change the conclusions.

About three to four decades ago, MANOVA was a widely used and popular technique particularly amongst psychologists and in particular for analysing repeated measures or longitudinal data sets. But this latter use of the technique has been largely superseded by the methods described in Chapters 8 to 10. And MANOVA is perhaps now largely only of historical interest.

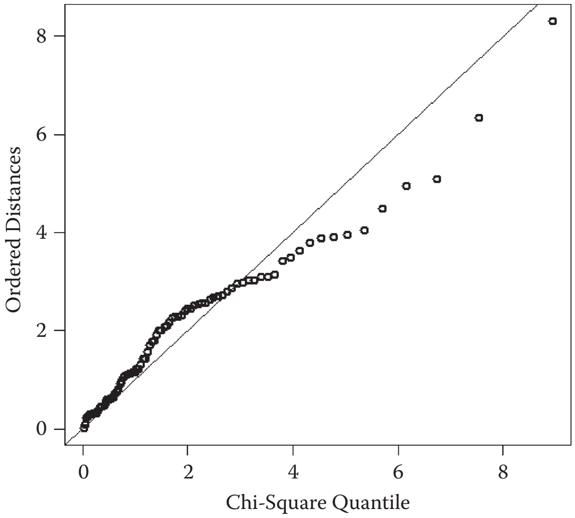


FIGURE 18.5
Chi-square plot of residuals from fitting one-way MANOVA to data from risk-taking experiment.

18.3.2 Classification Functions

In this section we will use data generated during a functional magnetic resonance imaging (fMRI) investigation. Two measures of intensity of each voxel in an image were recorded—PD and T_2. Part of the data is shown in Table 18.6. One aim of the investigation was to derive a rule for allocating each voxel in an image into one of three classes: grey matter, white matter, or cerebrospinal fluid (CSF). When more than two groups are involved, we can again derive classification functions by comparing the assumed multivariate normal densities for each group. Technical Section 18.5 explains how.

TABLE 18.6
Part of fMRI Data

Class	PD	T_2
Grey	124	58
Grey	107	44
White	142	122
White	144	148
CSF	98	45
CSF	87	34

Note: CSF = Cerebrospinal fluid.

Technical Section 18.5: Discriminant Analysis for Three Groups

Assuming that the observations in the three groups have multivariate normal densities with different means, $\boldsymbol{\mu}_1$, $\boldsymbol{\mu}_2$ and $\boldsymbol{\mu}_3$ but a common covariance matrix, $\mathbf{S}$, the allocation rule for an individual with vector of scores $\mathbf{x}$ becomes:

Allocate to group 1 if

$$MVN(\mathbf{x}, \boldsymbol{\mu}_1, \mathbf{S}) > MVN(\mathbf{x}, \boldsymbol{\mu}_2, \mathbf{S})$$

and

$$MVN(\mathbf{x}, \boldsymbol{\mu}_1, \mathbf{S}) > MVN(\mathbf{x}, \boldsymbol{\mu}_3, \mathbf{S})$$

Allocate to group 2 if

$$MVN(\mathbf{x}, \boldsymbol{\mu}_2, \mathbf{S}) > MVN(\mathbf{x}, \boldsymbol{\mu}_1, \mathbf{S})$$

and

$$MVN(\mathbf{x}, \boldsymbol{\mu}_2, \mathbf{S}) > MVN(\mathbf{x}, \boldsymbol{\mu}_3, \mathbf{S})$$

Allocate to group 3 if

$$MVN(\mathbf{x}, \boldsymbol{\mu}_3, \mathbf{S}) > MVN(\mathbf{x}, \boldsymbol{\mu}_1, \mathbf{S})$$

and

$$MVN(\mathbf{x}, \boldsymbol{\mu}_3, \mathbf{S}) > MVN(\mathbf{x}, \boldsymbol{\mu}_2, \mathbf{S})$$

This leads to sample-based allocation rules as follows:
Allocate to group 1 if $h_{12}(\mathbf{x}) > 0$ and $h_{13}(\mathbf{x}) > 0$
Allocate to group 2 if $h_{12}(\mathbf{x}) < 0$ and $h_{23}(\mathbf{x}) > 0$
Allocate to group 3 if $h_{13}(\mathbf{x}) < 0$ and $h_{23}(\mathbf{x}) < 0$
where

$$h_{ij}(\mathbf{x}) = (\bar{\mathbf{x}}_i - \bar{\mathbf{x}}_j)'\mathbf{S}^{-1}\left[\mathbf{x} - \frac{1}{2}(\bar{\mathbf{x}}_i + \bar{\mathbf{x}}_j)\right]$$

and $\bar{\mathbf{x}}_i$ and $\bar{\mathbf{x}}_j$ are group mean vectors, $\mathbf{S}$ is the sample estimate of the assumed common covariance matrix of the three groups and is given by

$$\mathbf{S} = \frac{(n_1 - 1)\mathbf{S}_1 + (n_2 - 1)\mathbf{S}_2 + (n_3 - 1)\mathbf{S}_3}{n_1 + n_2 + n_3 - 3}$$

and $\mathbf{S}_1$, $\mathbf{S}_2$, and $\mathbf{S}_3$ are the estimates of the covariance matrices of each group.

To begin, we can plot the data labeling the three classes. The plot is shown in Figure 18.6. To find the three discriminant functions, we first need to find the mean vectors and covariance matrices of each class and then the pooled

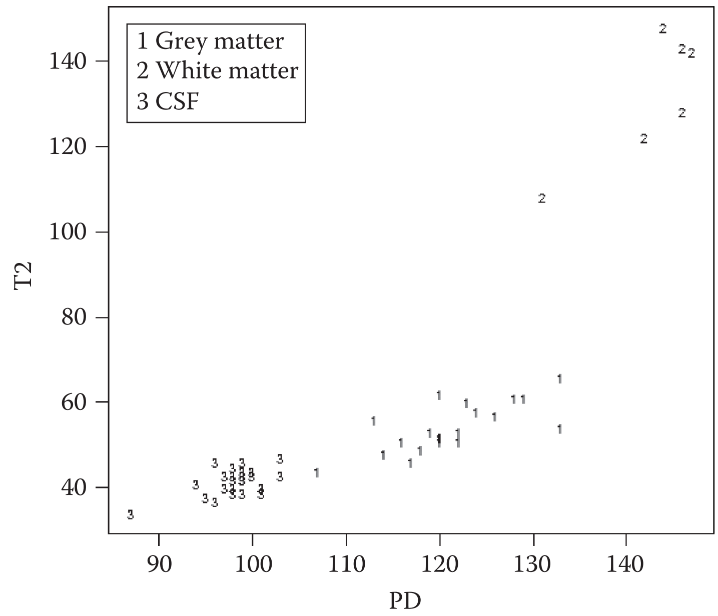


FIGURE 18.6
Scatterplot of imaging data with three classes labeled.

covariance matrix; all are shown in Table 18.7. The coefficients of each linear discriminant function and the thresholds calculated from the information in Table 18.7 are shown in Table 18.8. Each of the discriminant functions can

TABLE 18.7
Means and Covariance Matrices of Each Class in Imaging Data

	Grey Matter ($n = 20$)		**White Matter ($n = 6$)**		**CSF ($n = 24$)**	
	PD	T_2	PD	T_2	PD	T_2
Mean	121.20	54.25	142.67	131.83	98.08	41.67
			Covariance Matrix			
	PD	T_2	PD	T_2	PD	T_2
PD	42.48	26.95	35.87	74.93	10.34	5.77
T_2	26.95	33.25	74.93	233.77	5.77	9.62
			Pooled Covariance Matrix			
		PD		T_2		
PD		26.05		21.69		
T_2		21.69		43.02		

TABLE 18.8
Discriminant Functions and Thresholds for Imaging Data

	Grey Matter		**White Matter**		**CSF**	
	PD	T_2	PD	T_2	PD	T_2
Discriminant coefficients	1.17	−2.39	1.11	−0.27	−0.06	2.13
			Thresholds			
	Grey v White		Grey v CSF		White v CSF	
	−68.54		108.86		177.39	

now be shown on the scatterplot of the data using the same approach as that used for a discriminant function for two groups.

The scatterplot showing the three discriminant functions is shown in Figure 18.7. This plot would allow an investigator to classify new, unlabeled voxels, although in practice the three discriminant functions would need to be calculated from a much larger sample of previously labeled voxels.

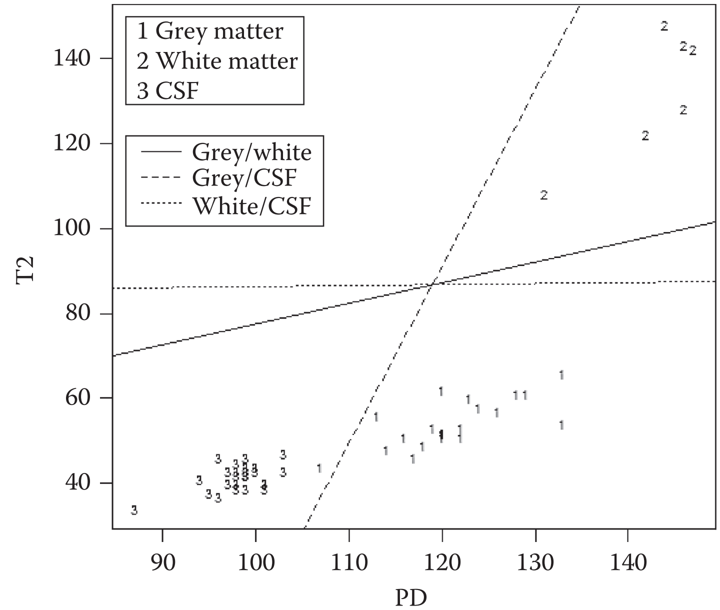


FIGURE 18.7
Scatterplot of imaging data showing the three discriminant functions.

18.4 Summary

- Grouped multivariate data frequently occur in practice.
- The appropriate method of analysis depends on the question of most interest to the investigator.
- Hotelling's T^2 test and MANOVA can be used to assess hypotheses about population mean vectors.
- Fisher's linear discriminant function can be used to construct formal classification rules for allocating new individuals into one of two a priori known groups. And similar rules can be found when there are more than two groups.
- Full details of discriminant function methods are given in Hand (2005).

18.5 Exercises

(excluded from MABS for IODS)

Part V

Dimensionality reduction techniques ("MABS for IODS")

Selected excerpts of the textbook *Multivariate Analysis for the Behavioral Sciences*, Second Edition (Vehkalahti and Everitt, 2019), produced exclusively for the students of IODS (Introduction to Open Data Science, University of Helsinki), with a permission from Chapman and Hall/CRC, London, UK.

13 Principal Components Analysis

The basic goal of principal components analysis is to describe variation in a set of correlated variables in terms of a new set of uncorrelated variables each of which is a linear combination of the original variables. The new variables are derived in decreasing order of “importance” in the sense that the first one accounts for as much as possible of the variation in the original data among all linear combinations of the original variables; then the second new variable is chosen to account for as much of the remaining variation, subject to being uncorrelated with the first new variable and so on. The new variables are the principal components and a small number of these may serve to provide a convenient summary of a set of multivariate data, useful, for example, in constructing informative graphics of the data.

14 Multidimensional Scaling and Correspondence Analysis

The concept of distance is important in multivariate analysis, for example, in assessing the structure in a scatterplot. In this chapter methods for dealing with matrices of distances between items of interest are discussed, the aim in general being to provide an informative graphic of the items, for example, a two-dimensional map. In addition an approach for representing cross tabulations of categorical data graphically will be briefly discussed.

13

Principal Components Analysis

13.1 Introduction

One of the problems with many sets of multivariate data is that there are simply too many variables to make the application of, say, some of the graphical techniques described in Chapter 2 successful in providing an informative initial assessment of the data. Further, having too many variables may cause problems for other statistical techniques that the researcher may want to apply to the data. The possible problem of too many variables is sometimes known as the curse of dimensionality. Clearly, the scatterplots, scatterplot matrices, and other graphics that might be applied to multivariate data for an initial assessment are likely to be more useful when the number of variables in the data, the dimensionality of the data, is relatively small rather than large. This brings us to *principal components analysis* (PCA), a multivariate technique with the central aim of reducing the dimensionality of a multivariate data set while retaining as much as possible of the variation present in it. This aim is achieved by transforming to a new set of variables the principal components that are uncorrelated and that are ordered, so that the first few of them account for most of the variation in all the original variables. In the best of all possible worlds, the result of a PCA would be the creation of a small number of new variables that can be used as surrogates for the originally large number of variables and, consequently, that provide a simpler basis for, say, graphing or summarizing the data and also, perhaps, when undertaking further multivariate analyses of the data.

13.2 Principal Components Analysis (PCA)

The basic goal of PCA is to describe variation in a set of correlated variables, $x_1, x_2, \dots, x_q$, in terms of a new set of uncorrelated variables, $y_1, y_2, \dots, y_q$, each of which is a linear combination of the x variables. The new variables are derived in decreasing order of "importance" in the sense that y_1 accounts for as much as possible of the variation in the original data among all linear combinations of $x_1, x_2, \dots, x_q$. Then, y_2 is chosen to account for as much as possible of the remaining variation, subject to being uncorrelated with y_1, and so on. The new variables defined by this process, $y_1, y_2, \ldots, y_q$, are the principal components. Principal components analysis was first suggested by Pearson (1901) and independently by Hotelling (1933).

The general hope of PCA is that the first few components will account for a substantial proportion of the variation in the original variables $x_1, x_2, \ldots, x_q$, and can, consequently, be used to provide a convenient lower-dimensional summary of these variables that might prove useful for a variety of reasons. Consider, for example, a set of data consisting of examination scores for several different subjects for each of a number of students. One question of interest might be how best to construct an informative index of overall examination performance. One obvious possibility would be to take the mean score for each student, although, if the possible or observed range of examination scores varied from subject to subject, it might be more sensible to weight the scores in some way before calculating the average or, alternatively, standardize the results for the separate examinations before attempting to combine them. In this way, it might be possible to spread the students out further and so obtain a better ranking. The same result could often be achieved by applying the principal components to the observed examination results and using the students' scores on the first principal component to provide a measure of examination success that maximally discriminated between them.

A further possible application for PCA arises in the field of economics, where complex data are often summarized by some kind of index number, for example, indices of prices, wage rates, cost of living, and so on. When assessing changes in prices over time, the economist will wish to allow for the fact that prices of some commodities are more variable than others or that the prices of some of the commodities are considered more important than others; in each case, the index will need to be weighted accordingly. In such examples, the first principal component can often satisfy the investigator's requirements.

However, it is not always the first principal component that is of most interest to a researcher. A taxonomist, for example, when investigating variation in morphological measurements on animals for which all the pairwise correlations are likely to be positive, will often be more concerned with the second and subsequent components since these might provide a convenient description of aspects of an animal's "shape"; this will often be of more interest to the researcher than aspects of an animal's "size," which here, because of the positive correlations, will be reflected in the first principal component. For essentially the same reasons, the first principal component derived from, say, clinical psychiatric scores on patients may only provide an index of the severity of symptoms, and it is the remaining components that will give the psychiatrist important information about the "pattern" of symptoms.

The principal components are most commonly (and properly) used as a means of constructing an informative graphical representation of the data (see examples later in the chapter) or as inputs to some other analysis. One example of the latter is provided by regression analysis; principal components may be useful here when

- There are too many explanatory variables relative to the number of observations.
- The explanatory variables are highly correlated.

Both situations lead to problems when applying regression techniques—problems that may be overcome by replacing the original explanatory variables with the first few principal component variables derived from them. An example will be given later, and other applications of the technique are described in Rencher and Christensen (2012).

A further example when the results from a PCA may be useful is in the application of multivariate analysis of variance (see Chapter 18), when there are too many original variables to ensure that the technique can be used with reasonable power. In such cases, the first few principal components might be used to provide a smaller number of variables for analysis.

In the behavioral sciences, particularly psychology, the principal components are often considered an end in themselves, and researchers may then try to interpret them in a similar fashion to the factors in an exploratory factor analysis (see Chapter 15). We shall make some comments about this practice later in that chapter.

13.3 Finding the Sample Principal Components

PCA is overwhelmingly an exploratory technique for multivariate data. Although there are inferential methods available for using the sample principal components derived from a random sample of individuals from a population to test hypotheses about population principal components (see Jolliffe, 2002), they are very rarely to be seen in the accounts of PCA analysis that appear in the literature. Quintessentially, PCA is an aid in helping us understand the sample data. We use this observation as the rationale for describing only sample principal components in this chapter.

The first principal component of the observations is that linear combination of the original variables whose sample variance is the greatest among all possible such linear combinations. The second principal component is defined as that linear combination of the original variables that accounts for a maximal proportion of the remaining variances, subject to being uncorrelated with the first principal component. Subsequent components are defined similarly. The question now arises as to how the coefficients specifying the linear combinations of the original variables defining each component are found. This question is answered in Technical Section 13.1.

Technical Section 13.1: Extracting Principal Components

The first principal component of the observations, y_1, is the linear combination

$$y_1 = a_{11}x_1 + a_{12}x_2 + \cdots + a_{1q}x_q$$

whose sample variance is the greatest among all such linear combinations. Because the variance of y_1 could be increased without limit simply by increasing the values of the coefficients $a_{11}, a_{12}, \ldots, a_{1q}$ (which we will write as the vector $\mathbf{a}_1$), a restriction must be placed on these coefficients. As we shall see later, a sensible constraint is to require that the sum of squares of the coefficients should take the value 1, although other constraints are possible, and any multiple of the vector $\mathbf{a}_1$ produces basically the same component. To find the coefficients defining the first principal component, we need to choose the elements of the vector $\mathbf{a}_1$ so as to maximize the variance of y_1 subject to the sum-of-squares constraint, which can be written as $\mathbf{a}_1'\mathbf{a}_1 = 1$. The sample variance of y_1, which is a linear function of the x variables, is given by (see Chapter 12)

$$\text{var}(y_1) = \mathbf{a}_1'\mathbf{S}\mathbf{a}_1$$

where $\mathbf{S}$ is the $q \times q$ sample covariance matrix of the x variables. To maximize a function of several variables subject to one or more constraints, the method of Lagrange multipliers is used. Full algebraic details are given in Morrison (1990) and Jolliffe (2002), and we will not give them here. (The algebra of an example with $q = 2$ is, however, given in Section 13.5.) We simply state that the Lagrange multiplier approach leads to the solution that $\mathbf{a}_1$ is what is called an *eigenvector* or *characteristic vector* of the sample covariance matrix $\mathbf{S}$, and that it is the eigenvector corresponding to the largest of what are called the *eigenvalues* or *characteristic roots* of $\mathbf{S}$. (Eigenvalues of $\mathbf{S}$ and the corresponding eigenvectors are found by numerical algorithms, the details of which are not necessary to know to understand PCA.)

The second principal component y_2 is defined to be the linear combination

$$y_2 = a_{21}x_1 + a_{22}x_2 + \cdots + a_{2q}x_q$$

that is,

$$y_2 = \mathbf{a}_2'\mathbf{x}, \text{ where } \mathbf{a}' = [a_{21}, a_{22}, \ldots, a_{2q}] \text{ and } \mathbf{x}' = [x_1, x_2, \ldots, x_q]$$

which has the greatest variance subject to the following two conditions:

$$\mathbf{a}_2'\mathbf{a}_2 = 1$$
$$\mathbf{a}_2'\mathbf{a}_1 = 0$$

(The second condition specifies that y_1 and y_2 are uncorrelated).

Similarly, the jth principal component is the linear combination $y_j = \mathbf{a}_j'\mathbf{x}$, which has the greatest variance subject to the conditions

$$\begin{aligned} \mathbf{a}_j'\mathbf{a}_j &= 1 \\ \mathbf{a}_j'\mathbf{a}_i &= 0 \qquad (i < j) \end{aligned}$$

Application of the Lagrange multiplier technique demonstrates that the vector of coefficients defining the jth principal component, that is, $\mathbf{a}_j$, is the eigenvector of $\mathbf{S}$ associated with its jth largest eigenvalue. If the q eigenvalues of $\mathbf{S}$ are denoted by $\lambda_1, \lambda_2, \ldots, \lambda_q$, then by requiring that $\mathbf{a}_i'\mathbf{a}_i = 1$, it can be shown that the variance of the ith principal component is given by λ_i. The total variance of the q principal components will equal the total variance of the original variables so that

$$\sum_{i=1}^{q} \lambda_i = s_1^2 + s_2^2 + \cdots + s_q^2$$

where s_i^2 is the sample variance of x_i. We can write this more concisely as

$$\sum_{i=1}^{q} \lambda_i = \text{trace}(\mathbf{S})$$

Consequently, the jth principal component accounts for a proportion of the total variation of the original data, where

$$P_j = \frac{\lambda_j}{\text{trace}(\mathbf{S})}$$

The first m principal components, where $m < q$, account for a proportion of the total variation in the original data, where

$$P^{(m)} = \frac{\sum_{i=1}^{m} \lambda_i}{\text{trace}(\mathbf{S})}$$

In geometrical terms, it is easy to show that the first principal component defines the line of best fit (in the least-squares sense) to the q-dimensional observations in the sample. These observations may therefore be represented in one dimension by taking their projection onto this line, that is, finding their first principal component score. If the observations happen to be collinear in q dimensions, this representation would completely account for the variation in the data, and the sample covariance matrix would have only one nonzero eigenvalue. In practice, of course, such collinearity is extremely unlikely, and an improved representation would be given by projecting the q-dimensional observations onto the space of the best fit, this being defined by the first two principal components. Similarly, the first m components give the best fit in m dimensions. If the observations fit exactly into a space of m dimensions, it would be indicated by the presence of $q - m$ zero eigenvalues of the covariance matrix. This would imply the presence of $q - m$ linear relationships between the variables. Such constraints are sometimes referred to as *structural relationships*. In practice, in the vast majority of applications of PCA, all the eigenvalues of the covariance matrix will be nonzero.

13.4 Should Principal Components Be Extracted from the Covariance or the Correlation Matrix?

The account of principal components given above has them extracted from the covariance matrix of the data. However, imagine a set of multivariate data in which the variables $x_1, x_2, \ldots, x_q$ are of completely different types, for example, length, temperature, blood pressure, anxiety rating, etc. With such a data set, the structure of the principal components derived from the covariance matrix will depend upon the essentially arbitrary choice of units of measurement; for example, changing lengths from centimeters to inches will alter the derived components. Additionally, if there are large differences between the variances of the original variables, then the ones whose variances are the largest will tend to dominate the early components. This difficulty is overcome in practice by extracting the components from the correlation matrix $\mathbf{R}$. Extracting the components as the eigenvectors of $\mathbf{R}$ is equivalent to calculating the principal components from the original variables after each has been standardized to have unit variance. It should be noted, however, that there is rarely any simple correspondence between the components derived from $\mathbf{S}$ and those derived from $\mathbf{R}$. In addition, choosing to work with $\mathbf{R}$ rather than $\mathbf{S}$ involves a definite, but possibly arbitrary, decision to make the variables "equally important."

To demonstrate how the principal components of the covariance matrix of a data set can differ from the components extracted from the data's correlation

TABLE 13.1
Correlations of Blood Chemistry Variables and Their Standard Deviations

	rBlood	**Plate**	**wBlood**	**Neut.**	**Lymph**	**Bilir.**	**Sodium**	**Potass.**
rBlood	1.000	0.290	0.202	−0.055	−0.105	−0.252	−0.229	0.058
Plate	0.290	1.000	0.415	0.285	−0.376	−0.349	−0.164	−0.129
wBlood	0.202	0.415	1.000	0.419	−0.521	−0.441	−0.145	−0.076
Neut.	−0.055	0.285	0.419	1.000	−0.877	−0.076	0.023	−0.131
Lymph	−0.105	−0.376	−0.521	−0.877	1.000	0.206	0.034	0.151
Bilir.	−0.252	−0.349	−0.441	−0.076	0.206	1.000	0.192	0.077
Sodium	−0.229	−0.164	−0.145	0.023	0.034	0.192	1.000	0.423
Potass.	0.058	−0.129	−0.076	−0.131	0.151	0.077	0.423	1.000
Std Dev	0.371	41.253	1.935	0.077	0.071	4.037	2.732	0.297

matrix, we will use the example given in Jolliffe (2002). The data in this example consist of eight blood chemistry variables measured on 72 patients in a clinical trial. The correlation matrix of the data, together with the standard deviations of each of the eight variables, is given in Table 13.1; there are considerable differences between these standard deviations. We can apply PCA to both the covariance and correlation matrix of the data (the covariance matrix is not given, but it can be easily calculated from the correlation matrix and the standard deviations—see Chapter 12). The details of the principal components of the covariance matrix are given in Table 13.2, and those of the correlation matrix in Table 13.3 (in both tables, very small values have been set to 0).

TABLE 13.2
Principal Components of the Covariance Matrix of Blood Chemistry Data

	Variances, etc. of the Components							
	Comp.1	**Comp.2**	**Comp.3**	**Comp.4**	**Comp.5**	**Comp.6**	**Comp.7**	**Comp.8**
Variance	1704.68	15.06	6.98	2.64	0.13	0.07	0.00	0.00
Proportion of variance	0.986	0.0087	0.00404	0.00153	0.000	0.000	0.000	0.000
Cumulative proportion	0.986	0.9943	0.99836	0.99989	1.000	1.000	1.000	1.000
	Component Loadings							
rBlood	0.000	0.000	0.000	0.000	0.943	0.329	0.000	0.000
Plate	−0.999	0.000	0.000	0.000	0.000	0.000	0.000	0.000
wBlood	0.000	−0.192	0.000	−0.981	0.000	0.000	0.000	0.000
Neut.	0.000	0.000	0.000	0.000	0.000	0.000	0.758	0.650
Lymph	0.000	0.000	0.000	0.000	0.000	0.000	−0.649	0.760
Bilir.	0.000	0.961	0.195	−0.191	0.000	0.000	0.000	0.000
Sodium	0.000	0.193	−0.979	0.000	0.000	0.000	0.000	0.000
Potass.	0.000	0.000	0.000	0.000	0.329	−0.942	0.000	0.000

TABLE 13.3
Principal Components of the Correlation Matrix of Blood Chemistry Data

	Variances, etc. of the Components							
	Comp.1	**Comp.2**	**Comp.3**	**Comp.4**	**Comp.5**	**Comp.6**	**Comp.7**	**Comp.8**
Variance	2.792	1.532	1.249	0.778	0.622	0.489	0.436	0.102
Proportion of variance	0.349	0.191	0.156	0.0973	0.0777	0.0611	0.0545	0.0128
Cumulative proportion	0.349	0.540	0.697	0.7939	0.8716	0.9327	0.9872	1.0000
	Component Loadings							
rBlood	−0.194	0.417	0.400	0.652	0.175	−0.363	0.176	0.102
Plate	−0.400	0.154	0.168	0.000	−0.848	0.230	−0.110	0.000
wBlood	−0.459	0.000	0.168	−0.274	0.251	0.403	0.677	0.000
Neut.	−0.430	−0.472	−0.171	0.169	0.118	0.000	−0.237	0.678
Lymph	0.494	0.360	0.000	−0.180	−0.139	0.136	0.157	0.724
Bilir.	0.319	−0.320	−0.277	0.633	−0.162	0.384	0.377	0.000
Sodium	0.177	−0.535	0.410	−0.163	−0.299	−0.513	0.367	0.000
Potass.	0.171	−0.245	0.709	0.000	0.198	0.469	−0.376	0.000

Examining the results in Tables 13.2 and 13.3, we see that each of the principal components of the covariance matrix is largely dominated by a single variable, whereas those for the correlation matrix have moderate-sized coefficients on several of the variables. In addition, the first component of the covariance matrix accounts for almost 99% of the total variance of the observed variables. The components of the covariance matrix are completely dominated by the fact that the variance of the plate variable is 100 times larger than the variance of any of the other seven variables. Consequently, the principal components from the covariance matrix simply reflect the order of sizes of the variances of the observed variables. The results from the correlation matrix tell us, in particular, that a weighted contrast of the first four and last four variables is the linear function with the largest variance. This example illustrates that, when variables are on very different scales or have very different variances, a PCA of the data should be performed on the correlation matrix, not on the covariance matrix.

13.5 Principal Components of Bivariate Data with Correlation Coefficient *r*

Before we move on to look at some practical examples of the application of PCA, it will be helpful to look in a little more detail at the mathematics of the method in one very simple case. We will do this in Technical Section 13.2, using bivariate data in which the two variables x_1 and x_2 have correlation coefficient r.

Technical Section 13.2: Principal Components of Bivariate Data

Suppose we have just two variables x_1 and x_2, measured on a sample of individuals, with sample correlation matrix given by

$$\mathbf{R} = \begin{bmatrix} 1.0 & r \\ r & 1.0 \end{bmatrix}$$

In order to find the principal components of the data, we need to find the eigenvalues and eigenvectors of $\mathbf{R}$. The eigenvalues are roots of the equation

$$|\mathbf{R} - \lambda \mathbf{I}| = 0$$

where the vertical lines indicate the determinant of the matrix enclosed by them. This leads to the following quadratic equation in λ:

$$(1 - \lambda)^2 - r^2 = 0$$

which has roots (eigenvalues) $\lambda_1 = 1+r$, $\lambda_2 = 1-r$. The first component has variance $1+r$, and the second has variance $1-r$. Note that the sum of the eigenvalues is 2, equal to trace($\mathbf{R}$), that is, the sum of the elements on the main diagonal. The eigenvector corresponding to λ_1 is obtained by solving the equation

$$\mathbf{R}\mathbf{a}_1 = \lambda_1 \mathbf{a}_1$$

This leads to the equations

$$\begin{aligned} a_{11} + r a_{12} &= (1+r)a_{11} \\ r a_{11} + a_{12} &= (1+r)a_{12} \end{aligned}$$

The two equations are identical, and both reduce to $a_{11} = a_{12}$. If we now introduce the normalization constraint $\mathbf{a}_1'\mathbf{a}_1 = 1$, we find that

$$a_{11} = a_{12} = \frac{1}{\sqrt{2}}$$

Similarly, we find the elements of the second eigenvector as $a_{21} = 1/\sqrt{2}$ and $a_{22} = -1/\sqrt{2}$. The two principal components are then given by

$$y_1 = \frac{1}{\sqrt{2}}(x_1 + x_2)$$

and

$$y_2 = \frac{1}{\sqrt{2}}(x_1 - x_2)$$

Notice that if $r < 0$, the order of the eigenvalues, and hence that of the principal components, is reversed; if $r = 0$, the eigenvalues are both equal to 1, and any two solutions at right angles could be chosen to represent the two components.

Three further points:

- There is an arbitrary sign in the choice of the elements of $\mathbf{a}_i$; it is customary to choose a_{i1} to be positive.
- The components do not depend on r, although the proportion of variance explained by each does change with r. As r tends to 1, the proportion of variance accounted for by y_1, namely, $(1+r)/2$, also tends to 1.
- When $r = 1$ the points all lie on a straight line, and the variation in the data is unidimensional.

13.6 Rescaling the Principal Components

The coefficients defining the principal components derived as described in Section 13.5 are often rescaled so that they are correlations or covariances between the original variables and the derived components. The rescaled coefficients are often more useful in interpreting a PCA. The covariance of variable x_i with component y_j is given by

$$\text{Cov}\left(x_i, y_j\right) = \lambda_j a_{ji}$$

The correlation of variable x_i with component y_j is therefore

$$r_{x_i,y_j} = \frac{\lambda_j a_{ji}}{\sqrt{\text{Var}\left(x_i\right)\text{Var}\left(y_j\right)}} = \frac{\lambda_j a_{ji}}{s_i\sqrt{\lambda_j}} = \frac{a_{ji}\sqrt{\lambda_j}}{s_i}$$

If the components are extracted from the correlation matrix rather than the covariance matrix, the correlation between variable and component becomes

$$r_{x_i,y_j} = a_{ji}\sqrt{\lambda_j}$$

because in this case the standard deviation s_i is 1. (Although for convenience we have used the same nomenclature for the eigenvalues and the eigenvectors extracted from the covariance matrix or the correlation matrix, they will, of course, not be equal.)

The rescaled coefficients from a PCA of a correlation matrix are analogous to factor loadings as we shall see in Chapter 15. It is often these rescaled coefficients that are presented as the results of a PCA and used in interpretation.

13.7 How the Principal Components Predict the Observed Covariance Matrix

In Technical Section 13.3, we will look at how the principal components reproduce the observed covariance or correlation matrix from which they were extracted.

Technical Section 13.3: How Principal Components Reproduce the Sample Covariance Matrix

To begin, let the initial vectors $\mathbf{a}_1, \mathbf{a}_2, \ldots, \mathbf{a}_q$ that define the principal components be used to form a $q \times q$ matrix $\mathbf{A} = [\mathbf{a}_1, \ldots, \mathbf{a}_q]$; these are vectors extracted from the covariance matrix $\mathbf{S}$ and scaled so that

$\mathbf{a}_i'\mathbf{a}_i = 1$. Arrange the eigenvalues $\lambda_1, \ldots, \lambda_q$ along the main diagonal of a diagonal matrix $\mathbf{\Lambda}$. Then, it can be shown that the covariance matrix of the observed variables $x_1, x_2, \ldots, x_q$ is given by

$$\mathbf{S} = \mathbf{A}\mathbf{\Lambda}\mathbf{A}'$$

Rescaling the vectors $\mathbf{a}_1, \mathbf{a}_2, \ldots, \mathbf{a}_q$ so that the sum of squares of their elements is equal to the corresponding eigenvalue, that is, calculating $\mathbf{a}_i^* = \lambda_i^{1/2}\mathbf{a}_i$, allows $\mathbf{S}$ to be written more simply as

$$\mathbf{S} = \mathbf{A}^*(\mathbf{A}^*)'$$

where $\mathbf{A}^* = \left[\mathbf{a}_1^*, \ldots, \mathbf{a}_q^*\right]$

If the matrix $\mathbf{A}^*{}_m$ is formed from, say, the first m components rather than from all q, then $\mathbf{A}^*{}_m(\mathbf{A}^*{}_m)'$ gives the predicted value of $\mathbf{S}$ based on these m components. It is often useful to calculate the predicted value based on the number of components considered to adequately describe the data. How this number might be chosen is considered in the next section.

13.8 Choosing the Number of Components

As described earlier, PCA is seen to be a technique for transforming a set of observed variables into a new set of variables that are uncorrelated with one another. The variation in the original q variables is only completely accounted for by all q principal components. The usefulness of these transformed variables, however, stems from their property of accounting for the variance in decreasing proportions. The first component, for example, accounts for the maximum amount of variation possible for any linear combination of the original variables. But, how useful is this artificial variate constructed from the observed variables? To answer this question, we would first need to know the proportion of the total variance of the original variables for which it accounted. If, for example, 80% of the variation in a multivariate data set involving six variables could be accounted for by a simple weighted average of the variable values, then almost all the variation can be expressed along a single continuum rather than in six-dimensional space. The PCA would have provided a highly parsimonious summary (reducing the dimensionality of the data from six to one) that might be useful in later analysis.

So, the question we need to ask is how many components are needed to provide an adequate summary of a given data set? A number of informal and more formal techniques are available. Here we shall concentrate on the former; examples of the use of formal inferential methods are given in Jolliffe (2002) and Rencher and Christensen (2012).

The most common of the relatively ad hoc procedures that have been suggested for deciding on the number of components to retain are the following:

- Retain just enough components to explain some specified, large percentage of the total variation of the original variables. Values between 70% and 90% are usually suggested, although smaller values might be appropriate as q or n, the sample size, increases.

- Exclude those principal components whose eigenvalues are less than the average, that is, $\sum_{i=1}^{q} \lambda_i / q$. Since $\sum_{i=1}^{q} \lambda_i = \text{trace}(\mathbf{S})$, the average eigenvalue is also the average variance of the original variables. This method then retains those components that account for more variance than the average for the observed variables.

- When the principal components are extracted from the correlation matrix, $\text{trace}(\mathbf{R}) = q$, and the average variance is, therefore, 1; so, applying the rule in the previous bullet point, components with eigenvalues less than 1 will be excluded. This rule was originally suggested by Kaiser (1958), but Jolliffe (1972), on the basis of a number of simulation studies, proposed that a more appropriate procedure would be to exclude components extracted from a correlation matrix whose associated eigenvalues are less than 0.7.

- Cattell (1965) suggested examination of the plot of λ_i against i, the so-called *scree diagram*. The number of components selected is the value of i corresponding to an "elbow" in the curve, that is, a change of slope from "steep" to "shallow." In fact, Cattell was more specific than this; he recommended looking for a point on the plot beyond which the scree diagram defines a more or less straight line, not necessarily horizontal. The first point on the straight line is then taken as the last component to be retained. Further, it should also be remembered that Cattell suggested the scree diagram in the context of factor analysis rather than as applied to PCA.

- A modification of the scree diagram described by Jolliffe (1989) is the log-eigenvalue diagram consisting of a plot of $\log(\lambda_i)$ against i.

Returning to the results of the PCA of the correlation matrix of the blood chemistry data given in Section 13.4, we find that the first four components account for nearly 80% of the total variance, but it takes a further two components to push this figure up to 90%. A cutoff of 1 for the eigenvalues leads to retaining three components, and with a cutoff of 0.7, four components are kept. Figure 13.1 shows the scree diagram and the log-eigenvalue diagram for the data. The former plot may suggest four components, although this is fairly subjective, and the latter seems to be of little help here because it appears to indicate retaining seven components, which is hardly much of a dimensionality reduction. The example illustrates that the proposed methods for deciding how many components to keep can (and often do) lead to different conclusions.

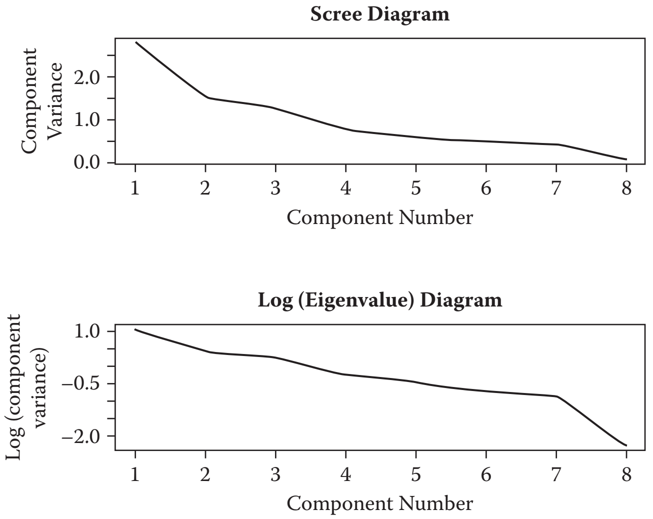


FIGURE 13.1
Scree diagram and log-eigenvalue diagram for the principal components of the correlation matrix of the blood chemistry data.

13.9 Calculating Principal Component Scores

If we decide that we need, say, m principal components to adequately represent our data (using one or other of the methods described in the previous section), then we will generally wish to calculate the scores on each of these components for each individual in our sample. How we do this is described in Technical Section 13.4.

Technical Section 13.4: Calculating Principal Component Scores

First, let us assume that we have derived the components from the covariance matrix **S**. The m principal component scores for individual i with original $q \times 1$ vector of variable values x_i are obtained as

$$\begin{aligned} y_{i1} &= \mathbf{a}_1'\mathbf{x}_i \\ y_{i2} &= \mathbf{a}_2'\mathbf{x}_i \\ &\vdots \\ y_{im} &= \mathbf{a}_m'\mathbf{x}_i \end{aligned}$$

If the components are derived from the correlation matrix, then $\mathbf{x}_i$ would contain the ith individual's standardized scores for each variable.

The principal component scores calculated as shown here have variances equal to λ_j for $j = 1, \dots, m$. Many investigators might prefer to have scores with means equal to 0 and variances equal to 1. Such scores can be found as follows:

$$\mathbf{z} = \mathbf{\Lambda}_m^{-1}\mathbf{A}_m'\mathbf{x}$$

where $\mathbf{\Lambda}_m$ is an $m \times m$ diagonal matrix with $\lambda_1, \lambda_2, \dots, \lambda_m$ on the main diagonal, $\mathbf{A}_m = [\mathbf{a}_1, \dots, \mathbf{a}_m]$, and $\mathbf{x}$ is the $q \times 1$ vector of standardized scores. We should note here that the first m principal component scores are the same whether we retain all possible q components or just the first m. As we shall see in Chapter 15, this is not the case with the calculation of factor scores.

13.10 Some Examples of the Application of PCA

In this section, we will look at the application of PCA to a number of data sets, beginning with one involving only two variables as this allows us to illustrate graphically an important point about this type of analysis.

13.10.1 Head Size of Brothers

The data in Table 13.4 give the head lengths (in millimeters) for each of the first two adult sons in 25 families. The mean vector and covariance matrix of the data are

$$\bar{\mathbf{x}}' = [185.72, 183.84] \quad \mathbf{S} = \begin{bmatrix} 95.29 & 69.66 \\ 69.66 & 100.81 \end{bmatrix}$$

The principal components of these data extracted from their covariance matrix are

$$y_1 = 0.693x_1 + 0.721x_2 \quad y_2 = -0.721x_1 + 0.693x_2$$

with variances 167.77 and 28.33. The first principal component accounts for a proportion $167.77/(167.77 + 28.33) = 0.86$ of the total variance in the original variables. Note that the total variance of the principal components is 196.10, which, as expected, is equal to the total variance of the original variables found by adding the relevant terms in the covariance matrix above, that is, $95.29 + 100.81 = 196.10$.

How should the two derived components be interpreted? The first component is essentially the sum of the head lengths of the two sons, and the

TABLE 13.4
Head Lengths (in Millimeters) of First and Second Sons of 25 Families

Family	**First Son**	**Second Son**
1	191	179
2	195	201
3	181	185
4	183	188
5	176	171
6	208	192
7	189	190
8	197	189
9	188	197
10	192	187
11	179	186
12	183	174
13	174	185
14	190	195
15	188	187
16	163	161
17	195	183
18	186	173
19	181	182
20	175	165
21	192	185
22	174	178
23	176	176
24	197	200
25	190	187

second component is the difference in head lengths. Perhaps we can label the first component "size" and the second component "shape," but see the next subsection for some comments about trying to give principal components such labels.

To calculate an individual's score on a component, we simply multiply the variable values, subtract the appropriate mean by the loading for the variable, and add these values over all variables. We can illustrate this calculation using the data for the first family, in which the head length of the first son is 191 mm and the second son, 179 mm. The score for this family on the first principal component is calculated as

$$0.693 \times (191 - 185.72) + 0.721 \times (179 - 183.84) = 0.169$$

and on the second component the score is

$$-0.721 \times (191 - 185.72) + 0.693 \times (179 - 183.84) = -7.61$$

The variance of the first principal component scores will be 167.77, and that of the second principal component scores will be 28.33.

We can plot the data showing the axes corresponding to the principal components. The first axis passes through the mean of the data and has a slope 0.721/0.693, and the second axis also passes through the mean and has a slope −0.693/0.721. The plot is shown in Figure 13.2. This example illustrates that a PCA is essentially simply a rotation of the axes of the multivariate data scatter. Further, we can also plot the principal component scores to give Figure 13.3. (Note that in this figure, the range of the x-axis and the range of the y-axis have been made the same so that the larger variance of the first principal component is clearly shown.)

We can use the PCA of the head size data to demonstrate how the principal components reproduce the observed covariance matrix. We first need to rescale the principal components we have at this point by multiplying them by the square roots of their respective variances to give the new components:

$$y_1 = 12.952[0.693x_1 + 0.721x_2], \quad \text{that is , } \; y_1 = 8.976x_1 + 9.338x_2$$

and

$$y_2 = 5.323[-0.721x_1 + 0.693x_2], \quad \text{that is , } \; y_2 = -3.837x_1 + 3.688x_2$$

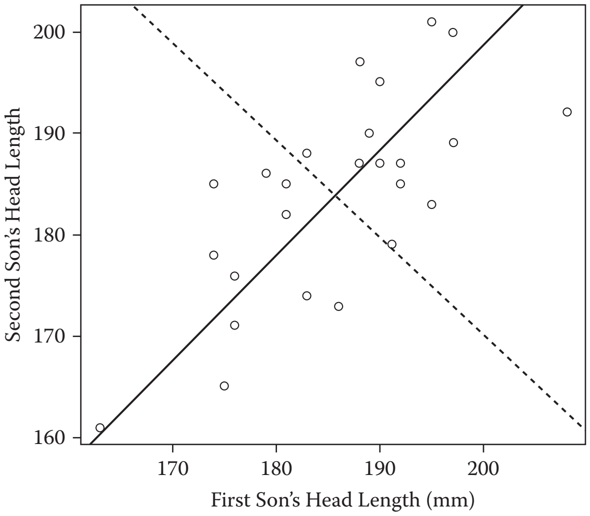


FIGURE 13.2
Head lengths of first and second sons of 25 families, showing axes corresponding to the principal components of the sample covariance matrix of the data.

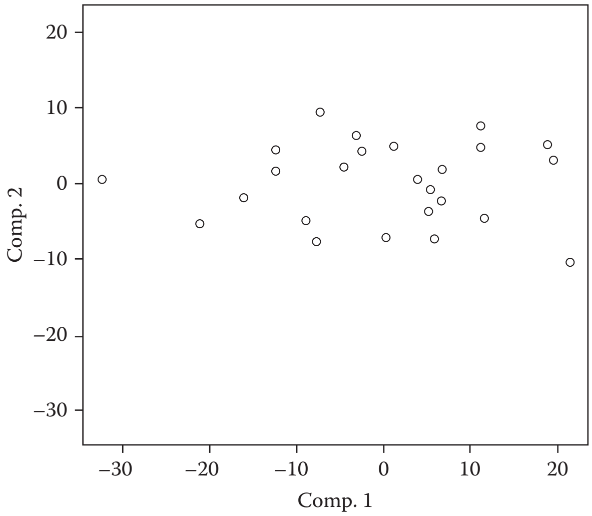


FIGURE 13.3
Plot of the first two principal components score for the head size data.

leading to the matrix $\mathbf{A}^*{}_2$ as defined in Section 13.7:

$$\mathbf{A}^*{}_2 = \begin{bmatrix} 8.976 & -3.837 \\ 9.338 & 3.688 \end{bmatrix}$$

Multiplying this matrix by its transpose should recreate the covariance matrix of the head length data; performing the matrix multiplication shows that it does recreate $\mathbf{S}$:

$$\mathbf{A}^*{}_2(\mathbf{A}^*{}_2)' = \begin{bmatrix} 95.29 & 69.66 \\ 69.66 & 100.81 \end{bmatrix}$$

As an exercise, readers might like to find the predicted covariance matrix using only the first component.

The head size example has been useful for discussing some aspects of PCA, but it is not, of course, typical of multivariate data sets encountered in behavioral research, where many more than two variables will be recorded for each individual in a study. In the following two subsections, we consider some more realistic examples.

13.10.2 Crime Rates in the United States

The *Statistical Abstract of the USA* (1988) gives rates of different types of crime per 100,000 residents of 50 states of the United States plus the District of Columbia for the year 1986. The data for the first five states are given

TABLE 13.5
Crime Rates in the United States

State	Murder	Rape	Robbery	Assault	Burglary	Theft	Vehicle
ME	2.0	14.8	28	102	803	2347	164
NH	2.2	21.5	24	92	755	2208	228
VT	2.0	21.8	22	103	949	2697	181
MA	3.6	29.7	193	331	1071	2189	906
RI	3.5	21.4	119	192	1294	2568	705

in Table 13.5. We shall use PCA to explore these data, but to start, it will be useful to look at the scatterplot matrix of the seven types of crime, and this is given in Figure 13.4. The plot shows that the relationships between crime rates are of varying strengths and that there are a number of outlying states in some of the panels, for example, the one for rape and murder rates. We shall ignore the outlier problem in the following analysis, but readers are encouraged to see how the results that follow are altered if the outliers are removed (see Exercise 13.1). In this example, the variables are all on the same scale, crimes per 100,000 of the resident population of a state, but if we look at the variances of each crime rate,

Murder	Rape	Robbery	Assault	Burglary	Theft	Vehicle
23.20	212.31	18993.37	22004.31	177912.83	582812.84	50007.37

we see that they are very different, and the results from a PCA on the unstandardized variables would be swamped by those variables with the largest variances. Consequently, we will apply the analysis to the standardized variables, that is, components will be extracted from the correlation rather than the covariance matrix.

The results of the PCA on the crime rate data are shown in Table 13.6. A scree plot of variances of principal components is shown in Figure 13.5. Only the variance of the first component is greater than 1, although that of the second component is very close to 1. The scree plot suggests that perhaps two components might be adequate to describe these data. Many users of PCA search for an interpretation of the derived components that allow them to be "labeled" in some sense. This requires examining the coefficients defining each component; in Table 13.6, the coefficients are scaled so that their sums of squares equal 1; "—" indicates near-zero values. (Remember also that the signs of the coefficients are arbitrary in the sense that the minus signs and positive signs could be reversed without altering the structure or the interpretation of the components.) Examining the coefficients defining the principal components in Table 13.6, we see that the first component might be regarded as some index of overall crime rate in a state, with states that have larger crime

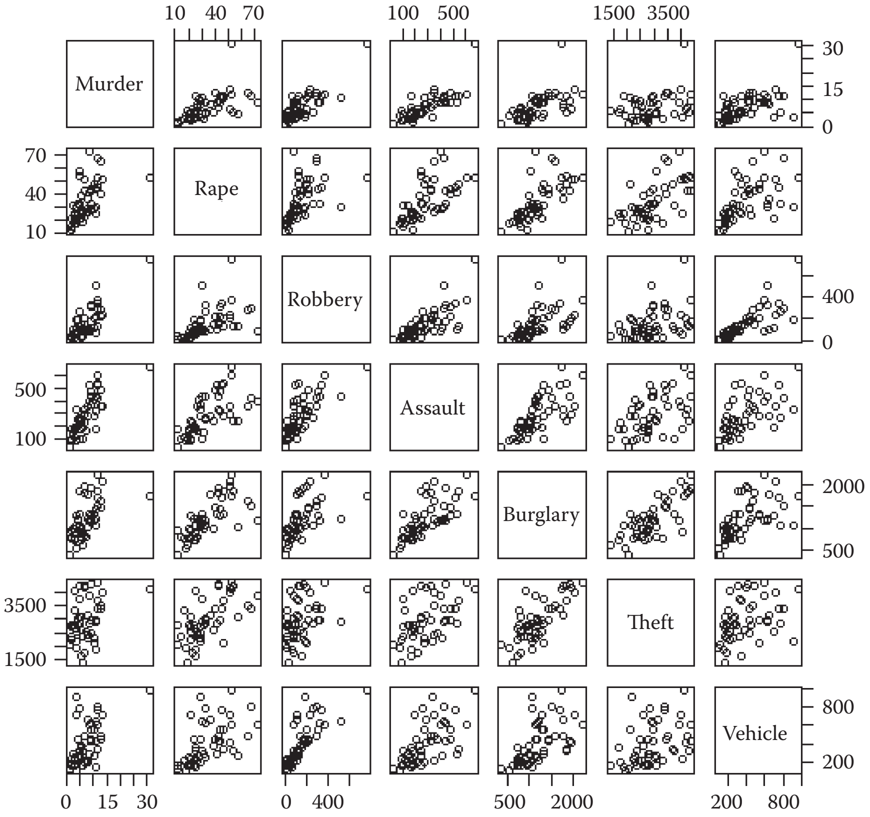


FIGURE 13.4
Scatterplot matrix of crime rate data.

rates having larger negative scores on this component (negative because of the minus signs attached to each loading); perhaps we could label this component "dangerousness." Labeling the second component is more difficult; in this component, the coefficients have a mixture of positive and negative signs, and the component appears to contrast "property crimes," that is, larceny and burglary, with crimes against the person, that is, robbery and murder. A not very inspired label might be "property versus person." The other components have very small variances, and we shall not try to interpret them.

Attempting to label components in this way is not without its critics; the following quotation from Marriott (1974) should act as a salutary warning about the dangers of overinterpretation:

> It must be emphasized that no mathematical method is, or could be, designed to give physically meaningful results. If a mathematical expression of this sort has an obvious physical meaning, it must be attributed to a lucky change, or to the fact that the data have a strongly marked structure

TABLE 13.6
Results from a PCA of the Correlation Matrix of Crime Rate Data

	Importance of Components						
	Comp.1	**Comp.2**	**Comp.3**	**Comp.4**	**Comp.5**	**Comp.6**	**Comp.7**
Variance	4.69	0.99	0.46	0.34	0.24	0.18	0.09
Proportion of Variance	0.67	0.14	0.07	0.05	0.03	0.03	0.01
Cumulative Proportion	0.67	0.81	0.88	0.93	0.96	0.99	1.00
	Coefficients Defining Components						
Murder	−0.381	−0.350	−0.538	—	−0.274	0.370	0.480
Rape	−0.377	0.279	—	−0.830	−0.250	—	−0.151
Robbery	−0.391	−0.420	0.131	0.275	−0.387	—	−0.651
Assault	−0.410	−0.124	−0.335	—	0.564	−0.620	—
Burglary	−0.394	0.367	—	0.162	0.466	0.622	−0.283
Theft	−0.321	0.628	—	0.449	−0.388	−0.282	0.256
Vehicle	−0.366	−0.282	0.758	—	0.163	—	0.422

Note: — indicates a coefficient that is almost zero.

that shows up in analysis. Even in the latter case, quite small sampling fluctuations can upset the interpretation; for example, the first two principal components may appear in reverse order or may become confused

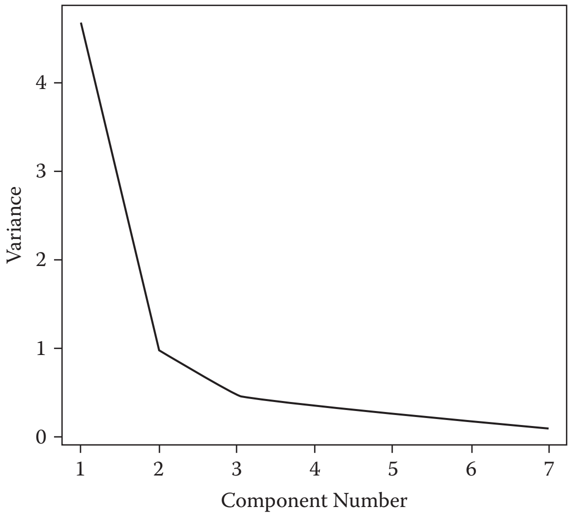


FIGURE 13.5
Scree plots of variances of principal components in the correlation matrix of crime rate data.

altogether. Reification then requires considerable skill and experience if it is to give a true picture of the physical meaning of the data.

Perhaps a more suitable use for the principal components of the crime rate data is as the basis of various graphical displays of cities. In fact, this is often the most useful aspect of a PCA and as a means to providing informative "views" of multivariate data, PCA has the advantage of making it less urgent or tempting to try to interpret and label the components. The first few component scores provide a low-dimensional "map" of the observations in which the Euclidean distances between the points representing the individuals best approximate in some sense the Euclidean distances between the individuals based on the original variables (for details, see the next chapter).

A plot of the crime rate data in the space of the first two principal components showing state labels is given in Figure 13.6. Clearly, DC is not a place to live in by choice! On the second component, WA has a high score because it has a low murder and robbery rate and relatively high burglary and larceny rates; contrast NY, which has relatively high murder and robbery rates and relatively low burglary and larceny rates and has a low score on the second component. Because the first two components account for over 80% of the variance in the crime rates, the two-dimensional plot in Figure 13.6 gives a very accurate description of the original seven-variable data. This claim is

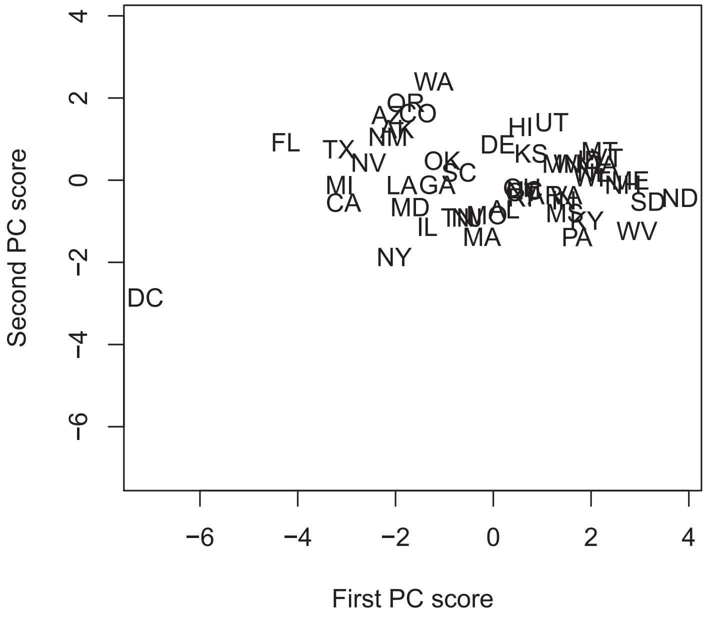


FIGURE 13.6
Plot of the crime rate data in the space of the first two principal components showing state labels.

TABLE 13.7
Observed Correlation Matrix for Crime Rate Data Compared to Matrix Constructed from the Two-Component Solution

				Observed			
	Murder	**Rape**	**Robbery**	**Assault**	**Burglary**	**Theft**	**Vehicle**
Murder	1.000	0.578	0.804	0.781	0.581	0.361	0.573
Rape	0.578	1.000	0.530	0.659	0.721	0.635	0.569
Robbery	0.804	0.530	1.000	0.740	0.551	0.400	0.786
Assault	0.781	0.659	0.740	1.000	0.710	0.512	0.638
Burglary	0.581	0.721	0.551	0.710	1.000	0.764	0.579
Theft	0.361	0.635	0.400	0.512	0.764	1.000	0.386
Vehicle	0.573	0.569	0.786	0.638	0.579	0.386	1.000
				Predicted			
Murder	0.801	0.578	0.843	0.775	0.578	0.357	0.752
Rape	0.578	0.745	0.576	0.691	0.799	0.741	0.571
Robbery	0.843	0.576	0.889	0.802	0.571	0.328	0.788
Assault	0.775	0.691	0.802	0.803	0.713	0.540	0.739
Burglary	0.578	0.799	0.571	0.713	0.862	0.821	0.576
Theft	0.357	0.741	0.328	0.540	0.821	0.872	0.377
Vehicle	0.752	0.571	0.788	0.739	0.576	0.377	0.708

backed up by comparing the observed correlation matrix with the correlation matrix "predicted" by the two-component solution after it has been rescaled, as described in Section 13.7. The two matrices are shown in Table 13.7. Corresponding elements of the two matrices are quite similar.

13.10.3 Drug Usage by American College Students

The majority of adult and adolescent Americans regularly use psychoactive substances and often do so for a substantial proportion of their lifetime. Various forms of licit and illicit psychoactive substance use are prevalent, suggesting that patterns of psychoactive substance taking are a major part of the individual's behavioral repertory and have pervasive implications on the performance of other behaviors. In an investigation of these phenomena, Huba et al. (1981) collected data on drug usage rates for 1634 students in the seventh to ninth grades in 11 schools in the greater metropolitan area of Los Angeles. Each participant completed a questionnaire about the number of times a particular substance had ever been used. The substances asked about were as follows:

1. Cigarettes
2. Beer
3. Wine
4. Liquor
5. Cocaine
6. Tranquilizers
7. Drugstore medications used to get "high"
8. Heroin and other opiates
9. Marijuana
10. Hashish
11. Inhalants (glue, gasoline)
12. Hallucinogenics (LSD, psilocybin, mescaline)
13. Amphetamine stimulants

Responses were recorded on a five-point scale:

1. Never tried
2. Only once
3. A few times
4. Many times
5. Regularly

The correlations between the usage rates of the 13 substances are shown in Table 13.8.

Applying a PCA to this correlation matrix gives the results shown in Table 13.9. A scree plot of the variances of the components is shown in Figure 13.7. The first two components have variances greater than 1, and the third has a variance slightly lower than 1. The scree plot suggests that perhaps three components need to be used to describe the correlations for these data, although these three components account for only 57% of the variance in drug usage rates. The first component is clearly a measure of overall drug usage, as might be expected since all the coefficients have relatively similar numerical values and all have the same sign. The second component contrasts "legal" with "illegal" substances (with the exception of marijuana, which has the same sign as the legal substances). This component might be seen as contrasting "soft" and "hard" drug usage. So, after overall usage has been accounted for, the main source of variation is between the different patterns of consumption of soft and hard drugs. The third component is essentially a contrast of drugstore and inhalant substance usage on the one hand, with marijuana, hashish, and amphetamine usage on the other.

We will return to the drug usage data in Chapter 16.

TABLE 13.8
Correlation Matrix for Drug Usage Data

	Drug	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**11**	**12**	**13**
1	Cigarettes	1												
2	Beer	0.447	1											
3	Wine	0.442	0.619	1										
4	Liquor	0.435	0.604	0.583	1									
5	Cocaine	0.114	0.068	0.053	0.115	1								
6	Tranquilizers	0.203	0.146	0.139	0.258	0.349	1							
7	Drugstore	0.091	0.103	0.110	0.122	0.209	0.221	1						
8	Heroin	0.082	0.063	0.066	0.097	0.321	0.355	0.201	1					
9	Marijuana	0.513	0.445	0.365	0.482	0.186	0.315	0.150	0.154	1				
10	Hashish	0.304	0.318	0.240	0.368	0.303	0.377	0.163	0.219	0.534	1			
11	Inhalants	0.245	0.203	0.183	0.255	0.272	0.323	0.310	0.288	0.301	0.302	1		
12	Hallucinogenics	0.101	0.088	0.074	0.139	0.279	0.367	0.232	0.320	0.204	0.368	0.304	1	
13	Amphetamine	0.245	0.199	0.184	0.293	0.278	0.545	0.232	0.314	0.394	0.467	0.392	0.511	1

TABLE 13.9
Results of Applying PCA to the Correlation Matrix of Drug Usage Rates

	Variances of Components												
	C1	**C2**	**C3**	**C4**	**C5**	**C6**	**C7**	**C8**	**C9**	**C10**	**C11**	**C12**	**C13**
Variance	4.38	2.05	0.96	0.81	0.76	0.69	0.63	0.62	0.57	0.40	0.39	0.38	0.36
Proportion of Variance	0.34	0.16	0.07	0.06	0.059	0.053	0.050	0.048	0.044	0.031	0.030	0.029	0.027
Cumulative Proportion	0.34	0.49	0.57	0.63	0.69	0.74	0.79	0.84	0.88	0.91	0.94	0.97	1.00

	Coefficients Defining Components												
Var	**C1**	**C2**	**C3**	**C4**	**C5**	**C6**	**C7**	**C8**	**C9**	**C10**	**C11**	**C12**	**C13**
1	−0.280	−0.283	—	—	−0.300	−0.387	−0.124	0.137	0.655	−0.139	−0.136	−0.169	−0.263
2	−0.287	−0.394	0.120	—	0.187	0.161	0.114	—	—	—	—	0.695	−0.410
3	−0.267	−0.393	0.207	−0.139	0.309	0.141	—	—	0.107	−0.421	0.210	−0.188	0.564
4	−0.318	−0.322	—	—	0.181	0.142	—	−0.164	−0.214	0.563	−0.181	−0.519	−0.219
5	−0.208	0.290	—	−0.582	−0.432	0.416	0.185	−0.244	0.204	—	0.154	—	—
6	−0.293	0.262	−0.165	—	0.122	—	−0.629	−0.399	—	−0.124	−0.421	0.170	0.138
7	−0.176	0.190	0.723	0.372	−0.178	0.277	−0.309	0.253	—	—	—	—	—
8	−0.201	0.317	0.153	−0.534	0.327	−0.359	—	0.525	−0.169	—	—	—	—
9	−0.340	−0.160	−0.228	0.112	−0.365	−0.129	—	0.285	−0.149	0.418	0.154	0.285	0.502
10	−0.329	—	−0.352	0.125	−0.256	0.243	0.167	0.274	−0.400	−0.496	−0.187	−0.240	−0.152
11	−0.274	0.163	0.330	0.159	−0.152	−0.531	0.466	−0.417	−0.228	—	—	—	—
12	−0.245	0.327	−0.144	0.272	0.379	0.210	0.413	0.162	0.440	0.179	−0.308	—	0.159
13	−0.328	0.235	−0.235	0.267	0.203	—	−0.132	−0.177	—	—	0.733	—	−0.269

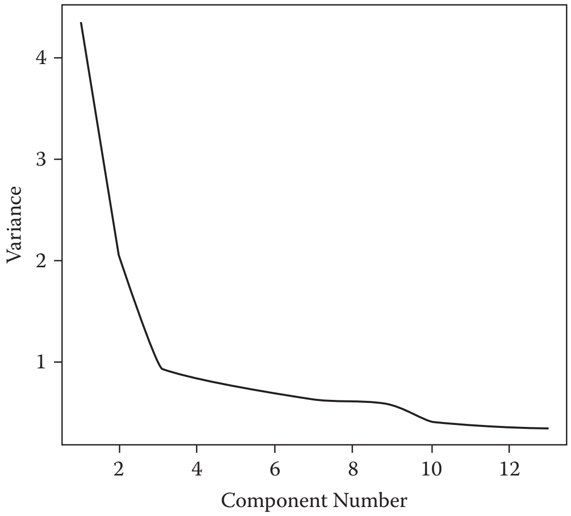


FIGURE 13.7
Scree plot of component variances for the drug usage data.

13.11 Using PCA to Select a Subset of the Variables

Although the first few principal component scores for each individual may provide a very useful summary for a set of multivariate data, all the original variables are needed in their computation. In many cases, an investigator might be happier with determining a subset of the original variables that contains, in some sense, virtually all the information contained in the complete set of these variables. In a series of papers, Jolliffe (1970, 1972, 1973) discusses a number of approaches to selecting subsets of variables, several of which are based on PCA. One such method is to first use one or other of the criteria for choosing the number of components described in Section 13.8; this number, say, m, is taken to indicate the effective dimensionality of the data and will be the size of the subset of the original variables to be retained. The variables are then chosen, one associated with each of the first m components and having the largest absolute coefficient value on the component but not already having been selected. If we use the eigenvalue criterion suggested by Jolliffe, namely, retain components with eigenvalues greater than 0.7 (assuming the correlation matrix is being used) for the drug usage data, then we keep the first five components. Examining the coefficients defining these components, we find that we are led to the following five variables:

1. Marijuana usage
2. Beer usage

3. Drugstore medication usage
4. Cocaine usage
5. Hallucinogenics usage

These variables could be used in future analyses of the data with little loss of information, compared to using all 13 of the original variables.

13.12 Summary

- PCA provides a way of reducing the complexity of multivariate data by reducing their dimensionality.
- The reduction in dimensionality that can often be achieved by a PCA is possible only if the original variables are correlated; if the original variables are independent of one another, a PCA cannot lead to any simplification.
- In most applications, variables will be on different scales, so components will need to be extracted from the correlation matrix of the data.
- In essence, PCA is simply a rotation of the axes of multivariate data scatter.
- The first few principal component scores can often be used to provide a convenient summary of a multivariate data set, particularly for looking at the data via simple scatterplots.
- Trying to give meaningful labels to components is often confusing and a waste of time.
- Two techniques that are related to principal components are multidimensional scaling and correspondence analysis; both topics are discussed in the next chapter.

13.13 Exercises

(excluded from MABS for IODS)

14

Multidimensional Scaling and Correspondence Analysis

14.1 Introduction

The concept of *distance* is at the heart of many methods for dealing with multivariate data. For example, in the scatterplots shown in Chapter 2 the relative ‘distances’ between points are obviously central to making interpretations about the plots; this is clear without giving an explicit definition of distance but simply appealing to its everyday usage. But in this chapter, we will need to consider the distance concept in more detail as we consider methods which aim to give useful low-dimensional ‘maps’ of particular types of data. We have, of course, already met one such technique, principal components analysis, in the previous chapter. As mentioned briefly there, this technique finds the required low-dimensional map in such a way that Euclidean distances between the observations in the space of the original variables are preserved as far as possible by the points representing the observations in the principal component plot. For the observations in the data matrix $\mathbf{X}$ (see Chapter 12), the Euclidean distance between observation i with variable values $x_{i1}, x_{i2}, \ldots, x_{iq}$, and observation j with variable values $x_{j1}, x_{j2}, \ldots, x_{jq}$ is defined as

$$d_{ij} = \sqrt{\sum_{k=1}^{q} (x_{ik} - x_{jk})^2}$$

Applying this formula to all pairs of observations results in an $n \times n$ Euclidean *distance matrix.* To illustrate the calculation of a distance matrix we shall use the data in Table 14.1 showing birth and death rates for seven countries; the Euclidean distance matrix for these data is shown in Table 14.2. The distance matrix is symmetric because $d_{ij} = d_{ji}$ and it has zeros on the main diagonal.

The distance matrix in Table 14.2 was derived from the raw data in Table 14.1 simply by applying the formula for Euclidean distance given above. But similar matrices can arise more directly. For example, Table 14.3 shows judgements about various brands of cola made by two subjects using a visual analogue scale with anchor points “same” (having a score of 0) and “different” (having a score of 100). In this example, the resulting rating for a pair of colas is labeled as a measure of *dissimilarity*—low values indicate that the two colas

TABLE 14.1
Birth and Death Rates for Seven Countries

Country	Birth rate	Death rate
Japan	8.4	9.9
Italy	8.6	10.2
Spain	9.4	8.6
United Kingdom	12.4	9.0
Finland	10.8	9.5
Cuba	11.2	7.6
United States	12.5	8.2

Note: Average data from 2010–2015 taken from the *World Population Prospects* by United Nations, Population Division (2017).

TABLE 14.2
Euclidean Distance Matrix Based on the Birth and Death Rates in Table 14.1

	Japan	Italy	Spain	UK	Finland	Cuba	US
Japan	0.00						
Italy	0.36	0.00					
Spain	1.64	1.79	0.00				
United Kingdom	4.10	3.98	3.03	0.00			
Finland	2.43	2.31	1.66	1.68	0.00		
Cuba	3.62	3.68	2.06	1.84	1.94	0.00	
United States	4.44	4.38	3.13	0.81	2.14	1.43	0.00

TABLE 14.3
Dissimilarity Data for All Pairs of 10 Colas for Two Subjects

Subject 1:											Subject 2:										
	Cola Number											Cola Number									
	1	2	3	4	5	6	7	8	9	10		1	2	3	4	5	6	7	8	9	10
1	0										1	0									
2	16	0									2	20	0								
3	81	47	0								3	75	35	0							
4	56	32	71	0							4	60	31	80	0						
5	87	68	44	71	0						5	80	70	37	70	0					
6	60	35	21	98	34	0					6	55	40	20	89	30	0				
7	84	94	98	57	99	99	0				7	80	90	90	55	87	88	0			
8	50	87	79	73	19	92	45	0			8	45	80	77	75	25	86	40	0		
9	99	25	53	98	52	17	99	84	0		9	87	35	50	88	60	10	98	83	0	
10	16	92	90	83	79	44	24	18	98	0	10	12	90	96	89	75	40	27	14	90	0

are regarded as more alike than high values, and vice versa. A *similarity measure* would have been obtained had the anchor points been reversed, although similarities are often scaled to lie in the interval $[0, 1]$.

Distance matrices, dissimilarity and similarity matrices however they arise are generally referred to collectively as *proximity matrices.* It is the analysis of such matrices that is the subject of this chapter where the aims are to clarify, display, and possibly explain any structure or pattern not readily apparent in the collection of numerical values. In some areas, particularly psychology, the ultimate goal in the analysis of a set of proximities is more specifically the development of theories for explaining similarity judgements, or, in other words, finding an answer to the question 'what makes things seem alike or different?' Here we will confine ourselves to discussing the methods for analysing proximity values without searching for the answer to this type of 'holy grail' question.

The two classes of techniques to be described in this chapter are *multidimensional scaling* which is used essentially to represent an observed proximity matrix geometrically and *correspondence analysis* which is quintessentially a method for displaying the associations among a set of categorical variables in a type of scatterplot or map, thus allowing a visual examination of any structure or pattern in the data. Both these methods are exploratory in nature and they share more similarities than differences with each other, so they fit extremely well in the same chapter. In addition, both methods, especially correspondence analysis, have interesting connections to factor analysis that is the topic of the next chapter. We will start from multidimensional scaling, covering its basic principles and practices.

14.2 Multidimensional Scaling

A spatial representation of a proximity matrix consists of a set of q-dimensional coordinates representing each of the observations, chosen so that the distances (generally Euclidean but not always) between the points in the q-dimensional space match closely in some sense the observed proximities. Finding both the 'best' fitting set of coordinates and the appropriate value of q (which we would like to be as low as possible) is the general aim of *multidimensional scaling* (MDS) techniques that have originated in psychometrics. The variety of methods that have been suggested differ largely in how agreement between fitted distances and observed proximities are measured, i.e., in their goodness-of-fit criteria. Here, we discuss only *classical scaling* and *nonmetric scaling.* Accounts of other methods are given in Everitt and Rabe-Hesketh (1997).

14.2.1 Classical Multidimensional Scaling

Classical multidimensional scaling seeks to represent a proximity matrix by a simple geometrical model or map. Such a model is characterized by a set of points $\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_n$, in q dimensions, each point representing one of the stimuli of interest, and a measure of the distance between pairs of points. The objective of MDS is to determine both the dimensionality, q, of the model, and the n, q-dimensional coordinates $\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_n$ so that the model gives a "good" fit for the observed proximities. Fit will often be judged by some numerical index that measures how well the proximities and the distances in the geometrical model match. In essence, this simply means that the larger an observed dissimilarity between two stimuli (or the smaller their similarity), the further apart should be the points representing them in the final geometrical model.

The question now arises as to how we estimate q, and the coordinate values $\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_n$, from the observed proximity matrix? *Classical scaling* provides an answer to this question based on the early work of Young and Householder (1938) and the development of the method due to Torgerson (1952, 1958). To begin, we must note that there is no unique set of coordinate values that give rise to these distances, since they are unchanged by shifting the whole configuration of points from one place to another, or by rotation or reflection of the configuration. In other words, we cannot uniquely determine either the location or the orientation of the configuration. The location problem is usually overcome by placing the mean vector of the configuration at the origin. The orientation problem means that any configuration derived can be subjected to an arbitrary orthogonal transformation. Such transformations can often be used to facilitate the interpretation of solutions as will be seen later.

The essential details of classical scaling are given in Technical Section 14.1.

Technical Section 14.1: Classical Multidimensional Scaling

To begin our account of the method, we shall assume that the proximity matrix we are dealing with is a matrix of Euclidean distances $\mathbf{D}$ derived from a raw data matrix $\mathbf{X}$. In the beginning of the chapter, we saw how to calculate Euclidean distances from $\mathbf{X}$. Now, MDS is essentially concerned with the reverse problem: Given the distances (arrayed in the $n \times n$ matrix $\mathbf{D}$) how do we find $\mathbf{X}$? To begin, define an $n \times n$ inner product matrix $\mathbf{B}$ as follows:

$$\mathbf{B} = \mathbf{X}\mathbf{X}' \tag{14.1}$$

where the elements of $\mathbf{B}$ are given by

$$b_{ij} = \sum_{k=1}^{q} x_{ik} x_{jk} \tag{14.2}$$

It is easy to see that the squared Euclidean distances between the rows of $\mathbf{X}$ can be written in terms of the elements of $\mathbf{B}$ as

$$d_{ij}^2 = b_{ii} + b_{jj} - 2b_{ij} \tag{14.3}$$

If the bs could be found in terms of the ds in the equation above, then the required coordinate values could be derived by factoring $\mathbf{B}$ as in (14.1). No unique solution exists unless a location constraint is introduced. Usually the center of the points $\bar{\mathbf{x}}$ is set at the origin, so that $\sum_{i=1}^n x_{ik} = 0$ for all $k = 1, 2, \dots, q$. These constraints and the relationship given in (14.2) imply that the sum of the terms in any row of $\mathbf{B}$ must be zero. Consequently, summing the relationship given in (14.3) over i, over j, and finally over both i and j, leads to the following series of equations:

$$\sum_{i=1}^n d_{ij}^2 = \text{trace}(\mathbf{B}) + nb_{jj}$$

$$\sum_{j=1}^n d_{ij}^2 = \text{trace}(\mathbf{B}) + nb_{ii}$$

$$\sum_{i=1}^n \sum_{j=1}^n d_{ij}^2 = 2n \times \text{trace}(\mathbf{B})$$

where $\text{trace}(\mathbf{B}) = \sum_{i=1}^n b_{ii}$. The elements of $\mathbf{B}$ can now be found in terms of squared Euclidean distances as

$$b_{ij} = -\frac{1}{2}\left[d_{ij}^2 - d_{i.}^2 - d_{.j}^2 + d_{..}^2\right],$$

where

$$d_{i.}^2 = \frac{1}{n}\sum_{j=1}^n d_{ij}^2$$

$$d_{.j}^2 = \frac{1}{n}\sum_{i=1}^n d_{ij}^2$$

$$d_{..}^2 = \frac{1}{n^2}\sum_{i=1}^n \sum_{j=1}^n d_{ij}^2$$

Having now derived the elements of $\mathbf{B}$ in terms of Euclidean distances, it remains to factor it to give the coordinate values. In terms of its spectral decomposition, $\mathbf{B}$ can be written as

$$\mathbf{B} = \mathbf{V}\boldsymbol{\Lambda}\mathbf{V}',$$

where $\boldsymbol{\Lambda} = \text{diag}(\lambda_1, \lambda_2, \dots, \lambda_n)$ is the diagonal matrix of eigenvalues of $\mathbf{B}$ and $\mathbf{V}$ the corresponding matrix of eigenvectors, normalized so that the sum of squares of their elements is unity, that is, $\mathbf{V}'\mathbf{V} = \mathbf{I}_n$. The eigenvalues are assumed labeled such that $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$.

When the matrix of Euclidean distances $\mathbf{D}$ arises from an $n \times k$ matrix of full column rank, then the rank of $\mathbf{B}$ is k, so that the last $n - k$ of its eigenvalues will be zero. So $\mathbf{B}$ can be written as $\mathbf{B} = \mathbf{V}_1 \mathbf{\Lambda}_1 \mathbf{V}_1'$, where $\mathbf{V}_1$ contains the first k eigenvectors and $\mathbf{\Lambda}_1$ the k non-zero eigenvalues. The required coordinate values are thus $\mathbf{X} = \mathbf{V}_1 \mathbf{\Lambda}_1^{1/2}$, where $\mathbf{\Lambda}_1^{1/2} = \text{diag}(\sqrt{\lambda_1}, \sqrt{\lambda_2}, \ldots, \sqrt{\lambda_k})$.

Using all q dimensions would lead to complete recovery of the original Euclidean distance matrix. The best-fitting k-dimensional representation is given by the k eigenvectors of $\mathbf{B}$ corresponding to the k largest eigenvalues. The adequacy of the k-dimensional representation can be judged by the size of the criterion

$$P_k = \sum_{i=1}^{k} \lambda_i \Big/ \sum_{i=1}^{n-1} \lambda_i$$

Values of P_k of the order of 0.8 suggest a reasonable fit.

When the observed dissimilarity matrix is not Euclidean, the matrix $\mathbf{B}$ is not positive-definite. In such cases, some of the eigenvalues of $\mathbf{B}$ will be negative; correspondingly, some coordinate values will be complex numbers. If, however, $\mathbf{B}$ has only a small number of small negative eigenvalues, a useful representation of the proximity matrix may still be possible using the eigenvectors associated with the k largest positive eigenvalues. The adequacy of the resulting solution might be assessed using one of the following two criteria suggested by Mardia et al. (1979):

$$P_k^{(1)} = \sum_{i=1}^{k} |\lambda_i| \Big/ \sum_{i=1}^{n} |\lambda_i| \quad \text{or} \quad P_k^{(2)} = \sum_{i=1}^{k} \lambda_i^2 \Big/ \sum_{i=1}^{n} \lambda_i^2$$

Again, we would look for values above 0.8 to claim a "good" fit. Alternatively, Sibson (1979) recommends one of the following criteria for deciding on the number of dimensions to adequately represent the observed proximities:

1. *Trace criterion:* Choose the number of coordinates so that the sum of the *positive* eigenvalues is approximately equal to the sum of *all* the eigenvalues.
2. *Magnitude criterion:* Accept as genuinely positive only those eigenvalues whose magnitude substantially exceeds that of the largest negative eigenvalue.

If, however, the matrix $\mathbf{B}$ has a considerable number of large negative eigenvalues, classical scaling of the proximity matrix may be inadvisable and some other methods of scaling, for example nonmetric or least-squares scaling, might be better employed (for details, see Everitt and Rabe-Hesketh, 1997).

As first example of applying classical scaling, we will return to the distance matrix in Table 14.2. The two-dimensional solution is shown in Table 14.4 and we can use these results to produce a two-dimensional 'map' of the data as shown in Figure 14.1. Of course, in this example the raw data consists of only two variables, so consequently the classical scaling solution achieves complete recovery of the observed distance matrix. For example, the Euclidean distance between Japan and Italy found from the relevant values given in Table 14.4 is calculated as

$$\sqrt{[-2.26-(-2.19)]^2+[0.03-0.39]^2}=0.36,$$

which is the distance between these two countries derived for the raw data values in Table 14.1 (see Table 14.2).

TABLE 14.4
Two-Dimensional Solution from Classical MDS Applied to the Distance Matrix in Table 14.2

Country	**Dimension 1**	**Dimension 2**
Japan	−2.26	0.03
Italy	−2.19	0.39
Spain	−0.83	−0.78
United Kingdom	1.78	0.74
Finland	0.11	0.59
Cuba	1.21	−1.01
United States	2.18	0.05

14.2.2 Connection to Principal Components

It should be mentioned here that when the proximity matrix of interest contains Euclidean distances derived from a raw data matrix (as in the previous example of the seven countries), classical scaling can be shown to be equivalent to principal components analysis (PCA, see Chapter 13), with the derived coordinate values corresponding to the scores on the principal components derived from the covariance matrix. One result of this duality is that the classical scaling is often referred to as *principal coordinates analysis* (see Gower, 1966). The low-dimensional representation achieved by classical scaling for Euclidean distances (and that produced by PCA) is such that the function ϕ given by

$$\phi=\sum_{r,s}^{n}(d_{rs}^2-\hat{d}_{rs}^2)$$

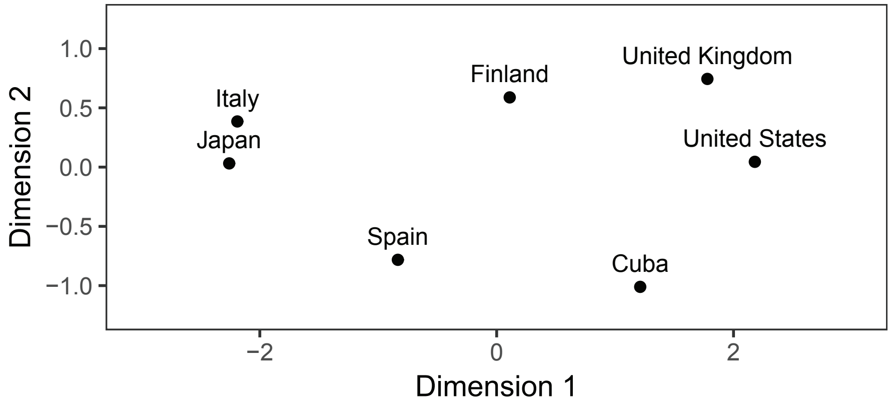


FIGURE 14.1
Resulting map from classical scaling of the seven countries' distance matrix in Table 14.2.

is minimized. In this expression, d_{rs} is the Euclidean distance between observations r and s in the original q-dimensional space, and $\hat{d}^2_{rs}$ is the corresponding distance in k-dimensional space ($k < q$) chosen for the classical scaling solution (equivalently the first k principal components).

For more details of the connections of MDS to other methods, see Groenen and van de Velden (2005).

14.2.3 Road Distances in Finland

It is almost *de rigueur* in any account of MDS to include an example involving road distances between towns or cities of a particular country, usually the country of origin of the author involved; see, for example, Kruskal and Wish (1978), Manly (1986), Krzanowski and Marriott (1994), Mustonen (1995), and Everitt and Rabe-Hesketh (1997). The present account is no exception and so Table 14.5 gives the road distances between 15 cities, towns etc. in Finland. Road distances are unlikely to be Euclidean (they are measured on the surface of a sphere for one thing) and, in fact, the eigenvalues of the matrix **B** (see Technical Section 14.1) arising from the distances in Table 14.6 include seven negative values (including one that is practically zero).

The first question that has to be addressed is how many coordinate values are needed to adequately represent the observed distance matrix? We could answer this question by using one or other of the fit criteria described in Technical Section 14.1, but here we shall simply use the two-dimensional solution and judge informally how this matches up to the usual map of Finland. This plot (after a convenient rotation to put Helsinki in the South) is shown in Figure 14.2. This diagram gives a good approximation to the map of Finland, as the mean absolute error of approximation between the 15 selected places

TABLE 14.5
Road Distances of 15 Selected Places in Finland

	Hel	**Joe**	**Jyv**	**Kil**	**Kok**	**Kot**	**Kuo**	**Kuu**	**Lap**	**Nuo**	**Oul**	**Rov**	**Tam**	**Tur**	**Vaa**
Helsinki	0														
Joensuu	438	0													
Jyväskylä	272	245	0												
Kilpisjärvi	1202	979	931	0											
Kokkola	491	429	241	789	0										
Kotka	134	343	244	1177	488	0									
Kuopio	383	136	144	878	315	316	0								
Kuusamo	802	459	551	620	411	735	417	0							
Lappeenranta	223	236	219	1144	460	108	264	682	0						
Nuorgam	1328	1045	1056	649	916	1303	1006	617	1271	0					
Oulu	612	393	339	592	196	585	286	212	551	719	0				
Rovaniemi	832	550	561	428	419	806	509	191	774	495	222	0			
Tampere	174	394	151	1079	324	243	293	702	275	1207	491	712	0		
Turku	166	549	304	1226	436	295	448	848	364	1353	633	856	153	0	
Vaasa	419	494	282	910	121	484	379	533	501	1035	318	541	244	331	0

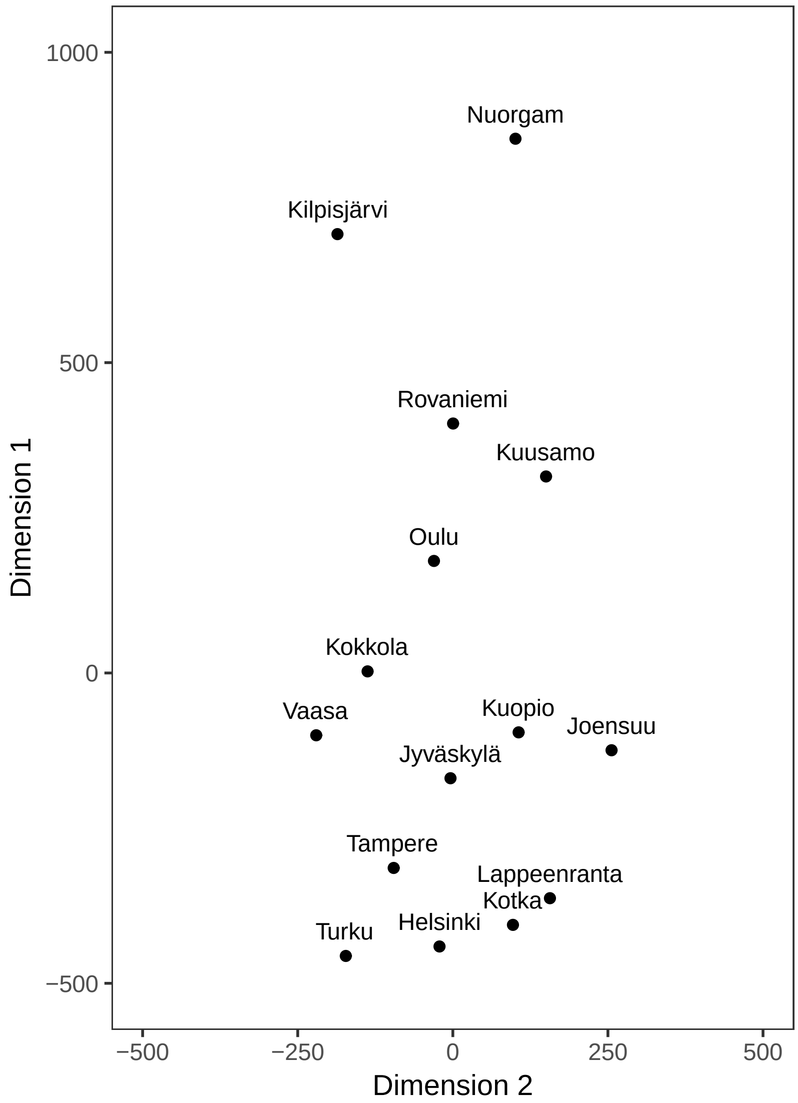


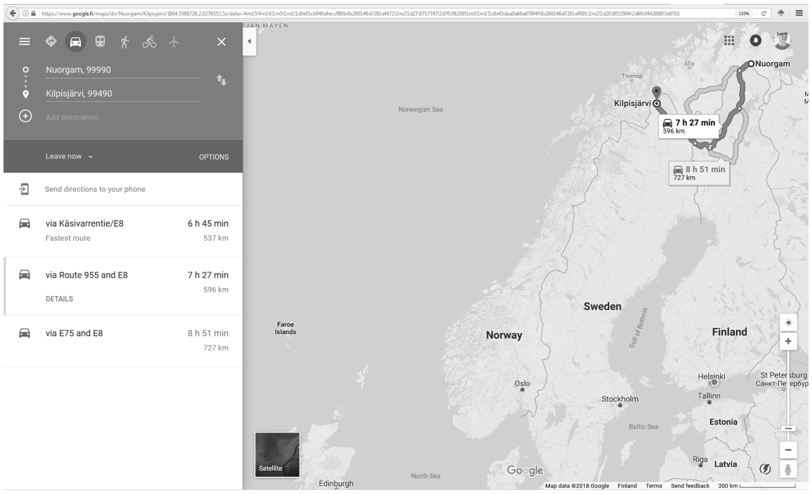
FIGURE 14.2
Resulting map from classical scaling of the Finnish road distances.

is only about 16 km. The case of the two northernmost places of these data, both located in rather extreme corners of Finland, reveals a huge exception, however, as the actual road distance between the villages of Nuorgam and Kilpisjärvi (based on these data) is 649 km, but the estimate based on the classical scaling is only about half of that (326 km). The reason for this error

TABLE 14.6
Eigenvalues and Eigenvectors Arising from Classical Scaling Applied to the Distance Matrix in Table 14.5

Eigenvalues	**City/Town/Village**	**Dim 1**	**Dim 2**
2395788	Helsinki	−440.7	−21.5
285542	Joensuu	−124.5	255.9
198140	Jyväskylä	−169.6	−3.8
56660	Kilpisjärvi	707.1	−186.0
16092	Kokkola	2.6	−137.4
15119	Kotka	−405.8	96.9
7806	Kuopio	−95.7	106.0
724	Kuusamo	316.6	150.3
0	Lappeenranta	−362.9	156.5
−995	Nuorgam	860.8	101.0
−5886	Oulu	180.5	−30.4
−13245	Rovaniemi	402.0	0.5
−21336	Tampere	−314.1	−95.3
−37055	Turku	−455.9	−172.5
−56468	Vaasa	−100.4	−220.2

should come quite clear by looking at the (true) map of Finland, for example, in Google Maps (see Figure 14.3).



Nuorgam, 99990

Kilpisjärvi, 99490

Add destination

Leave now OPTIONS

Send directions to your phone

via Käsivarrentie/E8 Fastest route	6 h 45 min 537 km	
via Route 955 and E8 DETAILS	7 h 27 min 596 km	
via E75 and E8	8 h 51 min 727 km	

https://www.google.fi/maps/dir/Nuorgam/Kilpisjärvi/@64.5588726,2.0276553,5z/data=!4m15!4m14!1m5!1m1!1s0x45cb940afeccf80b:0x260146d7261ef472!2m2!1d27.8717747!2d70.08209!1m5!1m1!1s0x45daa9a66a078f4f:0x260146d7261ef091!2m2!1d20.8032994!2d69.0442888!3e0!5i1
133%
JAN MAYEN
Norwegian Sea
Tromsø
Alta
Nuorgam
Kilpisjärvi
7 h 27 min
596 km
8 h 51 min
727 km
Faroe Islands
Norway
Sweden
Finland
Gulf of Bothnia
Oslo
Stockholm
Helsinki
Tallinn
St Petersburg
Санкт-Петербург
Estonia
Baltic Sea
Riga
Latvia
Satellite
Edinburgh
North Sea
Google
Map data ©2018 Google Finland Terms Send feedback 200 km

FIGURE 14.3
Routes and road distances between the villages of Nuorgam and Kilpisjärvi, Finland (source: Google Maps).

TABLE 14.7
Proximity Matrix of Ten Remarkable Classical Music Composers Selected and Compared by Olli Mustonen

	Bac	**Hay**	**Moz**	**Bee**	**Sch**	**Bra**	**Sib**	**Deb**	**Bar**	**Šos**
Bach	0									
Haydn	50	0								
Mozart	30	10	0							
Beethoven	20	15	20	0						
Schubert	40	30	25	10	0					
Brahms	40	70	40	20	15	0				
Sibelius	40	90	70	25	60	20	0			
Debussy	50	50	50	80	50	70	35	0		
Bartók	30	80	80	60	70	70	35	15	0	
Šostakovitš	30	40	50	40	60	70	20	40	20	0

14.2.4 Mapping Composers of Classical Music

Our final example of the use of classical scaling involves data on composers of classical music, taken with permission from Mustonen (1996, 156–159) and Mustonen (1995, 167–170). Seppo Mustonen (a Finnish professor of Statistics) asked his son Olli Mustonen (a Finnish pianist, conductor, and composer) to select ten remarkable composers from different era of classical music and compare those composers with each other intuitively based on their entire production and style. Olli Mustonen made his comparisons using a scale from 0 to 100 in a way that the more he considered the composers to differ, the higher the score he gave. After about half an hour's reflection, he presented the proximity matrix given in Table 14.7, where the selected composers appear roughly in chronological order. We can see that the scale was applied with intervals of five units, and that the greatest difference was 90 units, occurring between Sibelius and Haydn.

Applying classical scaling to the data in Table 14.7 leads to four negative eigenvalues for the matrix **B** (see Technical Section 14.1) and so the dissimilarity matrix shown there is clearly non-Euclidean. Here we will look at the fit criteria described in Technical Section 14.1 as a guide to the number of dimensions needed to adequately represent the dissimilarity values in Table 14.7. For the one-dimensional solution we obtain the values

$$P_1^{(1)} = 0.35 \text{ and } P_1^{(2)} = 0.58$$

while for the two-dimensional solution, the values obtained are

$$P_2^{(1)} = 0.58 \text{ and } P_2^{(2)} = 0.83$$

which would seem to suggest two dimensions (although the first one does not approach 0.8 before eight dimensions). Also both the alternative criteria (the

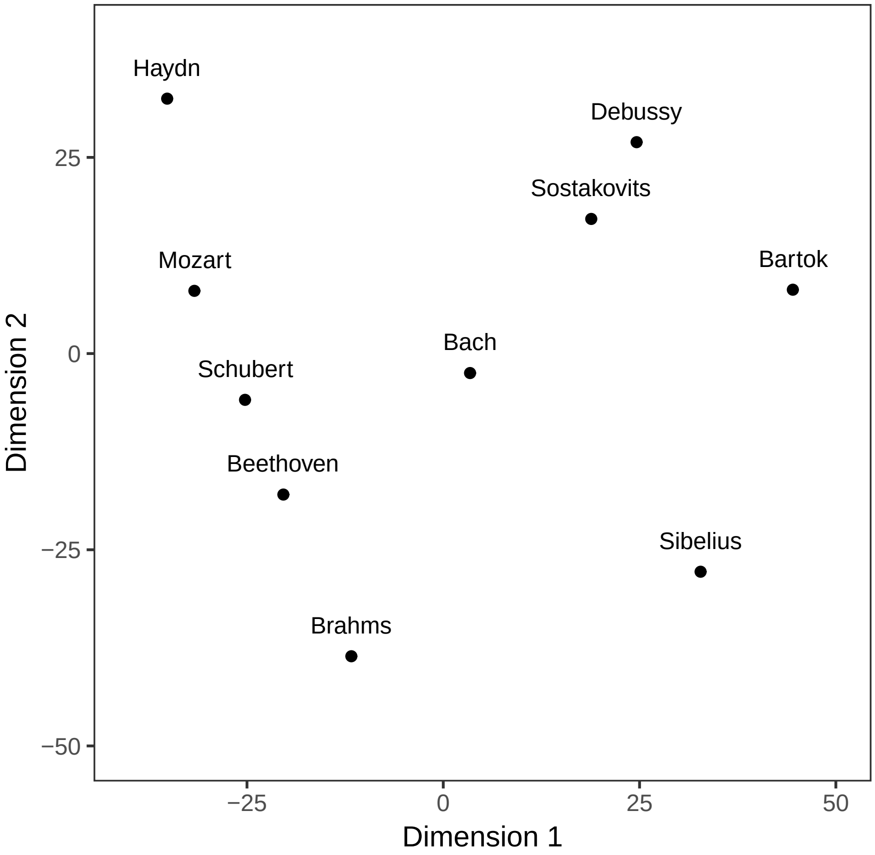


FIGURE 14.4
Resulting map from classical scaling of the classical composers.

trace and the magnitude) support the conclusion, so we shall proceed with two dimensions, following the original lines of interpretations of Mustonen (1996).

The resulting map of composers is shown in Figure 14.4. The first dimension (from left to right) appears to be related to time, with one significant exception: the “timeless” Bach is placed in the middle. The second dimension (from top to bottom) can be interpreted as a transition from ”light” music to “heavy” music. Indeed, the *Viennese Classics* (Haydn, Mozart, Schubert, and Beethoven) form a logical chain, accompanied by Brahms, who, together with Sibelius, is located in the “heavyweight division”. The modern composers (Debussy, Šostakovitš, and Bartók) seem to form a cluster of their own, and it is perfectly understandable that, of these composers, it is Šostakovitš who gets settled nearest to Bach. A rather lonely Sibelius is placed at a considerable distance from all other composers.

One feature of the proximity matrix in Table 14.7 which we should point to, involves the rating between Debussy and Beethoven which is the second largest in the whole matrix. According to the rater, Olli Mustonen, this rating was 'coloured' by the fact that he was aware that Debussy hated Beethoven's music!

We shall close this subsection by noting that obviously musicians do not have a uniform perception of the relations between the composers (see Georges, 2017). The reader might easily make experiments in this respect and compare the resulting maps to the one we have presented here. For further analysis and interesting ways of studying the behavioral dimensions of music, including emotions, see, for example, Eerola (2011). And about the term 'classic' in the context of music, take a look at Bennett (2009).

14.2.5 Nonmetric Multidimensional Scaling

In some psychological work and in market research, proximity matrices arise from asking human subjects to make judgements about the similarity or dissimilarity of objects or stimuli of interest. When collecting such data, the investigator may feel that realistically subjects are only able to give "ordinal" judgements; for example, when comparing a range of colours they might be able to specify with some confidence that one colour is brighter than another but would be far less confident if asked to put a value to how much brighter. Such considerations led, in the 1960s, to the search for a method of multidimensional scaling that uses only the *rank order* of the proximities to produce a spatial representation of them. In other words, a method was sought that would be invariant under *monotonic transformations* of the observed proximity matrix; i.e., the derived coordinates will remain the same if the numerical values of the observed proximities are changed but their rank order is not.

The essential details of nonmetric multidimensional scaling are given briefly in Technical Section 14.2.

Technical Section 14.2: Nonmetric Multidimensional Scaling

Nonmetric MDS was proposed in landmark papers by Shepard (1962a,b) and by Kruskal (1964a). The quintessential component of the method is that the coordinates in the spatial representation of the observed proximities give rise to fitted distances, d_{ij}, and that these distances are related to a set of numbers which we will call *disparities*, $\hat{d}_{ij}$, by the formula $d_{ij} = \hat{d}_{ij} + \epsilon_{ij}$, where the ϵ_{ij} are error terms representing errors of measurement plus distortion errors arising because the distances do not correspond to a configuration in the particular number of dimensions chosen. The disparities are monotonic with the observed proximities and, subject to this constraint, resemble the fitted distances as closely as possible.

Monotonic regression (see Barlow et al., 1972) is used to find the disparities, and then the required coordinates in the spatial representation of the observed dissimilarities, are found by minimizing a criterion known as *stress*, which is defined as

$$stress = \min \frac{\sum_{i<j}(\hat{d}_{ij} - d_{ij})^2}{\sum_{i<j} d_{ij}^2},$$

where the minimum is taken over the disparities $\hat{d}_{ij}$ such that $\hat{d}_{ij}$ is monotonic with the observed dissimilarities. In essence, *stress* represents the extent to which the rank order of the fitted distances disagrees with the rank order of the observed dissimilarities. The denominator in the formula for *stress* is chosen to make the final spatial representation invariant under changes of scale; that is, uniform stretching or shrinking.

An algorithm to minimize the *stress* criterion (see the Technical Section 14.2) and so find the coordinates of the required spatial representation is described in Kruskal (1964b). For each value of the number of dimensions, q, in the spatial configuration, the configuration that has the smallest *stress* is called the best-fitting configuration in q dimensions. For judging the goodness (or badness) of fit, Kruskal (1964a) gave the following verbal evaluation of various values of *stress* (typically expressed in percentages):

Stress (%)	**Goodness-of-fit**
20	Poor
10	Fair
5	Good
2.5	Excellent
0	Perfect

(The last one, 'perfect,' only occurs if the rank order of the fitted distances matches the rank order of the observed dissimilarities, an event, which is, of course, very rare in practise).

14.2.6 Re-mapping Composers of Classical Music

We now apply the nonmetric MDS to the classical music composers' proximity matrix in Table 14.7. The resulting two-dimensional map is shown in Figure 14.5. There are small differences between this plot and that resulting from classical scaling (Figure 14.4), but in general the interpretation of each diagram is very similar. The value of *stress* (defined earlier) for Figure 14.5 is 5.5%.

Now let us look at the plot provided by coordinates one and three from the nonmetric scaling solution for the composers' data; this is shown in Figure 14.6. The third dimension seems to highlight the previously mentioned closeness of Šostakovitš and Bach. The same applies to Sibelius and Bartók.

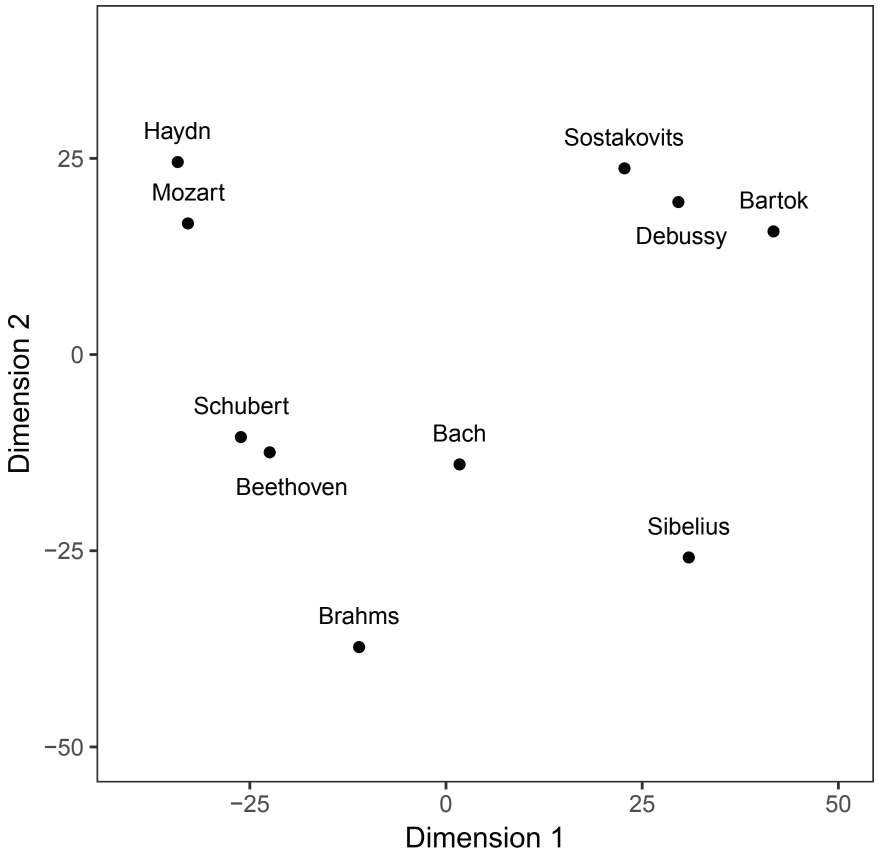


FIGURE 14.5
Resulting map from nonmetric scaling of the classical composers (dimensions 1 and 2).

A further feature of nonmetric scaling that might aid in evaluating solutions is the *Shepard diagram*; this involves a plot of the observed dissimilarities against the corresponding distances obtained from the scaling solution. In an ideal world, the plotted points would fall on a straight line corresponding to a perfect match between the rank order of the dissimilarities and that of the fitted distances. But the world is rarely ideal and such a perfect fit is extremely unlikely in practice. However, such a plot is useful in indicating how far from ‘perfection’ is the scaling solution. The Shepard diagram for the two-dimensional solution from the application of nonmetric scaling to the data on composers is shown in Figure 14.7. Clearly the fit is not perfect but the step function shows that the departure from a straight line is relatively small; this reflects the small value of the stress associated with this solution.

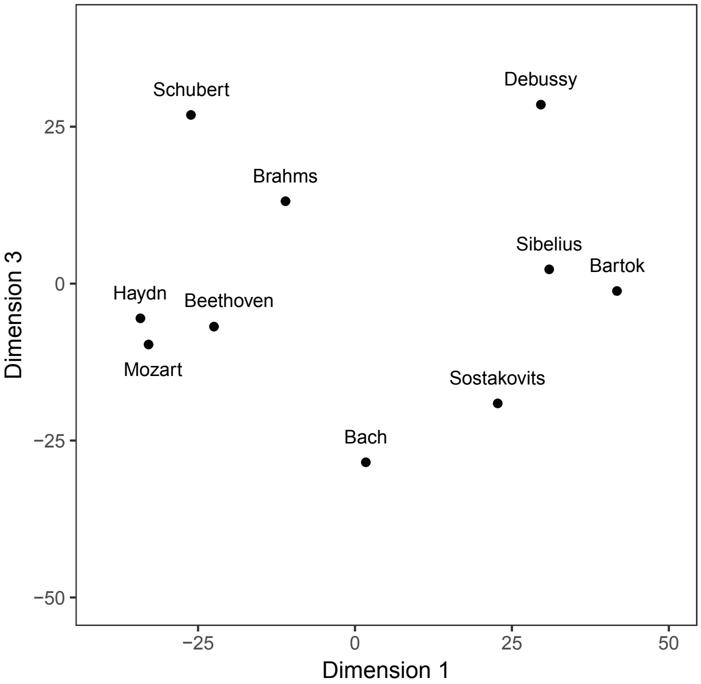


FIGURE 14.6
Resulting map from nonmetric scaling of the classical composers (dimensions 1 and 3).

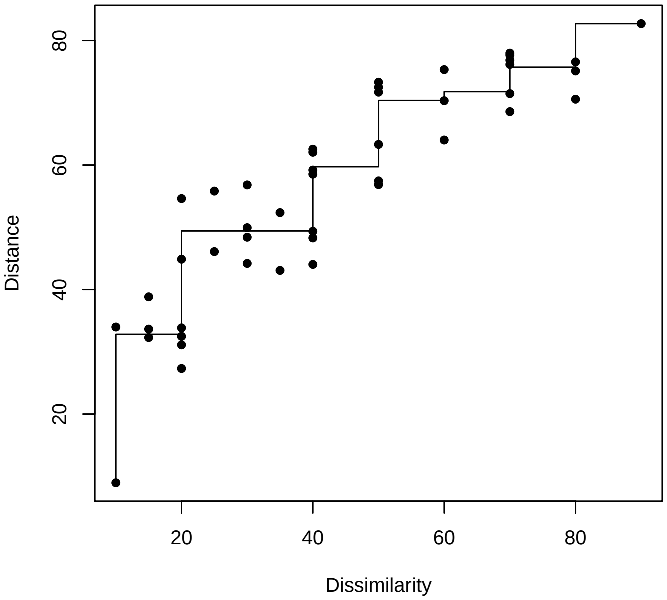


FIGURE 14.7
Shepard diagram for the classical composers' nonmetric scaling.

14.3 Correspondence Analysis

Correspondence analysis (CA) is a versatile method for displaying and analysing categorical data. As with many other multivariate methods, its history can be traced back in the 1930s and 1940s, to the publications of Fisher, among others. However, the essential development of the method took place in France in the 1960s, based on the visionary work of a French linguist and data analyst Jean-Paul Benzécri and his co-workers (Benzécri 1973). The wider dissemination of correspondence analysis outside France began with the books by Lebart et al. (1984), Greenacre (1984), and Benzécri (1992). The French tradition of correspondence analysis and other methods of exploratory multivariate analysis is continued in the recent book by Husson et al. (2017). A detailed bibliographical account of the history of correspondence analysis, spanning (or spinning!) the French, Japanese, and Dutch schools of data analysis, is included in Greenacre (2016). See also Blasius and Greenacre (2014).

Mathematically speaking, correspondence analysis can be regarded as either

- a method for decomposing the chi-squared statistic used to test for independence in a contingency table into components corresponding to different dimensions of the heterogeneity between its columns; or
- a method for simultaneously assigning a scale to the rows and a separate scale to the columns of a table in order to maximize the correlation between the two scales.

Quintessentially, correspondence analysis is a technique for displaying multivariate (often bivariate) categorical data graphically, by deriving coordinates to represent the categories of both the row and the column variables, which may then be plotted to display the pattern of association between the variables graphically.

The basic details of correspondence analysis are given in Technical Section 14.3.

Technical Section 14.3: Correspondence Analysis

Correspondence analysis (CA) is based on straightforward, classical results on matrix theory. The central result is the *singular value decomposition* (SVD), which is the basis of many multivariate statistical methods. We shall briefly summarize the theory behind correspondence analysis. For a more general account of the subject, see Greenacre (2016).

Let $\mathbf{N}$ denote an $I \times J$ data matrix, with positive row and column sums. Typically, the elements of $\mathbf{N}$ represent some form of count data, such as frequencies. Dividing $\mathbf{N}$ by its grand total, $n = \sum_i \sum_j n_{ij}$, converts $\mathbf{N}$ to the *correspondence matrix*, denoted by $\mathbf{P}$:

$$\mathbf{P} = \frac{1}{n}\mathbf{N}$$

The concept of a set of relative frequencies, or a *profile*, is fundamental to correspondence analysis. Profiles have special geometric features, because their elements add up to 1 (or 100%), and that is why graphical representations of data, especially scatterplots, are so central in the method.

The weights assigned to the profiles are called *row and column masses* and they are denoted by

$$r_i = \sum_{j=1}^{J} p_{ij} \quad \text{and} \quad c_i = \sum_{i=1}^{I} p_{ij}$$

or, in matrix form, as vectors

$$\mathbf{r} = \mathbf{P1} \quad \text{and} \quad \mathbf{c} = \mathbf{P}'\mathbf{1}$$

where $\mathbf{1}$ is the vector of ones (either $J \times 1$ or $I \times 1$, to match the dimensions of $\mathbf{P}$ and $\mathbf{P}'$). The coordinates of the row and column profiles are obtained using the SVD as follows.

To begin, we calculate the matrix $\mathbf{S}$ of standardized residuals:

$$\mathbf{S} = \mathbf{D}_r^{-\frac{1}{2}}(\mathbf{P} - \mathbf{rc}')\mathbf{D}_c^{-\frac{1}{2}}$$

where $\mathbf{D}_r = \text{diag}(\mathbf{r})$ and $\mathbf{D}_c = \text{diag}(\mathbf{c})$. The crucial step is the SVD of the matrix $\mathbf{S}$:

$$\mathbf{S} = \mathbf{UD}_\alpha\mathbf{V}'$$

where $\mathbf{U}'\mathbf{U} = \mathbf{V}'\mathbf{V} = \mathbf{I}$ and $\mathbf{D}_\alpha$ is the diagonal matrix of (positive) singular values in descending order ($\alpha_1 \geq \alpha_2 \geq \cdots$) as all essential results are included in these three output matrices of the SVD.

First, from the results of the SVD, we obtain the *principal coordinates* of rows and columns as matrices $\mathbf{F}$ and $\mathbf{G}$, respectively:

$$\mathbf{F} = \mathbf{D}_r^{-\frac{1}{2}}\mathbf{UD}_\alpha \quad \text{and} \quad \mathbf{G} = \mathbf{D}_c^{-\frac{1}{2}}\mathbf{VD}_\alpha$$

We also obtain the eigenvalues or *principal inertias* λ_k:

$$\lambda_k = \alpha_k^2, \quad k = 1, 2, \ldots, K$$

where $K = \min(I - 1, J - 1)$.

The concept of *inertia* refers to the measure of variance in the categorical data. The principal inertia λ_k refers to the inertia accounted for by each of the principal axes $k = 1, 2, \ldots, K$ obtained from the SVD.

The square root of the principal inertia, i.e., the first singular value α_1, can be interpreted as the maximum correlation (also called *canonical correlation*) between the scale values assigned to the categories of the row and column variables.

The principal coordinates **F** and **G** refer to the profiles with respect to principal axes. In the so-called *symmetric map*, where the separate configurations of row profiles and column profiles are overlaid in a joint display, all points are displayed in principal coordinates. This is the most typical way of mapping the results of correspondence analysis as a *biplot*, a general graphical display for multivariate data, see Gabriel (1971), Gabriel and Odoroff (1990), and Greenacre (2010). Strictly speaking, the symmetric map is not a true biplot, but it can be interpreted in the biplot style, see Gabriel (2002).

In a symmetric map summarizing the results of correspondence analysis, the row-to-row and column-to-column Euclidean distances are approximate chi-squared distances between the respective profiles, but there is no specific row-to-column distance interpretation. For a contingency table with I rows and J columns, it can be shown that the chi-squared distances can be represented *exactly* in $\min(I-1, J-1)$ dimensions. When both I and J are greater than three, an exact two-dimensional representation of the chi-squared distances is not possible, so the question of the adequacy of the fit will need to be addressed. In some of these cases, more than two dimensions may be required to give an acceptable fit (again for details, see Greenacre, 2016).

The symmetric map is interpreted by examining the positions of the points representing the categories of the row and column variables. Assuming that a two-dimensional solution provides an adequate fit for the data, row points that are close together represent row categories that have similar profiles across columns. Accordingly, column points that are close together indicate columns with similar profiles down the rows. Finally, row points that lie close to column points represent a row/column combination that occurs more frequently in the table than would be expected if the row and column variables were independent. Conversely, row and column points that are distant from one another indicate a cell in the table where the count is lower than would be expected under independence.

Next we will consider a simple example of the application of correspondence analysis.

14.3.1 Simple Example of the Application of Correspondence Analysis

The data shown in Table 14.8 is concerned with the influence of a girl's age on her relationship with her boyfriend. In this table, each of 139 girls has been classified into one of three groups:

TABLE 14.8
The Influence of Age of Relationship Status with Boyfriends: Observed Frequencies along with Expected Frequencies (in Parentheses)

	Age group					
Relationship	**< 16**	**16–17**	**17–18**	**18–19**	**19–20**	**Total**
No boyfriend	21	21	14	13	8	77
(expected)	(17.2)	(18.3)	(13.3)	(17.2)	(11.1)	
Boyfriend: No sex	8	9	6	8	2	33
(expected)	(7.4)	(7.8)	(5.7)	(7.4)	(4.7)	
Boyfriend: Sex	2	3	4	10	10	29
(expected)	(6.5)	(6.9)	(5.0)	(6.5)	(4.2)	
Total	31	33	24	31	20	139

- No boyfriend,
- Boyfriend: No sex(ual intercourse),
- Boyfriend: Sex(ual intercourse).

In addition, the age of each girl was recorded and used to divide the girls into five age groups. According to the labels in Table 14.8 the groups might seem overlapping but to be precise, 16–17 means ‘16 but less than 17’, and hence all the girls in the data are teenagers.

The standard analysis for such a contingency table would involve the calculation of the usual chi-square statistic for assessing independence of row and column variables. This involves first calculating the expected values under the assumption of independence—these are given in Table 14.8; details of their calculation and of the chi-square test itself are given in any introductory statistics text. For Table 14.8 the value of the statistic is 20.6 with eight degrees of freedom. The associated p-value is 0.008. Clearly the relationship groups and age are not independent, a result that will only be a surprise to our readers who have lived a rather sheltered life.

Now let us apply correspondence analysis to the data. The result is the two-dimensional map of the categories shown in Figure 14.8. The adequacy of the fit need not to be addressed, as the relationship variable includes only three categories and hence the chi-squared distances are represented exactly by the Euclidean distances in two dimensions. The principal inertia (defined earlier) is 0.141 (95.4%) for the first dimension and only 0.007 (4.6%) for the second dimension. It can be inferred that actually one dimension would be enough to account for the associations of the relationship data. Interpretation of the diagram involves examination of the positions of the points representing the row and column categories of Table 14.8.

Examining the plot in Figure 14.8, we see that it tells the age-old story of girls travelling through their teenage years, initially having no boyfriend, then acquiring a boyfriend, and then having sex with their boyfriend, a story

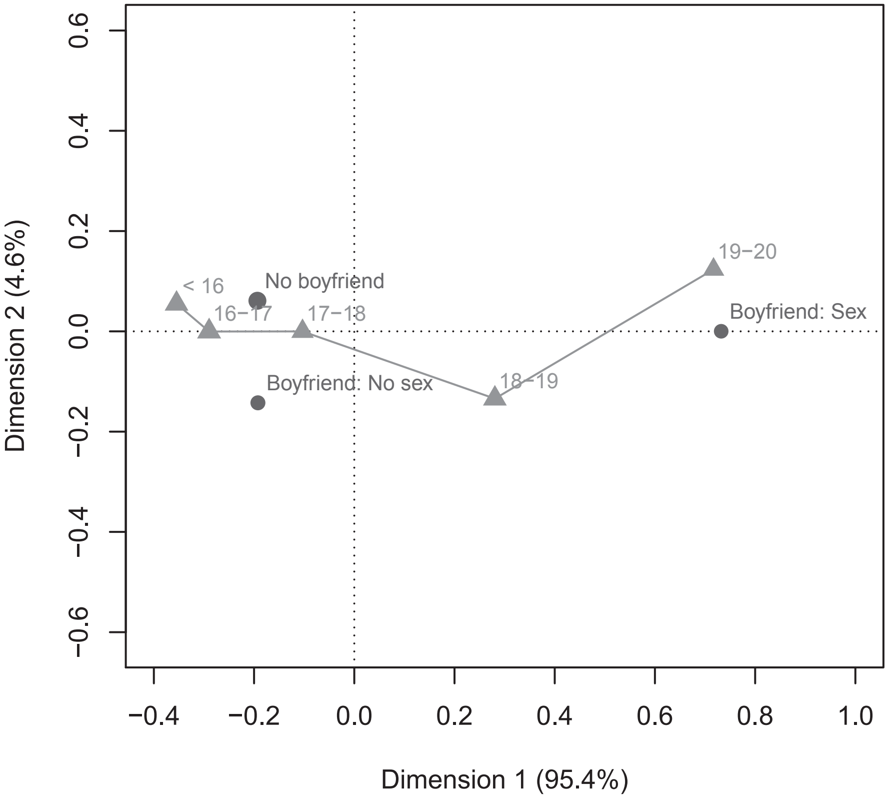


FIGURE 14.8
Resulting map from correspondence analysis of the age and the relationships with boyfriends of 139 girls.

that has broken the hearts of fathers everywhere, at least temporarily, until their wives suggest they reflect back to the time when they themselves were teenagers.

14.3.2 Connections of Work Activities and Job Advantages

Let us look at another example of CA that will be a bit more challenging for the interpretation compared to the simple example in the previous subsection. The main reason is that the following example, taken from Lebart et al. (1984), involves larger dimensions, both in respect to the number of observations and the number of categories in the data. The context of the study is a typical survey research, where people fill up a questionnaire with many of the questions being categorical. In one of the questions, the respondents had to select a type of work activity that best describes their job (e.g., 'farming', 'construction', 'social services', 'teaching', 'domestic work', 'small business' etc.). In another question, they had to choose the main advantage in their job, again from a

TABLE 14.9
Types of Work Activities and Main Advantages of Job from 6933 Survey Respondents (Lebart et al., 1984)

	Main Advantage of Job							
Type of Work Activity	**VARIETY**	**FREEDOM**	...	**LIKE IT**	**OTHER**	**NONE**	**OUTDOORS**	**NO ANS**
Farming–fishing	4	189	...	11	15	12	8	1
Farm–food industry	1	13	...	9	5	11	0	0
Energy–mines	1	9	...	4	3	6	1	0
Steel	5	5	...	2	3	22	0	0
Chemical–glass–oil	2	7	...	3	0	5	0	1
Wood–paper	2	5	...	1	0	3	0	2
Auto–aviation–shipping	2	3	...	6	1	24	0	1
Textile–leather–shoes	3	18	...	6	2	26	0	2
Pharmaceutical industries	3	7	...	2	1	8	0	0
Manufacturing	0	18	...	10	4	26	0	6
Construction	7	63	...	14	8	35	2	2
Food–grocery	2	43	...	6	1	7	0	3
Small business	8	95	...	13	4	18	1	3
Miscellaneous business	5	32	...	8	3	18	0	3
Administrative services	8	26	...	6	9	16	3	4
Telecommunications	1	7	...	1	3	5	0	2
Social services	4	10	...	3	2	1	0	1
Health services	3	31	...	24	1	5	0	5
Teaching–research	2	33	...	18	3	11	1	3
Transportation	2	19	...	3	3	13	0	1
Insurance–banking	8	12	...	3	1	10	0	3
Domestic workers	0	8	...	2	2	11	1	1
Other services	8	35	...	11	4	14	0	1
Printing–publishing	2	13	...	5	4	11	0	2
Private services	3	26	...	10	3	8	0	2
No answer	0	14	...	5	1	3	0	3

set of given alternatives (e.g., 'variety', 'freedom', 'salary', 'being outdoors' etc.) including categories 'other' and 'none'. Missing answers constituted their own categories on both questions. After the usual, time-consuming hard work of data cleanup, recoding, joining of some categories as well as other initial tasks and necessary checkings, the data set, consisting of 6933 observations was ready for the analyses.

Again we begin with a cross table, as both variables of interest are clearly nominal measurements with no real order within their categories. The variables have been cross-classified to form a contingency table of 26 categories for the type of the work activity and 17 categories for the main advantage of job. Part of the table is shown in Table 14.9. The result of the correspondence analysis is the two-dimensional map of the categories shown in Figure 14.9. A clear difference to the earlier example is that only about 57% of the total inertia of the table is explained. The first dimension accounts for 36.4% and the second dimension for 21.3% of the inertia. The adequacy of the fit

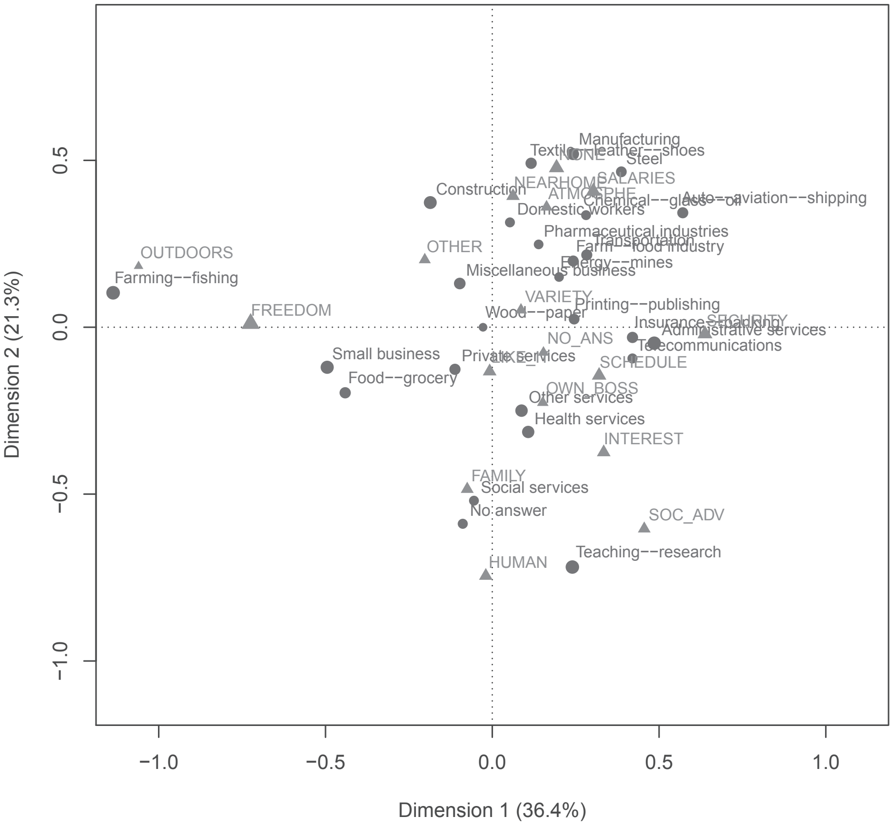


FIGURE 14.9
Resulting map from correspondence analysis of the work activities and main advantages of jobs (symbol sizes proportional to the row and column masses of the points).

would need to be addressed in more detail and perhaps additional dimensions should be analyzed. Another difference is that, because of the size of the data, understanding any associations in the data by looking at the plain numbers is quite impossible. A graph will certainly reveal to the eye much more than $26 \times 17 = 442$ numbers.

We restrict ourselves to a brief interpretation of the map in Figure 14.9. The horizontal dimension seems to be related to the size of the workplace, from smaller ones on the left to the various large companies on the right. The corresponding advantages vary from being outdoors, having freedom, through family and human aspects to salaries, social advantages, schedules, and security. The vertical dimension goes from various service activities on the bottom to factory work, where again the different advantages (including 'near home' and a bit depressed sounding 'none'!) correspond to the work activities perhaps in a quite expected way. The 'no answer' categories of both variables appear about in the middle of their scales.

Correspondence analysis and its variations such as multiple correspondence analysis, joint correspondence analysis, and canonical correspondence analysis are described in detail in Greenacre (2016). Examples of the application of multiple correspondence analysis appear in Greenacre and Blasius (2006). Readers contemplating using correspondence analysis are strongly advised to consult such references using the necessarily brief account given in this chapter only as an initial stepping stone.

14.4 Summary

- Multidimensional scaling and correspondence analysis both aim to help in understanding particular types of data by displaying the data graphically.
- Multidimensional scaling applied to proximity matrices is often useful in uncovering the dimensions on which similarity judgements are made.
- For more complete accounts of multidimensional scaling, including least-squares and other methods, see, for example, Groenen and Borg (2014), Cox and Cox (2001) or Everitt and Rabe-Hesketh (1997).
- Correspondence analysis is often a useful supplement to the routine chi-square test applied to contingency tables.
- For more information of the connections between correspondence analysis and other multivariate methods, together with more general biplot techniques to visualize the results of these methods, see Greenacre (2010).

14.5 Exercises

(excluded from MABS for IODS)

Part VI

Analysis of longitudinal data (“MABS for IODS”)

Selected excerpts of the textbook *Multivariate Analysis for the Behavioral Sciences*, Second Edition (Vehkalahti and Everitt, 2019), produced exclusively for the students of IODS (Introduction to Open Data Science, University of Helsinki), with a permission from Chapman and Hall/CRC, London, UK.

8 Analysis of Longitudinal Data I: Graphical Displays and Summary Measure Approach

Many studies in the behavioral sciences involve several measurement or observations of the response variable of interest on each subject in the study. For example, the response variable may be measured under a number of different experimental conditions or on a number of different occasions over time; such data are labelled repeated measures or longitudinal data. In this chapter useful methods for the graphical exploration of this type of data are described and a simple method for their analysis is introduced, with the warning that although simple the method should be used only in the initial stage of dealing with the data; more appropriate methods will be the subjects of the next two chapters.

9 Analysis of Longitudinal Data II: Linear Mixed Effects Models for Normal Response Variables

Longitudinal data, where a response variable is measured on each subject on several different occasions poses problems for their analysis because the repeated measurements on each subject are very likely to be correlated rather than independent. In this chapter methods for dealing with longitudinal data which aim to account for the correlated nature of the data and where the response is assumed to be normally distributed are discussed, and then applied to several sets of data including a study of the use of computerized delivery of cognitive behavioral therapy.

8

Analysis of Longitudinal Data I: Graphical Displays and Summary Measure Approach

8.1 Introduction

Previous chapters (3–7) have looked at ways to model and analyse data where there is a single random response variable and a number of explanatory variables considered to be fixed rather than random; it is sometime helpful to refer to such data as *multivariable* rather than *multivariate* keeping the latter for data sets containing a number of variables but with no division into response and explanatory and where all variables are considered random. Analysing such data will be the subject of Chapters 13–18. In this chapter and the following two chapters we consider data that comes somewhere between multivariable and multivariate. As with the former there is a division into explanatory and response variables, but now the response variable (and possibly some or all of the explanatory variables) is observed more than once on each individual in the study and so could be labelled multivariate.

In behavioral research, data with a multivariate response are common; for example, a response variable may be measured under a number of different experimental conditions, leading to what are generally called *repeated measures data*, or a response variable may be recorded on several different occasions over some period of time, in which case we have *longitudinal data*. (Although we think distinguishing two different types of data here is useful, it has to be said that the repeated measures label is often used for both types of data.) The variation among the repeated measures of the response is *within-subject variation*. But often one of the covariates will be a factor such as gender or treatment that will give rise to *between-subject variation*. Longitudinal data occur most frequently in the behavioral sciences in the clinical trials frequently undertaken by psychologists, psychiatrists and others to assess the effectiveness or otherwise of different treatments; it is largely this type of data which will be the subject of this chapter and the two following chapters.

As several observations of the response variable are made on the same individual, it is likely that the repeated measurements of the response will be correlated rather than independent even after conditioning on the explanatory variables. Consequently, for the analysis of repeated measures data and for longitudinal data, models are needed that can both assess the effects of

TABLE 8.1
BPRS Measurements from 40 Subjects

		Week								
Treatment	**Subject**	**0**	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**
1	1	42	36	36	43	41	40	38	47	51
1	2	58	68	61	55	43	34	28	28	28
1	3	54	55	41	38	43	28	29	25	24
1	4	55	77	49	54	56	50	47	42	46
1	5	72	75	72	65	50	39	32	38	32
1	6	48	43	41	38	36	29	33	27	25
1	7	71	61	47	30	27	40	30	31	31
1	8	30	36	38	38	31	26	26	25	24
1	9	41	43	39	35	28	22	20	23	21
1	10	57	51	51	55	53	43	43	39	32
1	11	30	34	34	41	36	36	38	36	36
1	12	55	52	49	54	48	43	37	36	31
1	13	36	32	36	31	25	25	21	19	22
1	14	38	35	36	34	25	27	25	26	26
1	15	66	68	65	49	36	32	27	30	37
1	16	41	35	45	42	31	31	29	26	30
1	17	45	38	46	38	40	33	27	31	27
1	18	39	35	27	25	29	28	21	25	20
1	19	24	28	31	28	29	21	22	23	22
1	20	38	34	27	25	25	27	21	19	21
2	1	52	73	42	41	39	38	43	62	50
2	2	30	23	32	24	20	20	19	18	20
2	3	65	31	33	28	22	25	24	31	32
2	4	37	31	27	31	31	26	24	26	23
2	5	59	67	58	61	49	38	37	36	35
2	6	30	33	37	33	28	26	27	23	21
2	7	69	52	41	33	34	37	37	38	35
2	8	62	54	49	39	55	51	55	59	66
2	9	38	40	38	27	31	24	22	21	21
2	10	65	44	31	34	39	34	41	42	39
2	11	78	95	75	76	66	64	64	60	75
2	12	38	41	36	27	29	27	21	22	23
2	13	63	65	60	53	52	32	37	52	28
2	14	40	37	31	38	35	30	33	30	27
2	15	40	36	55	55	42	30	26	30	37
2	16	54	45	35	27	25	22	22	22	22
2	17	33	41	30	32	46	43	43	43	43
2	18	28	30	29	33	30	26	36	33	30
2	19	52	43	26	27	24	32	21	21	21
2	20	47	36	32	29	25	23	23	23	23

explanatory variables on the multiple measures of the response variable and account for the likely correlations between these multiple measures. Suitable models for longitudinal data will be described in Chapters 9 and 10. But before consideration of such models we will in this chapter look at how to display such data graphically and a possible “quick and dirty” approach to their analysis.

8.2 Graphical Displays of Longitudinal Data

Graphical displays of data are almost always useful for exposing patterns in the data, particularly when these are unexpected; this might be of great help in suggesting which class of models might be most sensibly applied in the later more formal analysis. According to Diggle et al. (2002), there is no single prescription for making effective graphical displays of longitudinal data, although they do offer the following simple guidelines:

- Show as much of the relevant raw data as possible rather than only data summaries;
- Highlight aggregate patterns of potential scientific interest;
- Identify both cross-sectional and longitudinal patterns;
- Try to make the identification of unusual individuals or unusual observations simple.

A number of graphical displays which can be useful in the preliminary assessment of longitudinal data from clinical trials will now be illustrated using the data shown in Table 8.1 taken from Davis (2002). Here 40 male subjects were randomly assigned to one of two treatment groups and each subject was rated on the brief psychiatric rating scale (BPRS) measured before treatment began (week 0) and then at weekly intervals for eight weeks. The BPRS assesses the level of 18 symptom constructs such as hostility, suspiciousness, hallucinations and grandiosity; each of these is rated from one (not present) to seven (extremely severe). The scale is used to evaluate patients suspected of having schizophrenia.

To begin we shall plot the BPRS values for all 40 men, differentiating between the treatment groups into which the men have been randomized. The resulting diagram is shown in Figure 8.1. This simple graph makes a number of features of the data readily apparent. First, the BPRS score of almost all the men is decreasing over the eight weeks of the study. Second, the men who have higher BPRS values at the beginning tend to have higher values throughout the study. This phenomenon is generally referred to as *tracking.*

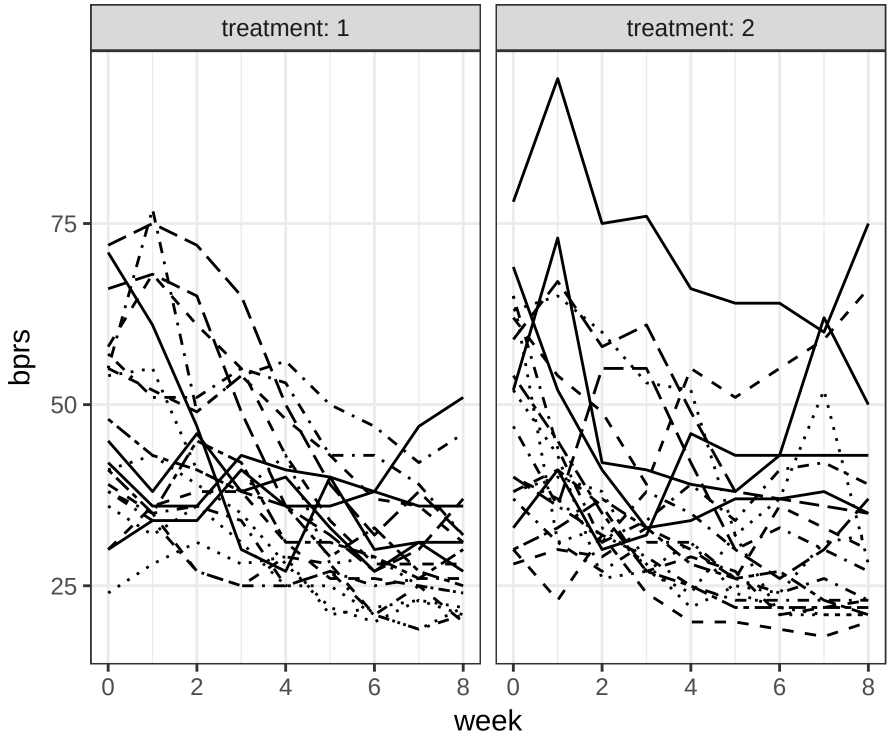


FIGURE 8.1
Individual response profiles by treatment group for the BPRS data.

Third, there are substantial individual differences and variability appears to decrease with time.

The tracking phenomenon can be seen more clearly in a plot of the standardized values of each observation, i.e., the values obtained by subtracting the relevant occasion mean from the original observation and then dividing by the corresponding visit standard deviation. This plot is shown in Figure 8.2.

With large numbers of observations, graphical displays of individual response profiles are of little use and investigators then commonly produce graphs showing average profiles for each treatment group along with some indication of the variation of the observations at each time point. The result is Figure 8.3. There is considerable overlap in the mean profiles of the two treatment groups suggesting perhaps that there is little difference between the two groups with respect to the mean BPRS values.

A possible alternative to plotting the mean profiles as in Figure 8.3 is to graph side-by-side box plots of the observations at each time point. The resulting plot is shown in Figure 8.4. The plot suggests the presence of some possible "outliers" at a number of time points and indicates again the general

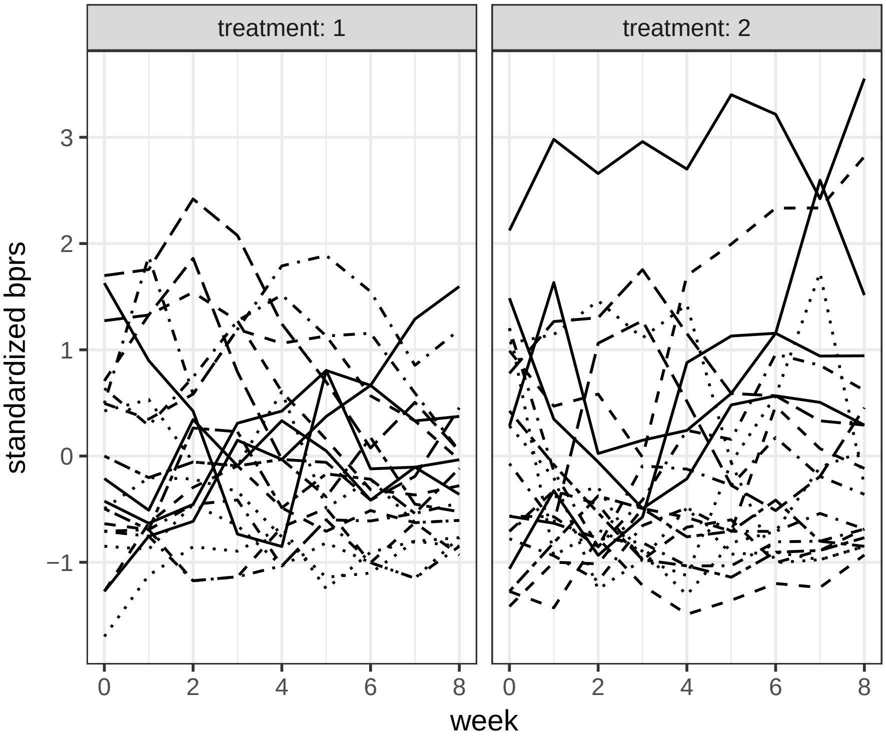


FIGURE 8.2
Individual response profiles for BPRS data after standardization.

decline in BPRS values over the eight weeks of the study in both treatment groups.

Another graphic for longitudinal data that is often helpful in making informed decisions about models that might be appropriate for the data is the scatterplot matrix. But we shall leave consideration of this type of plot until the next chapter when we begin to discuss possible models for longitudinal data.

8.3 Summary Measure Analysis of Longitudinal Data

According to Matthews (2005) "the use of summary measures is one of the most important and straightforward methods for the analysis of longitudinal data". The approach is certainly straightforward but as to "most important" we think not. The models to be described in the next two chapters are of far

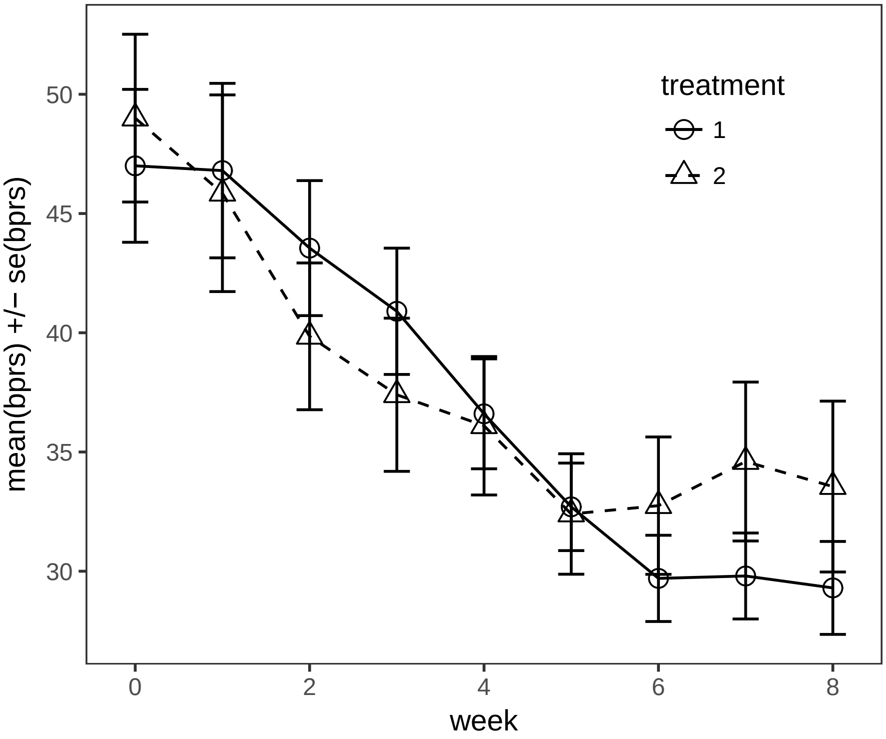


FIGURE 8.3
Mean response profiles for the two treatment groups in the BPRS data.

greater importance for dealing appropriately with longitudinal data. Nevertheless we will describe the summary measure method (often also called the response feature method) here because it may be helpful in some cases for an initial assessment of longitudinal data.

The summary measure method operates by transforming the repeated measurements made on each individual in the study into a single value that captures some essential feature of the individual's response over time. Analysis then proceeds by applying standard univariate methods to the summary measures from the sample of subjects (see later examples). The approach has been in use for many years, and is described in Oldham (1962), Yates (1982) and Matthews et al. (1990).

8.3.1 Choosing Summary Measures

The key step to a successful summary measure analysis of longitudinal data is the choice of a relevant summary measure. The chosen measure needs to be

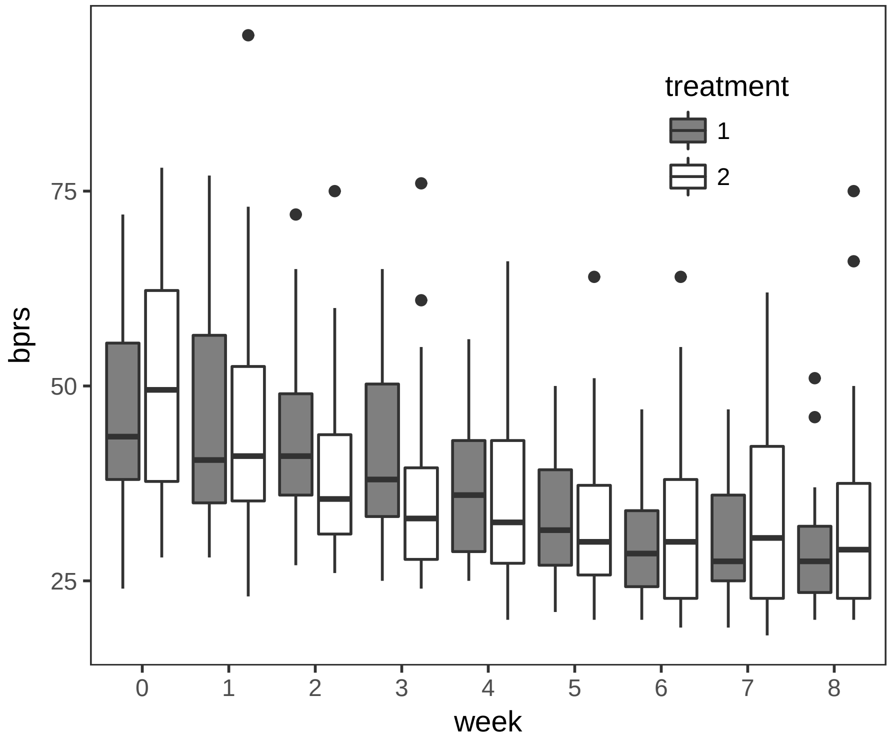


FIGURE 8.4
Boxplots for the BPRS data.

relevant to the particular questions of interest in the study and in the broader scientific context in which the study takes place. In some longitudinal studies, more than a single summary measure might be deemed relevant or necessary, in which case the problem of combined inference may need to be addressed. More often in practice, however, it is likely that the different measures will deal with substantially different questions so that each will have a notional interpretation in its own right. In most investigations, the decision over what summary measure to use needs to be made before the data are collected.

A wide range of possible summary measures have been proposed. Those given in Table 8.2, for example, were suggested by Matthews et al. (1990). Frison and Pocock (1992) argue that the average response to treatment over time is often likely to be the most relevant summary statistic in treatment trials. In some cases the response on a particular visit may be chosen as the summary statistic of most interest, but this must be distinguished from the generally flawed approach which separately analyses the observations at each and every time point.

TABLE 8.2
Possible Summary Measures

Type of Data	Question of Interest	Summary Measure
Peaked	Is overall value of outcome variable the same in different groups?	Overall mean (equal time intervals) or area under curve (unequal intervals)
Peaked	Is maximum (minimum) response different between groups?	Maximum (minimum) value
Peaked	Is time to maximum (minimum) response different between groups?	Time to maximum (minimum) response
Growth	Is rate of change of outcome different between groups?	Regression coefficient
Growth	Is eventual value of outcome different between groups?	Final value of outcome or difference between last and first values or percentage change between first and last values
Growth	Is response in one group delayed relative to the other?	Time to reach a particular value (e.g. a fixed percentage of baseline)

8.3.2 Applying the Summary Measure Approach

As our first example of the summary measure approach it will be applied to the post treatment values of the BPRS in Table 8.1. The mean of weeks 1 to 8 will be the chosen summary measure. We first calculate this measure and then look at boxplots of the measure for each treatment group. The resulting plot is shown in Figure 8.5. The diagram indicates that the mean summary measure is more variable in the second treatment group and its distribution in this group is somewhat skew. The boxplot of the second group reveals an outlier, a subject whose mean BPRS score of the eight weeks is over 70. It might bias the conclusions from further comparisons of the groups, so we decide to remove that subject from the data. The new version of the boxplots is shown in Figure 8.6. Without the outlier, the eight-week mean of the second treatment group is lower than of the first group, but there is still little evidence of a difference in location of the summary measure distributions in each group.

Although the informal graphical material presented up to now has all indicated a lack of difference in the two treatment groups, most investigators would still require a formal test for a difference. Consequently we shall now apply a t-test to assess any difference between the treatment groups, and also

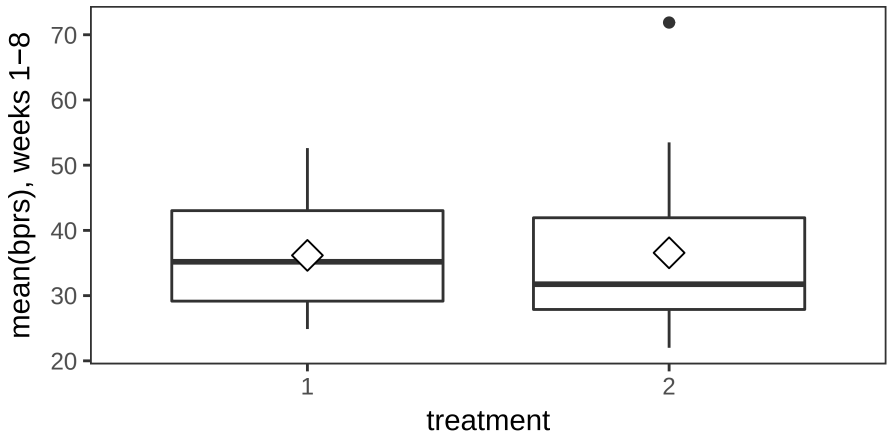


FIGURE 8.5
Boxplots of mean summary measures for the two treatment groups in the BPRS data.

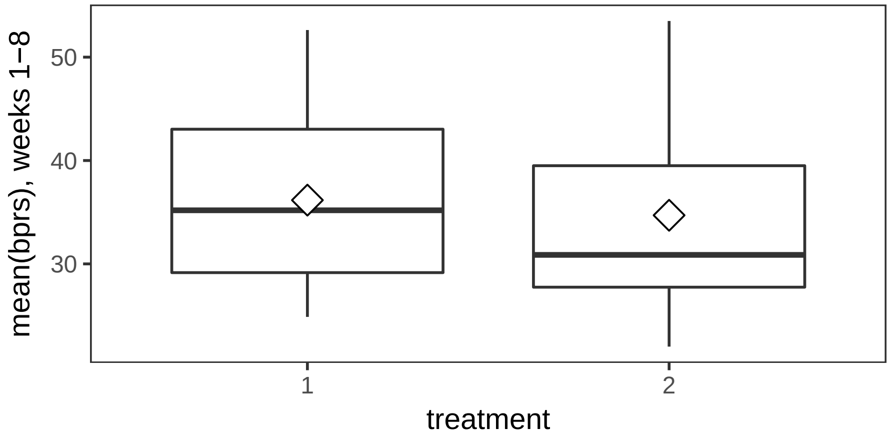


FIGURE 8.6
Boxplots of mean summary measures for the two treatment groups in the BPRS data, without the outlier shown in Figure 8.5.

calculate a confidence interval for this difference. We use the data without the outlier that was revealed in Figure 8.5. The results are shown in Table 8.3. The *t*-test confirms the lack of any evidence for a group difference. Also the 95% confidence interval is wide and includes the zero, allowing for similar conclusions to be made.

TABLE 8.3
Results From an Independent Samples *t*-test on the Mean Summary Measure for the BPRS Data, Without the Outlier Shown in Figure 8.5

	Treatment 1	**Treatment 2**	**Difference**	**t-Value**	**Pr(>|t|)**
Mean	36.16875	34.70395	1.4648	0.52095	0.6055
	95% confidence interval for the mean difference: [−4.23, 7.16]				

Note: Student's two sample *t*-test (two-sided) on 37 DF.

8.3.3 Incorporating Pre-Treatment Outcome Values into the Summary Measure Approach

Baseline measurements of the outcome variable in a longitudinal study are often correlated with the chosen summary measure and using such measures in the analysis can often lead to substantial gains in precision when used appropriately as a covariate in an analysis of covariance (see Everitt and Pickles, 2004). We can illustrate the analysis on the data in Table 8.1 using the BPRS value corresponding to time zero taken prior to the start of treatment as the baseline covariate. The results are shown in Table 8.4. We see that the baseline BPRS is strongly related to the BPRS values taken after treatment has begun, but there is still no evidence of a treatment difference even after conditioning on the baseline value.

TABLE 8.4
Results from an Analysis of Covariance of the BPRS Data with Baseline BPRS and Treatment Group as Covariates

Source	**Sum of Squares**	**Df**	**Mean Square**	**F**	**p-Value**
Baseline	1868.07	1	1868.07	30.1437	3.077e-06
Treatment	3.45	1	3.45	0.0557	0.8148
Residuals	2292.97	37	61.97	–	–

8.3.4 Dealing with Missing Values when Using the Summary Measure Approach

One of the problems that often occurs in the collection of longitudinal data is that a subject may not have values of the outcome measure recorded on all the occasions intended. This problem will be considered in detail in later chapters, but as an example of where it has arisen we can examine the data shown in Table 8.5 (taken from Davis, 2002). The data come from a clinical trial comparing two treatments for maternal pain relief during labour. In this study 83 women in labour were randomized to receive an experimental pain medication (43 subjects) or placebo (40 subjects). Treatment was initiated

TABLE 8.5
Pain Scores from 83 Women in Labour: 43 Subjects in Group 1 (Medication) and 40 Subjects in Group 2 (Placebo); First 20 Subjects in Each Group

Self-reported Pain Scores at 30-minute intervals								
Group	**Subject**	**0**	**30**	**60**	**90**	**120**	**150**	**180**
1	1	0.0	0.0	0.0	0.0			
1	2	0.0	0.0	0.0	0.0	2.5	2.3	14.0
1	3	38.0	5.0	1.0	1.0	0.0	5.0	
1	4	6.0	48.0	85.0	0.0	0.0		
1	5	19.0	5.0					
1	6	7.0	0.0	0.0	0.0			
1	7	44.0	42.0	42.0	45.0			
1	8	1.0	0.0	0.0	0.0	0.0	6.0	24.0
1	9	24.5	35.0	13.0				
1	10	1.0	30.5	81.5	67.5	98.5	97.0	
1	11	35.5	44.5	55.0	69.0	72.5	39.5	26.0
1	12	0.0	0.0	0.0	0.0	0.0	0.0	0.0
1	13	8.0	30.5	26.0	24.0	29.0	45.0	91.0
1	14	7.0	6.5	7.0	4.0	10.0		
1	15	6.0	8.5	19.5	16.5	42.5	45.5	48.5
1	16	32.5	9.5	7.5	5.5	4.5	0.0	7.0
1	17	10.5	10.0	18.0	32.5	0.0	0.0	0.0
1	18	11.5	20.5	32.5	37.0	39.0		
1	19	72.0	91.5	4.5	32.0	10.5	10.5	10.5
1	20	0.0	0.0	0.0	0.0	13.54	7.0	
2	1	4.0	9.0	30.0	75.0	49.0	97.0	
2	2	0.0	0.0	1.0	27.5	95.0	100.0	
2	3	9.0	6.0	25.0				
2	4	52.5	18.0	12.5				
2	5	90.5	99.0	100.0	100.0	100.0	100.0	100.0
2	6	74.0	70.0	81.5	94.5	97.0		
2	7	0.0	0.0	0.0	1.5	0.0	18.0	71.0
2	8	0.0	51.5	56.0				
2	9	6.5	7.0	7.0	9.0	25.0	36.0	20.0
2	10	19.0	31.0	41.0	58.0			
2	11	6.0	23.0	45.0	67.0	90.5		
2	12	42.0	64.0	6.0				
2	13	86.5	53.0	88.0	100.0	100.0		
2	14	50.0	100.0	100.0	100.0	100.0		
2	15	27.5	36.5	74.0	97.0	100.0	100.0	95.0
2	16	0.0	0.0	6.0	6.0			
2	17	62.0	79.0	80.5	85.0	90.0	97.5	97.0
2	18	17.5	27.5	21.0	60.0	80.0	97.0	
2	19	6.5	5.5	18.5	20.0	36.5	63.5	81.5
2	20	8.0	9.0	35.5	39.0	70.0	92.0	98.0

when the cervical dilation was 8cm. At 30-minute intervals, the amount of pain was self-reported by placing a mark on a 100mm line (0 = no pain, 100 = very much pain). Table 8.5 gives the data for the first 20 subjects in each group.

If we use the mean as a summary measure for these data, the missing values can be dealt with by (a) simply leaving out the subjects with any missing values or (b) calculating, for each subject, the mean of their available values. So, for example, for subject one in group one this would be the mean of four values, and for subject five in the same group, the mean of only two values. Both approaches are very straightforward but there are a number of possible problems which for the moment we shall conveniently ignore. The difficulties of missing values in data in general, and longitudinal data in particular will be considered in Chapter 11. Here we shall carry out both possibilities mentioned to see how the results compare. These results are shown in Table 8.6.

In both cases, the mean difference is statistically significant, but in alternative a) about 60 % of the values are discarded, when the means are computed. The alternative b) uses all available values, and therefore the *p*-value is even smaller and the corresponding confidence interval for the mean difference (that now does not include the zero) is narrower.

TABLE 8.6
Results from an Independent Samples *t*-test for the Mean Summary Measure Used on the Data Partially Shown in Table 8.5. (a) Leaving Out Subjects with Any Missing Value, (b) Mean of Available Values for Each Subject

	Treatment 1	**Treatment 2**	**Difference**	**t-Value**	**Pr(>|t|)**
Mean a)	16.74286	46.80000	−30.05714	−3.8465	0.00054
Mean b)	18.34181	41.03771	−22.69590	−4.1455	0.00008

a) 95% confidence interval for the mean difference: [−45.97, −14.14]
b) 95% confidence interval for the mean difference: [−33.59, −11.80]

Note: Student's two sample *t*-test (two-sided) on a) 32 DF, b) 81 DF.

8.4 Summary

- The methods described in this chapter are most (only) suitable for an initial exploration and initial analysis of longitudinal data.

- The graphical methods can provide insights into both potentially interesting patterns of response over time and the structure of any treatment differences. In addition, they can indicate possible outlying observations that may need special attention.

- The response feature approach to analysis has the distinct advantage that it is straightforward, can be tailored to consider aspects of the data thought to be particularly relevant, and produces results which are relatively simple to understand.

- Depending on the chosen summary measure, the approach can often accommodate data containing missing values without difficulty, although it might be misleading if the observations are anything other than missing completely at random (see Chapter 11).

- But, although simple to apply, the summary measure approach has a number of distinct drawbacks; one such is that it forces the investigator to focus on only a single aspect of the repeated measurements over time.

- It seems intuitively clear that when several repeated measures are replaced by a single number summary, there must necessarily be some loss of information. And it is possible for individuals with quite different response profiles to have the same or similar values for the chosen summary measure.

- Finally, the simplicity of the summary measure method is lost when there are missing data or the repeated measures are irregularly spaced as is the methods efficiency; the methods to be described in the next two chapters are more efficient than a summary measure analysis and can also handle missing data with minimal difficulty.

8.5 Exercises

(excluded from MABS for IODS)

9

Analysis of Longitudinal Data II: Linear Mixed Effects Models for Normal Response Variables

9.1 Introduction

The summary measure approach to the analysis of longitudinal data described in the previous chapter sometimes provides a useful first step in making inferences about the data, but it is really only ever a first step, and a more complete and a more appropriate analysis will involve fitting a suitable model to the data and estimating parameters that link the explanatory variables of interest to the repeated measures of the response variable.

The main objective in the analysis of data from a longitudinal study is to characterize change in the repeated values of the response variable and to determine the explanatory variables most associated with any change. Because several observations of the response variable are made on the same individual, it is likely that the measurements will be correlated rather than independent, even after conditioning on the explanatory variables. Consequently models for longitudinal data need to include parameters analogous to the regression coefficients in the usual multiple regression model (see Chapter 4) that relate the explanatory variables to the repeated measurements, and, in addition, parameters that account adequately for the correlational structure of the repeated measurements of the response variable.

It is the regression coefficients that are generally of most interest with the correlational structure parameters often being regarded as *nuisance parameters*. However, providing an adequate model for the correlational structure of the repeated measures is necessary to avoid misleading inferences about those parameters that are of primary relevance to the researcher, as is made clear in Fitzmaurice et al. (2011); these authors emphasize that although the estimation of the correlational structure of the repeated measurements is usually regarded as a secondary aspect of any analysis (relative to the mean response over time), the estimated correlational structure must describe the actual correlational structure present in the data relatively accurately to avoid making misleading inferences on the substantive parameters.

Over the last decade or two, methodology for the analysis of repeated measures data has been the subject of much research and development, and there are now a variety of powerful techniques available. A comprehensive account of these methods is given in Diggle et al. (2002) and Davis (2002). In this chapter we will concentrate on a single class of methods, *linear mixed effects models*, suitable for responses that can be assumed to be approximately normally distributed after conditioning on the explanatory variables. Non-normal responses will be the subject of Chapter 10.

9.2 Linear Mixed Effects Models for Repeated Measures Data

Linear mixed effects models for repeated measures data formalize the idea that an individual's pattern of responses is likely to depend on many characteristics of that individual, including some that are unobserved. These unobserved variables are included in the model as random variables, that is, *random effects*. The essential feature of the model is that the (usually positive) correlation among the repeated measurements on the same individual arises from shared, unobserved variables. Fitzmaurice et al. (2011) suggest several possible sources of correlation in longitudinal data including the following:

- Between-individual heterogeneity reflecting natural variation in individuals' propensity to respond—some consistently respond higher than the average and others consistently lower—the result being positive correlation between the repeated measurements of the response.

- Within-individual biological variation—the notion here is that some underlying biological process (or processes) that change through time in a relatively smooth and continuous fashion leads to random deviations from an individual's underlying response trajectory being more similar when measurements are obtained very close together in time—with the consequence that measurements taken closely together will typically be more highly correlated than measurements that are further separated in time.

Conditional on the values of the random effects, the repeated measurements are assumed to be independent, the so-called *local independence assumption*.

Two examples of linear mixed effects models, namely the *random intercept model* and the *random intercept and slope model* are introduced and described in Technical Section 9.1.

Technical Section 9.1: Introducing Linear Mixed Effects Models

Consider a simple set of longitudinal data in which a number of individuals each has values of a response variable recorded at times $t_1, t_2, \dots, t_r$. (We assume the same set of time points for each individual to make the description of linear mixed effects models simpler, but longitudinal data in which each individual is observed at a different set of time points present no problems for such models.)

Let y_{ij} represent the value of the response for individual i at time t_j with $j = 1, 2, \dots, r$ and $i = 1, 2, \dots, n$. If the repeated measurements of the response variable are independent of one another, then the fact that sets of r observations come from the same individual could be ignored, and the data might be described by a simple linear regression model of the form

$$y_{ij} = \beta_0 + \beta_1 t_j + \varepsilon_{ij}$$

but for repeated measures data, independence is very unlikely, so this model is not appropriate. A possible model for the y_{ij} that does not assume independence is

$$y_{ij} = \beta_0 + \beta_1 t_j + u_i + \varepsilon_{ij}$$

which is often helpful to write as

$$y_{ij} = (\beta_0 + u_i) + \beta_1 t_j + \varepsilon_{ij}$$

for reasons that will (hopefully) become clear later.

In the model above, the total residual that would be present in the usual linear regression model has been partitioned into a subject-specific random component u_i, which is constant over time, plus a residual ε_{ij}, which varies randomly over time. The u_i is assumed to be normally distributed with zero mean and variance σ_u^2. Similarly, the ε_{ij} is, as always, assumed normally distributed with zero mean and variance σ^2. The u_i and ε_{ij} are assumed to be independent of each other and of the time t_j. This model is known as a *random intercept model*, the u_i terms producing the random intercepts. The repeated measurements made over time for an individual vary about that individual's own regression line, which can differ in intercept but not in slope from the regression lines of other individuals. The random effects u_i model possible heterogeneity in the intercepts of the individuals' regression lines.

Let us now look at how the presence of the random effects introduces covariance between the repeated measurements over time. The random intercept model implies that the total variance of each repeated measurement is

$$\mathrm{Var}(y_{ij}) = \mathrm{Var}(u_i + \varepsilon_{ij}) = \sigma_u^2 + \sigma^2$$

Due to this decomposition of the total residual variance into a between-subject component, σ_u^2, and a within-subject component, σ^2, the model is sometimes referred to as a *variance component model.* The covariance between the total residuals at two time points t_j and t_k, in the same individual i is given by

$$\mathrm{Cov}(u_i + \varepsilon_{ij}, u_i + \varepsilon_{ik}) = \sigma_u^2$$

Note that these covariances are induced by the shared random intercept; for individuals with $u_i > 0$, the total residuals will tend to be greater than the mean; for individuals with $u_i < 0$, they will tend to be less than the mean. It follows from the two relations above that the residual correlations are given by

$$\mathrm{Cor}(u_i + \varepsilon_{ij}, u_i + \varepsilon_{ik}) = \frac{\sigma_u^2}{\sigma_u^2 + \sigma^2}$$

This is an *intraclass correlation* interpreted as the proportion of the total residual variance that is due to residual variability between subjects.

The formulae given earlier for the variance of each repeated measurement and for the covariance of each pair of repeated measurements do not involve time, and demonstrate that the random intercept model constrains the variance of each repeated measurement to be the same and the correlation of each pair of measurements to be equal. This particular correlational structure is known as *compound symmetry.* Fitting a random intercept model to longitudinal data implies that the compound symmetry structure is considered appropriate for the data. However, this is very often not the case; for example, it is more common for measures taken closer to each other in time to be more highly correlated than those taken further apart. In addition, the variances of the measurements taken later in time are often greater than those measurements taken earlier. Consequently, for many longitudinal data sets, the random intercept model will not do justice to the observed pattern of variances and correlations between the repeated measurements, and will, therefore, not be the most appropriate model for the data.

A model that allows a more realistic structure for covariances is one that allows heterogeneity in both intercepts and slopes, namely, the *random slope and intercept model.* In this model, there are two types of random effects: the first modeling heterogeneity in intercepts, u_i, and the second modeling heterogeneity in slopes, v_i. Explicitly, the model is

$$y_{ij} = \beta_0 + \beta_1 t_j + u_i + v_i t_j + \varepsilon_{ij}$$

which may also be written as

$$y_{ij} = (\beta_0 + u_i) + (\beta_1 + v_i)t_j + \varepsilon_{ij}$$

so as to show more clearly how the two subject random effects alter the intercept and the slope in the model. The two random effects are assumed to have a bivariate normal distribution with zero means for both variables and variances σ_u^2 and σ_v^2 with covariance σ_{uv}. With this model, the total residual is $u_i + v_i t_j + \varepsilon_{ij}$ with variance

$$\mathrm{Var}(u_i + v_i t_j + \varepsilon_{ij}) = \sigma_u^2 + 2\sigma_{uv} t_j + \sigma_v^2 t_j^2 + \sigma^2$$

which is now no longer constant for different values of t_j. Similarly, the covariance between two total residuals of the same individual is

$$\mathrm{Cov}(u_i + v_i t_j + \varepsilon_{ij}, u_i + v_i t_k + \varepsilon_{ik}) = \sigma_u^2 + \sigma_{uv}(t_j + t_k) + \sigma_v^2 t_j t_k$$

and this is now not constrained to be the same for all pairs t_j and t_k. The random intercept and slope model allows for both variances of the repeated measurements that change with time, and covariances of pairs of repeated measurements that are not all the same.

In the model we have been considering, time has a fixed effect measured by the parameter β_1. It is this parameter that is likely to be of more interest to the investigator than the other parameters in the model, namely, the variance of the error terms and the variance (and possibly covariance) of the random effects. However, if the estimate of β_1 and its estimated standard error are derived from the simple regression model assuming independence, the standard error will be larger than it should be because of ignoring the likely within-subject dependences that will reduce the error variance in the model. Consequently, use of the simple regression model may give a misleading inference for β_1. As we shall see later, the situation for between-subject fixed effects is the reverse of that for within-subject fixed effects, with the estimated standard error of the effect being smaller in the (usually) inappropriate independence model than in a linear mixed effects model.

Linear mixed effects models can be estimated by maximum likelihood (ML). However, this method tends to underestimate the variance components. A modified version of ML, known as restricted maximum likelihood (REML), is therefore often recommended. Details are given in Diggle et al. (2002) and Longford (1993). Competing linear mixed effects models for a data set, for example, a random intercept model and a random intercept and slope model, can be compared using a likelihood ratio test (although see later comments about this test). The distinction between ML and REML is relevant when using the likelihood ratio test to compare two nested models because, unlike ML, which places no restrictions on likelihood ratio tests involving fixed and random effects, when REML is used, such tests are only appropriate when both models have the same set of fixed effects (see Longford, 1993).

9.3 How Do Rats Grow?

To begin to see how linear mixed effects models are applied in practice, we shall use some data from a nutrition study conducted in three groups of rats (Crowder and Hand, 1990). The three groups were put on different diets, and each animal's body weight (grams) was recorded repeatedly (approximately weekly, except in week seven when two recordings were taken) over a 9-week period. The question of most interest is whether the growth profiles of the three groups differ. The data are shown in Table 9.1.

9.3.1 Fitting the Independence Model to the Rat Data

To begin, we shall ignore the repeated-measures structure of the data and assume that all the observations are independent of one another. It is easier to imagine this if we write the data in what is known as the long form (in Table 9.1, the data are their wide form); the data for the first two rats in group 1 are shown in their long form in Table 9.2. Now if we simply ignore that the sets of 11 weights come from the same rat, we have a data set consisting of 176 weights, times, and group memberships that we see can easily be analyzed using multiple linear regression. To begin, we will plot the data, identifying the observations in each group but ignoring the longitudinal nature of the

TABLE 9.1
Body Weights of Rats Recorded Over a 9-Week Period

		Day										
ID	**Group**	**1**	**8**	**15**	**22**	**29**	**36**	**43**	**44**	**50**	**57**	**64**
1	1	240	250	255	260	262	258	266	266	265	272	278
2	1	225	230	230	232	240	240	243	244	238	247	245
3	1	245	250	250	255	262	265	267	267	264	268	269
4	1	260	255	255	265	265	268	270	272	274	273	275
5	1	255	260	255	270	270	273	274	273	276	278	280
6	1	260	265	270	275	275	277	278	278	284	279	281
7	1	275	275	260	270	273	274	276	271	282	281	284
8	1	245	255	260	268	270	265	265	267	273	274	278
9	2	410	415	425	428	438	443	442	446	456	468	478
10	2	405	420	430	440	448	460	458	464	475	484	496
11	2	445	445	450	452	455	455	451	450	462	466	472
12	2	555	560	565	580	590	597	595	595	612	618	628
13	3	470	465	475	485	487	493	493	504	507	518	525
14	3	535	525	530	533	535	540	525	530	543	544	559
15	3	520	525	530	540	543	546	538	544	553	555	548
16	3	510	510	520	515	530	538	535	542	550	553	569

data to give Figure 9.1. Clearly, there is a difference between the weights of the group 1 rats and those in the other two groups. Continuing to ignore the repeated-measures structure of the data, we might fit a multiple linear regression model with weight as response and time and group (coded as two dummy variables D_1 and D_2, with both D_1 and D_2 taking the value 0 for rats in group 1, D_1 being 1 and D_2 being 0 for rats in group 2, and D_1 being 0 and D_2 being 1 for rats in group 3) as explanatory variables. Fitting the model gives the results shown in Table 9.3. As we might have anticipated from Figure 9.1, both group 2 and group 3 differ significantly from group 1 conditional on time; the regression on time is also highly significant. We might go on to fit a model with a group × time interaction, but we will not do this because we know from the structure of the data that the model considered here is wrong. The model assumes independence of the repeated measures of weight, and this assumption is highly unlikely. So, now we will move on to consider both some more appropriate graphics and appropriate models.

TABLE 9.2
Long Form of the Data for the First Two Rats in Group 1 in Table 9.1

	ID	**Group**	**Time**	**Weight**
1	1	1	1	240
2	1	1	8	250
3	1	1	15	255
4	1	1	22	260
5	1	1	29	262
6	1	1	36	258
7	1	1	43	266
8	1	1	44	266
9	1	1	50	265
10	1	1	57	272
11	1	1	64	278
12	2	1	1	225
13	2	1	8	230
14	2	1	15	230
15	2	1	22	232
16	2	1	29	240
17	2	1	36	240
18	2	1	43	243
19	2	1	44	244
20	2	1	50	238
21	2	1	57	247
22	2	1	64	245

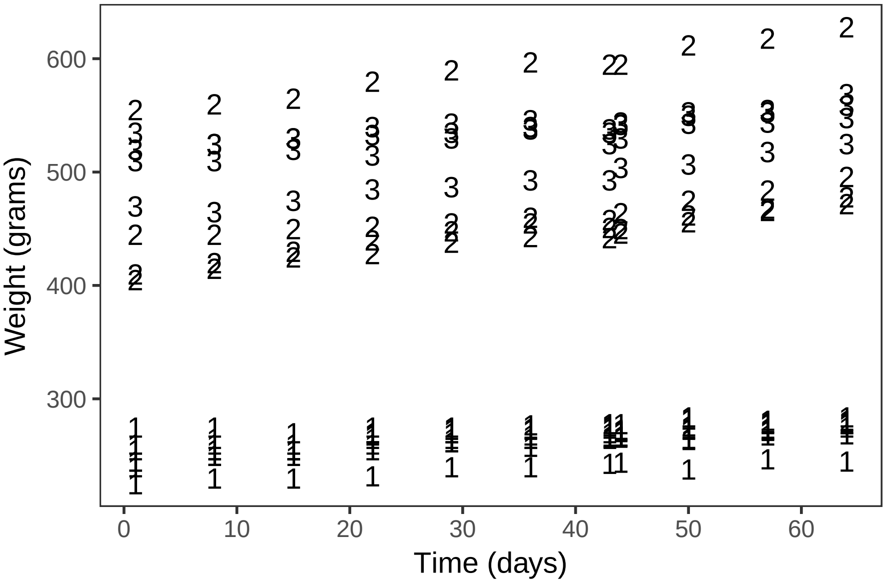


FIGURE 9.1
Plot of weight against time for rat data, ignoring the repeated-measures structure of the data but identifying the group to which each observation belongs.

9.3.2 Fitting Linear Mixed Models to the Rat Data

We begin with a graphical display of the rat growth data that takes into account the longitudinal structure of the data by joining together the points belonging to each rat to show the weight growth profiles of individual rats; the plot appears in Figure 9.2. In Figure 9.3, a scatterplot matrix of the repeated measures of weight, although not a terribly helpful graphic, does demonstrate that the repeated measures are certainly not independent of one another.

TABLE 9.3
Results from Fitting a Linear Regression Model to Rat Data with Weight as Response Variable, and Group and Time as Explanatory Variables, and Ignoring the Repeated-Measures Structure of the Data

	Estimate	**Standard Error**	**t-Value**	**Pr(>|t|)**
Intercept	244.0689	5.7725	42.281	<2e-16
Time	0.5857	0.1331	4.402	1.88e-05
D_1	220.9886	6.3402	34.855	<2e-16
D_2	262.0795	6.3402	41.336	<2e-16

Note: Multiple R-squared: 0.9283; F-statistic: 742.6 on 3 and 172 DF; p-value: <2.2e-16.

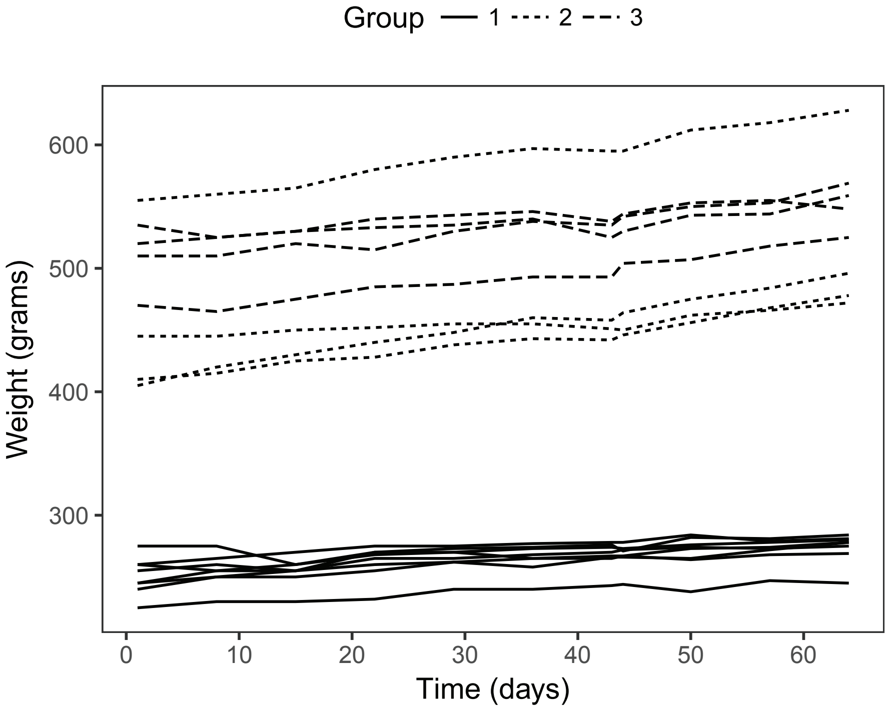


FIGURE 9.2
Plot of individual rat growth profiles.

To begin the more formal analysis of the rat growth data, we will first fit the random intercept model and include the two explanatory variables: time and group (coded as two dummy variables). If we represent the weight of the ith rat at time t_j by y_{ij}, the model can be written as

$$y_{ij} = (\beta_0 + u_i) + \beta_1 t_j + \beta_2 D_{i1} + \beta_3 D_{i2} + \varepsilon_{ij}$$

where u_i is the random effect specific to the ith subject, with these random effects having a normal distribution with zero mean and variance σ_u^2; the ε_{ij} are the usual "error" terms with a normal distribution with zero mean and variance σ^2, and D_{i1} and D_{i2} are the same two dummy variables used to code the group membership of the ith rat as in the independence model fitted earlier. This model allows the linear regression fit for each rat to differ in intercept from other rats. Fitting this model gives the results shown in Table 9.4. The estimated variance of the rat random effects is quite large, indicating the considerable variation in the intercepts of the regression fits of the individual rat growth profiles. The estimated regression parameters for time and the two dummy variables are very similar to those from fitting the independence model shown in Table 9.3, and all are highly significant again

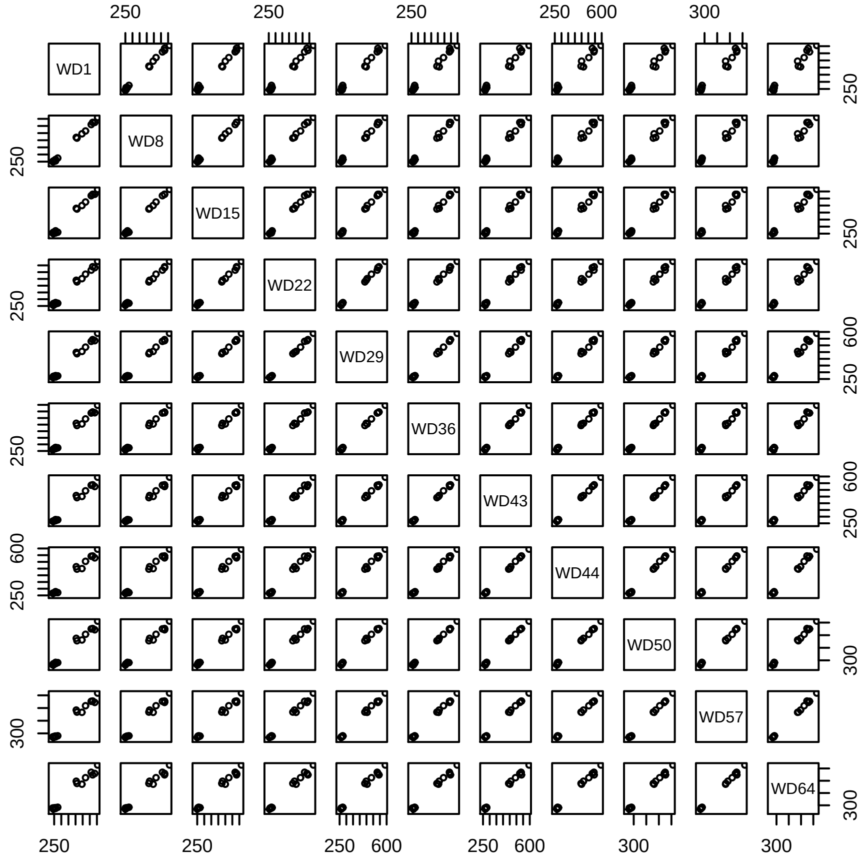


FIGURE 9.3
Scatterplot matrix of repeated measures in rat growth data.

as they were in Table 9.3. However, the estimated standard error of time is much smaller in Table 9.4 than it is in Table 9.3, reflecting the point made in Technical Section 9.1 that assuming independence will lead to the standard error of a within-subject covariate such as time being larger than it should be because of ignoring the likely within-subject dependences, which will reduce the error variance in the model. In contrast, the standard errors of each dummy variable in Table 9.4 are about three times the size of those in Table 9.3. The dummy variables are between-subject effects, and the reason for the smaller standard errors with the independence model is that the effective sample size for estimating these effects is less than the actual sample size because of the correlated nature of the data, and so the estimates for the independence model are unrealistically precise. In this example, the conclusions from the independence model and the random intercept model are the same, but in other examples this will not necessarily be so, as we shall see later.

Now we can move on to fit the random intercept and random slope model to the rat growth data; explicitly, the model is

$$y_{ij} = (\beta_0 + u_i) + (\beta_1 + v_i)t_j + \beta_2 D_{i1} + \beta_3 D_{i2} + \varepsilon_{ij}$$

where the extra term from the random intercept model is the random effect v_i that allows the linear regression fits for each individual to differ in slope; these random effects are assumed to have a normal distribution with zero mean and variance σ_v^2, and are allowed to be correlated with the u_i random intercept effects (see Technical Section 9.1). The results from fitting the random intercept and slope model to the rat growth data are shown in Table 9.5. The results for the fixed effects are very similar to those in Table 9.4, but the likelihood ratio test for the random intercept model versus the random intercept and slope model gives a chi-squared statistic of 142.94 with 2 degrees of freedom (DF) (the two additional parameters in the latter model are the variance of the v random effects and the covariance of the u and v random effects), and the associated p-value is very small. The random intercept and slope model provides a better fit for these data. (There are some technical problems with this likelihood ratio test, which are discussed in detail in Rabe-Hesketh and Skrondal, 2012; fortunately, the correct p-value for testing which of the two models is to be preferred can be found simply by dividing the p-value from the flawed likelihood ratio test by 2.)

Finally, we can fit a random intercept and slope model that allows for a group × time interaction. Explicitly, this model can be written as

$$y_{ij} = (\beta_0 + u_i) + (\beta_1 + v_i)t_j + \beta_2 D_{i1} + \beta_3 D_{i2} + \beta_4(D_{i1} \times t_j) + \beta_5(D_{i2} \times t_j) + \varepsilon_{ij}$$

TABLE 9.4
Results from Fitting Random Intercept Model, with Time and Group as Explanatory Variables, to Rat Growth Data

Random Effects			
$\hat{\sigma}_u^2 = 1085.92$, $\hat{\sigma}^2 = 66.44$			
Fixed Effects			
	Estimate	**Standard Error**	**t-Value**
Intercept	244.06890	11.73107	20.80
Time	0.58568	0.03158	18.54
D_1	220.98864	20.23577	10.92
D_2	262.07955	20.23577	12.95

TABLE 9.5

Results from Fitting the Random Intercept and Slope Model, with Time and Group as Explanatory Variables, to Rat Growth Data

Random Effects[a]			
$\hat{\sigma}_u^2 = 1140.54$, $\hat{\sigma}_v^2 = 0.11$, $\hat{\sigma}^2 = 19.75$			
Fixed Effects			
	Estimate	**Standard Error**	**t-Value**
Intercept	246.45727	11.81526	20.859
Time	0.58568	0.08548	6.852
D_1	214.58735	20.17983	10.634
D_2	258.92732	20.17983	12.831

[a] Estimated correlation between the u and v random effects is −0.22.

Fitting this model gives the results in Table 9.6. The likelihood ratio test of the interaction random intercept and slope model against the corresponding model without an interaction is 12.36 with 2 DF; the associated p-value is very small, and we can conclude that the interaction model provides a better fit for the rat growth data. The estimated regression parameters for the interaction in Table 9.6 indicate that the growth rate slopes are considerably higher for rats in group 2 than for rats in group 1 (on average 0.61 higher with an approximate 95% confidence interval [CI] of [0.33, 0.89]) but less so when comparing group 3 rats with those in group 1 (on average 0.30 higher, CI [0.02, 0.58]).

We can find the fitted values from the interaction model and plot the fitted growth rates for each rat; these are shown in Figure 9.4 alongside the

TABLE 9.6

Results from Fitting the Random Intercept and Slope Model that Allows for a Group × Time Interaction to Rat Growth Data

Random Effects[a]			
$\hat{\sigma}_u^2 = 1107.0$, $\hat{\sigma}_v^2 = 0.05$, $\hat{\sigma}^2 = 19.75$			
Fixed Effects			
	Estimate	**Standard Error**	**t-Value**
Intercept	251.65165	11.80279	21.321
Time	0.35964	0.08215	4.378
D_1	200.66549	20.44303	9.816
D_2	252.07168	20.44303	12.330
D_1 × Time	0.60584	0.14229	4.258
D_2 × Time	0.29834	0.14229	2.097

[a] Estimated correlation between the u and v random effects is −0.15.

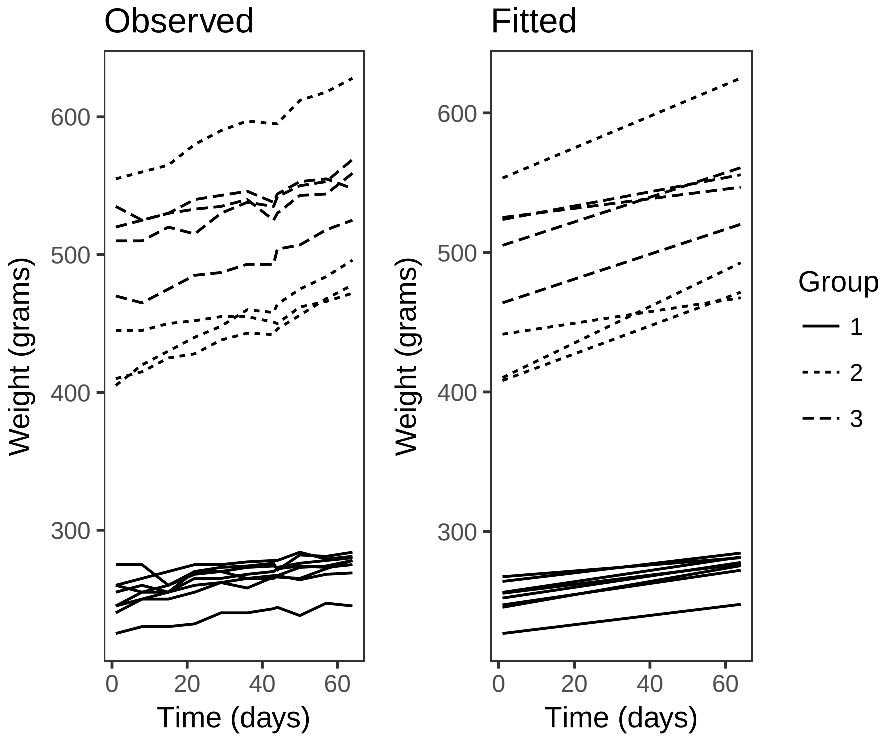


FIGURE 9.4
Fitted growth rate profiles from the interaction model and observed growth rate profiles.

observed values. This graphic underlines how well the interaction model fits the observed data. (The fitted values for each rat include “predicted” values of the u and v random effects for the rat; details of how these predicted values are calculated are given in Rabe-Hesketh and Skrondal, 2012.)

9.4 Computerized Delivery of Cognitive Behavioral Therapy—Beat the Blues

Depression is a major public health problem across the world. Antidepressants are the frontline treatment, but many patients either do not respond to them or do not like taking them. The main alternative is psychotherapy, and the modern “talking treatments” such as cognitive behavioral therapy (CBT) have been shown to be as effective as drugs, and probably more so when it comes

TABLE 9.7
First Five Patients in Each Treatment Group of the "Beat the Blues" (BtB) Clinical Trial of CBT for Depression

Drug	Length	Treatment	BDIpre	BDI2m	BDI4m	BDI6m	BDI8m
No	>6m	TAU	29	2	2	NA	NA
Yes	>6m	BtheB	32	16	24	17	20
Yes	<6m	TAU	25	20	NA	NA	NA
No	>6m	BtheB	21	17	16	10	9
Yes	>6m	BtheB	26	23	NA	NA	NA
Yes	<6m	BtheB	7	0	0	0	0
Yes	<6m	TAU	17	7	7	3	7
No	>6m	TAU	20	20	21	19	13
Yes	<6m	BtheB	18	13	14	20	11
No	>6m	TAU	30	32	24	12	2

to relapse (Watkins and Williams, 1998). But there is a problem, namely, availability—there are simply nothing like enough skilled therapists to meet the demand, and little prospect at all of this situation changing.

A number of alternative modes of delivery of CBT have been explored, including interactive systems making use of new computer technologies. The principles of CBT lend themselves reasonably well to computerization, and, perhaps surprisingly, patients adapt well to this procedure, and do not seem to miss the physical presence of the therapist as much as one might expect. Workers at the Institute of Psychiatry in the United Kingdom have developed one particular program, known as Beating the Blues (BtB). Full details are given by Proudfoot et al. (2004), but in essence, BtB is an interactive program using multimedia techniques, in particular, video vignettes. The computer-based intervention consists of nine sessions, followed by eight therapy sessions, each lasting about 50 minutes. Nurses are used to explain how the program works, but are instructed to spend no more than 5 minutes with each patient at the start of each session, and are there simply to assist with the technology. In a randomized controlled trial of the program, patients with depression recruited in primary care were randomized to either the BtB program or to "Treatment as Usual" (TAU). Patients randomized to BtB also received pharmacology and/or general practitioner (GP) support and practical/social help, offered as part of TAU, with the exception of any face-to-face counseling or psychological intervention. Patients allocated to TAU received whatever treatment their GP prescribed. The latter included, besides any medication, discussion of problems with GP, provision of practical/social help, referral to a counselor, referral to a practice nurse, referral to mental health professionals (psychologist, psychiatrist, community psychiatric nurse, counselor, etc.), or further physical examination.

A number of outcome measures were used in the trial, but here we concentrate on the Beck Depression Inventory II (BDI; Beck et al., 1996). Measurements on this variable were made on the following five occasions:

- Prior to treatment,
- 2, 4, 6, and 8 months after treatment began.

Data from 100 patients will be analyzed in this section; these data are a subset of the original and are used with the kind permission of the organizers of the study, in particular, Dr. Judy Proudfoot. Data for the first five patients from each treatment group are shown in Table 9.7. Two additional explanatory variables are also available for each patient: the first, drug, is whether the patient was taking antidepressant drugs (yes or no), and the second, length, is the length of the current episode of depression categorized into less than six months (<6m) or more than six months (>6m). The NAs (not available) in Table 9.7 indicate where a protocol-specified measurement of the BDI was not made; here, all the NAs are due to patients dropping out of the study. How dropouts might affect the results obtained from the analysis of the data will be discussed later in the chapter. The main question of interest here is to estimate the treatment effect of the BtB program.

In the distant past, the analysis of the BtB data would have involved only those patients with a complete set of five BDI values. At best, a "completers only" analysis would have been inefficient because the subset of BDI values for patients who dropped out are not used, thus lowering the sample size on which the analysis is based. But using only the completers in an analysis could have more dire consequences such as giving rise to biased parameter estimates and thus incorrect inferences. By considering the data in the long form, however, we see that analyses that use all the available data, including the BDI values that are recorded for patients who eventually drop out of the study, are straightforward. However, before considering models for the data, we should, as with any data set, try to discover some features of the data from some graphical material. So, we will begin by looking at boxplots of the BDI scores at each occasion of recording for each treatment group; the plot is shown in Figure 9.5. We see that the BDI scores decrease over time in each treatment group, but perhaps a little more in the BtB group, and the variance of the observations in the TAU group appears to be greater than those in the BtB group on each posttreatment time of recording. As a second graphic for these data, Figure 9.6 shows the scatterplot matrix of the five BDI scores; clearly, the repeated BDI values are not independent of one another.

We now move on to considering models for the BtB data. Again, we begin with an unrealistic multiple linear regression model that assumes that the repeated measures of the BDI are independent and contains the explanatory variables drug (coded 0 for no and 1 for yes), length (coded 0 for <6 months and 1 for >6 months), treatment (coded 0 for TAU and 1 for BtB), time, and BDI prevalue. The results are shown in Table 9.8. As we might have expected, the regression parameters for time and pretreatment BDI (BDIpre) are highly

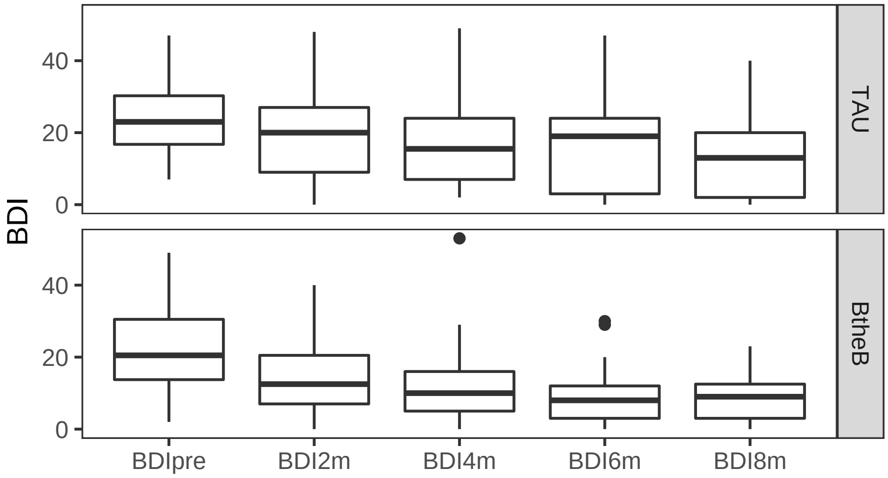


FIGURE 9.5
Box plots of BDI scores by occasion of recording and treatment group.

significant. The negative value for the time coefficient tells us what we have already surmised from the boxplots in Figure 9.5, namely, that the BDI scores decrease over time. The positive regression coefficient for BDIpre simply indicates that patients with, say, a higher-than-average BDI score before treatment begins, will tend to have higher-than-average values posttreatment. The regression coefficient for drug is also very significant, and its negative value tells us that patients taking antidepressant drugs will tend to have lower BDI scores than those not taking such medication. The regression coefficient for length is not significant at the 5% level; there is no evidence that the length of the current episode of depression affects the BDI score. Finally, we see that the regression coefficient for treatment is also highly significant; treatment with BtB rather than TAU is estimated to lower depression scores on average by 3.36 BDI units conditional on the other explanatory variables with an approximate 95% CI of $[-3.36-2\times1.10, -3.36+2\times1.10]$, that is, $[-5.56, -1.16]$ (this estimated treatment difference applies to all posttreatment occasions because, in the model fitted, there is no allowance for a treatment × time interaction). However, we know from Figure 9.6 that the independence assumption for the repeated BDI scores is almost certainly incorrect, and so we need to consider some linear mixed models for these data that do allow for departures from independence.

So, we start with a random intercept model including the same explanatory variables as the independence model. The results are shown in Table 9.9. The regression parameters for both time and BDIpre remain highly significant, but those for treatment and drug are now not significant primarily because

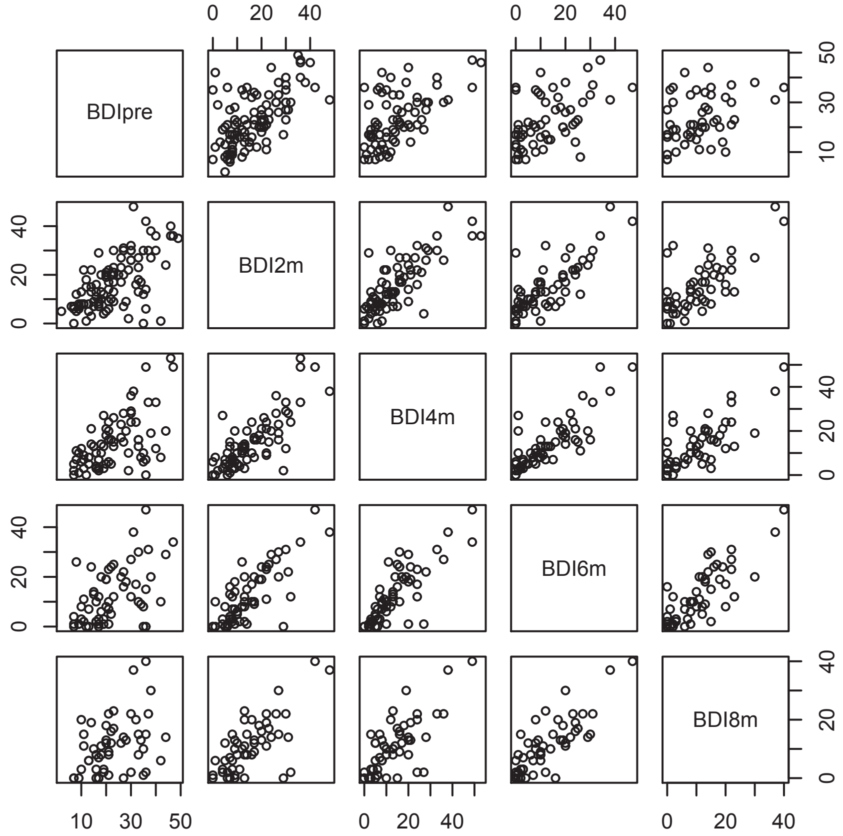


FIGURE 9.6
Scatterplot matrix of BDI scores.

TABLE 9.8
Results from Fitting a Multiple Linear Regression Model to BtB Data Assuming the Repeated Measurements of BDI are Independent

	Estimate	**Standard Error**	**t-Value**	**Pr(>|t|)**
Intercept	7.88307	1.78049	4.427	1.38e-05
BDIpre	0.57237	0.05486	10.433	<2e-16
Time	−0.96081	0.23263	−4.130	4.82e-05
Treatment	−3.35397	1.09832	−3.054	0.00248
Drug	−3.54601	1.14469	−3.098	0.00215
Length	1.75308	1.10850	1.581	0.11492

Note: Multiple R-squared: 0.3978; F-statistic: 36.2 on 5 and 274 DF; p-value: <2.2e-16.

the associated estimated standard errors of these parameters have increased considerably. However, before using the estimates in Table 9.9 for interpretation, we should perhaps consider whether a random intercept and slope model gives a better fit. If we fit such a model, the likelihood ratio test comparing the random intercept model with the random intercept and slope model has a value of 0.82 with 2 DF; it appears that the more complicated model is not needed for these data. So, returning to Table 9.9 and, in particular, the estimated regression parameter for treatment, we find that treatment with BtB is estimated to lower the average BDI score by 2.36 units conditional on the other covariates with 95% CI of $[-5.78, 1.06]$; there is no compelling evidence that treatment with BtB is effective, a different conclusion from that produced by using the independence model.

TABLE 9.9
Results from Fitting a Random Intercept Model to BtB Data

Random Effects			
$\hat{\sigma}_u^2 = 51.44$, $\hat{\sigma}^2 = 25.27$			
Fixed Effects			
	Estimate	**Standard Error**	**t-Value**
Intercept	5.92148	2.30586	2.568
BDIpre	0.63888	0.07961	8.025
Time	−0.71353	0.14664	−4.866
Treatment	−2.35900	1.70841	−1.381
Drug	−2.78885	1.76594	−1.579
Length	0.23810	1.67537	0.142

9.5 Summary

- Repeated measurements of a response under different experimental conditions or over a period of time occur often in behavioral research.
- The analysis of such data requires special techniques because of the likely nonindependence of the repeated measurements.
- Linear mixed models allow for correlations between the repeated measurements by introducing random effects for subjects.
- The essential feature of such models is that there is natural heterogeneity across individuals in their responses over time and that this heterogeneity can be represented by an appropriate probability distribution. Correlation

between observations from the same individual arises from unobserved or unmeasured characteristics of the individual that remain the same over time, for example, an increased propensity to the condition under investigation, or perhaps a predisposition to exaggerate symptoms.

- Conditional on the values of the random effects, the repeated measurements of the response variable are assumed independent—the local independence assumption.
- Linear mixed effects models can be fitted by maximum likelihood, and competing models can be assessed by a likelihood ratio test.
- Longitudinal data often suffer from missing values of the response variable. In particular, patients often drop out of a study for a variety of reasons. Every effort needs to be made to avoid the problem as far as possible because if there are a large number of dropouts the conclusions drawn from any analysis of the data may be compromised. Missing values are considered in detail in Chapter 11, but it is worth pointing out here that the models described in this chapter can be shown to give valid results under the relatively weak assumption that the missing data mechanism is MAR as defined in Chapter 11 (see Carpenter et al., 2002).
- In this chapter, only responses that can be assumed to have a normal distribution conditional on the explanatory variables have been considered. Non-normal responses will be the subject of the next chapter.

9.6 Exercises

(excluded from MABS for IODS)

References

Agresti, A. (1996). *An Introduction to Categorical Data Analysis.* John Wiley & Sons, New York.

Aitkin, M. (1978). The analysis of unbalanced cross-classification. *Journal of the Royal Statistical Society, Series A*, 141, 195–223.

Alwin, D. F. (2007). *Margins of Error: A Study of Reliability in Survey Measurement.* John Wiley & Sons, New York.

Anderson, J. A. (1972). Separate sample logistic discrimination. *Biometrika*, 59, 19–35.

Anscombe, F. (1973). Graphs in statistical analysis. *The American Statistician*, 27, 17–21.

Banfield, J. D. and Raftery, A. E. (1993). Model based Gaussian and non-Gaussian clustering. *Biometrics*, 49, 803–821.

Barlow, R. E., Bartholomew, D. J., Bremner, J. M. and Brunk, H. D. (1972). *Statistical Inference under Order Restrictions.* John Wiley & Sons, New York.

Barnard, J. and Rubin, D. B. (1999). Small sample degrees of freedom with multiple imputation. *Biometrika*, 86, 948–955.

Barnard, J., Rubin, D. B. and Schenker, N. (2005). Multiple imputation methods. In *Encyclopedia of Biostatistics*, 2nd edition (eds. P. Armitage and T. Colton). John Wiley & Sons, Chichester, U.K.

Barnett, V., ed. (1981). *Interpreting Multivariate Data.* John Wiley & Sons, Chichester, U.K.

Bartholomew, D. J., Knott, M. and Moustaki, I. (2011). *Latent Variable Models and Factor Analysis: A Unified Approach*, 3rd edition. John Wiley & Sons, Chichester, U.K.

Beck, A. T., Steer, A. and Brown, G. K. (1996). *Beck Depression Inventory Manual.* The Psychological Corporation, San Antonio, Texas.

Bennett, A. (2009). "Heritage rock": Rock music, representation and heritage discourse. *Poetics*, 37, 474–489.

Bentler, P. M. (1980). Multivariate analysis with latent variables: Causal modeling. *Annual Review of Psychology*, 31, 419–456.

Benzécri, J.–P. et al. (1973). *Analyse des Données. Tôme 1: La Classification. Tôme 2: L'Analyse des Correspondances.* [*Data Analysis. Volume 1: Classification. Volume 2: Correspondence Analysis*, in French.] Dunod, Paris.

Benzécri, J.–P. et al. (1992). *Correspondence Analysis Handbook.* Marcel Dekker, New York.

Bertin, J. (1981). *Semiology of Graphics.* University of Wisconsin Press, Wisconsin.

Bickel, P. J., Hammel, E. A. and O'Connell, J. W. (1975). Sex bias in graduate admissions: Data from Berkeley. *Science*, 187, 398–404.

Blackith, R. E. and Reyment, R. A. (1971). *Multivariate Morphometrics.* Academic Press, London.

Blalock, H. M. (1961). Correlation and causality: The multivariate case. *Social Forces*, 39, 246–251.

Blalock, H. M. (1963). Making causal inferences for unmeasured variables from correlations among indicators. *American Journal of Sociology*, 69, 53–62.

Blasius, J. and Greenacre, M., eds. (2014). *Visualization and Verbalization of Data.* Chapman and Hall/CRC, Boca Raton, Florida.

Bollen, K. A. (1989). *Structural Equations with Latent Variables.* John Wiley & Sons, New York.

Bollen, K. A. and Long, J. S., eds. (1993). *Testing Structural Equation Models.* Sage, London.

Borg, I. and Groenen, P. J. F. (2005). *Modern Multidimensional Scaling*, 2nd edition. Springer, New York.

Bradburn, N. M., Sudman, S. and Wansink, B. (2004). *Asking Questions: The Definitive Guide to Questionnaire Design—For Market Research, Political Polls, and Social and Health Questionnaires*, revised edition. Jossey-Bass, San Francisco, California.

Browne, M. W. (1974). Generalized least squares estimators in the analysis of covariance structures. *South African Statistical Journal*, 8, 1–24.

Byrne, B. M. (2005). Factor analytic models: Viewing the structure of an assessment instrument from three perspectives. *Journal of Personality Assessment*, 85, 17–32.

Calsyn, R. J. and Kenny, D. A. (1977). Self-concept of ability and perceived evaluation of others: Cause or effect of academic achievement? *Journal of Educational Psychology*, 69, 136–145.

Carpenter, J., Pocock, S. and Lamm, C. J. (2002). Coping with missing data in clinical trials: A model-based approach applied to asthma trials. *Statistics in Medicine*, 21, 1043–1066.

Carroll, J. B. (1953). An analytical solution for approximating simple structure in factor analysis. *Psychometrika*, 18, 23–38.

Cattell, R. B. (1965). Factor analysis: An introduction to essentials. I: The purpose and underlying models. *Biometrics*, 21, 190–215.

Chambers, J. M., Cleveland, W. S., Kleiner, B. and Tukey, P. A. (1983). *Graphical Methods for Data Analysis.* Wadsworth, Belmont, California.

Chatterjee, S. and Hadi, A. S. (2012). *Regression Analysis by Example*, 5th edition. John Wiley & Sons, New York.

Cleveland, W. S. (1979). Robust locally weighted regression and smoothing scatterplots. *Journal of the American Statistical Association*, 74, 829–836.

Cleveland, W. S. (1993). *Visualizing Data.* Hobart Press, Summit, New Jersey.

Cleveland, W. S. (1994). *The Elements of Graphing Data.* Hobart Press, Summit, New Jersey.

Cleveland, W. S. and McGill, M. E., eds. (1988). *Dynamic Graphics for Statistics.* Wadsworth, Belmont, California.

Cochran, W. G. (1965). The planning of observational studies of human populations. *Journal of the Royal Statistical Society*, Series A, 128, 134–155.

Collett, D. (2003). *Modelling Binary Data*, 2nd edition. Chapman and Hall/CRC, London.

Collett, D. (2015). *Modelling Survival Data in Medical Research*, 3rd edition. Chapman and Hall/CRC, London.

Colman, A. M., ed. (1994). *The Companion Encyclopedia of Psychology.* Routledge, London.

Cook, R. D. and Weisberg, S. (1999). *Applied Regression Including Computing and Graphics.* John Wiley & Sons, New York.

Cook, R. J. (2005). Generalized linear model. In *Encyclopedia of Biostatistics*, 2nd edition (eds. P. Armitage and T. Colton). John Wiley & Sons, Chichester, U.K.

Cox, D. R. (1972). Regression models and life-tables (with discussion). *Journal of the Royal Statistical Society, Series B*, 34, 187–220.

Cox, T. F. and Cox, M. A. A. (2001). *Multidimensional Scaling*, 2nd edition. Chapman and Hall/CRC, London.

Crowder, M. J. and Hand, D. J. (1990). *Analysis of Repeated Measurements.* Chapman and Hall, London.

Cudeck, R. and MacCallum, R. C., eds. (2007). *Factor Analysis at 100: Historical Developments and Future Directions.* Lawrence Elbaum, Mahwah, New Jersey.

Davis, C. S. (1991). Semi-parametric and non-parametric methods for the analysis of repeated measurements with applications to clinical trials. *Statistics in Medicine*, 10, 1959–1980.

Davis, C. S. (2002). *Statistical Methods for the Analysis of Repeated Measurements.* Springer, New York.

De Leeuw, E. D., Hox, J. and Dillman, D., eds. (2008). *International Handbook of Survey Methodology.* Routledge, London.

Dempster, A. P., Laird, N. M. and Rubin, D. B. (1977). Maximum likelihood from incomplete data via the EM algorithm (with discussion). *Journal of the Royal Statistical Society, Series B*, 39, 1–38.

Diggle, P. J. and Kenward, M. G. (1994). Informative drop-out in longitudinal data analysis (with discussion). *Journal of the Royal Statistical Society, Series C (Applied Statistics)*, 43, 49–93.

Diggle, P. J., Heagerty, P., Liang, K. and Zeger, S. L. (2002). *Analysis of Longitudinal Data*, 2nd edition. Oxford University Press, Oxford.

Dizney, H. and Gromen, L. (1967). Predictive validity and differential achievement on three MLA comparative foreign language tests. *Educational and Psychological Measurement*, 27, 1127–1130.

Dobson, A. J. and Barnett, A. G. (2018). *An Introduction to Generalized Linear Models*, 4th edition. Chapman and Hall/CRC, London.

Donati, M. A., Chiesi, F. and Primi, C. (2013). A model to explain at-risk/problem gambling among male and female adolescents: Gender similarities and differences. *Journal of Adolescence*, 36, 129–137.

Duncan, O. D. (1966). Path analysis: Sociological examples. *American Journal of Sociology*, 72, 1–16.

Eerola, T. (2011). Are the emotions expressed in music genre-specific? An audio-based evaluation of datasets spanning classical, film, pop and mixed genres. *Journal of New Music Research*, 40, 349–366.

Efron, B. (1998). Foreword in special issue on analyzing non-compliance in clinical trials. *Statistics in Medicine*, 17, 249–250.

Everitt, B. S. (1984). *An Introduction to Latent Variable Models.* Chapman and Hall, London.

Everitt, B. S. (1987). *An Introduction to Optimization Methods and Their Applications in Statistics.* Chapman and Hall, London.

Everitt, B. S. and Dunn, G. (2001). *Applied Multivariate Data Analysis.* Edward Arnold, London.

Everitt, B. S. and Hay, D. F. (1992). *Talking about Statistics: A Psychologist's Guide to Design & Analysis.* Edward Arnold, London.

Everitt, B. S. and Hothorn, T. (2009). *A Handbook of Statistical Analyses Using R*, 2nd edition. Chapman and Hall/CRC, Boca Raton, Florida.

Everitt, B. S. and Howell, D. C., eds. (2005). *Encyclopedia of Statistics in Behavioral Science.* John Wiley & Sons, Chichester, U.K.

Everitt, B. S. and Pickles, A. (2004). *Statistical Aspects of the Design and Analysis of Clinical Trials*, 2nd edition. Imperial College Press, London.

Everitt, B. S. and Rabe-Hesketh, S. (1997). *The Analysis of Proximity Data.* Edward Arnold, London.

Everitt, B. S. and Rabe-Hesketh, S. (2001). *Analysing Medical Data Using S-PLUS.* Springer, New York.

Everitt, B. S. and Wessely, S. (2008). *Clinical Trials in Psychiatry*, 2nd edition. John Wiley & Sons, Chichester, U.K.

Everitt, B. S., Landau, S., Leese, M. and Stahl, D. (2011). *Cluster Analysis*, 5th edition. John Wiley & Sons, Chichester, U.K.

Fisher, R. A. (1940). The precision of discriminant functions. *Annals of Eugenics*, 10, 422–429.

Fitzmaurice, G. M., Laird, N. M. and Ware, J. H. (2011). *Applied Longitudinal Analysis*, 2nd edition. John Wiley & Sons, Hoboken, New Jersey.

Fleiss, J. L. (1986). *The Design and Analysis of Clinical Experiments.* John Wiley & Sons, New York.

Fraley, C. and Raftery, A. E. (1998). How many clusters? Which cluster method? Answers via model-based cluster analysis. *Computer Journal*, 41, 578–588.

Fraley, C. and Raftery, A. E. (1999). MCLUS: Software for the model-based cluster analysis. *Journal of Classification*, 16, 297–306.

Fraley, C. and Raftery, A. E. (2002). Model based clustering, discriminant analysis and density estimation. *Journal of the American Statistical Association*, 97, 611–631.

Friedman, H. P. and Rubin, J. (1967). On some invariant criteria for grouping data. *Journal of the American Statistical Association*, 62, 1159–1178.

Friedman, J. H. (1989). Regularized discriminant analysis. *Journal of the American Statistical Association*, 84, 165–175.

Friendly, M. (2002). Corrgrams. *The American Statistician*, 56, 316–324.

Frison, L. and Pocock, S. J. (1992). Repeated measures in clinical trials: Analysis using mean summary statistics and its implications for design. *Statistics in Medicine*, 11, 1685–1704.

Gabriel, K. R. (1971). The biplot graphic display of matrices with application to principal component analysis. *Biometrika*, 58, 453–467.

Gabriel, K. R. (2002). Goodness of fit of biplots and correspondence analysis. *Biometrika*, 89, 423–436.

Gabriel, K. R. and Odoroff, C. L. (1990). Biplots in biomedical research. *Statistics in Medicine*, 9, 469–485.

Gardner, M. J. and Altman, D. G. (1986). Confidence intervals rather than P values: Estimation rather than hypothesis testing. *British Medical Journal*, 292, 746–750.

Gelman, A. and Unwin, A. (2013). Infovis and statistical graphics: Different goals, different looks. *Journal of Computational and Graphical Statistics*, 22, 2–28.

Georges, P. (2017). Western classical music development: a statistical analysis of composers similarity, differentiation and evolution. *Scientometrics*, 112, 21–53.

Giardiello, F. M., Hamilton, S. R., Krush, A. J. et al. (1993). Treatment of colonic and rectal adenomas with sulindac in familial adenomatous polyposis. *The New England Journal of Medicine*, 328, 1313–1316.

Goldberg, B. P. (1972). *The Detection of Psychiatric Illness by Questionnaire*. Oxford University Press, Oxford.

Goldberg, K. M. and Iglewicz, B. (1992). Bivariate extensions of the boxplot. *Technometrics*, 34, 307–320.

Gordon, A. D. (1987). A review of hierarchical classification. *Journal of the Royal Statistical Society, Series A*, 150, 119–137.

Gordon, A. D. (1999). *Classification*, 2nd edition. Chapman and Hall, London.

Gower, J. C. (1966). Some distance properties of latent root and vector methods used in multivariate analysis. *Biometrika*, 53, 325–338.

Grana, C., Chinol, M., Robertson, C. et al. (2002). Pretargeted adjuvant radioimmunotherapy with Yttrium-90-biotin in malignant glioma patients: A pilot study. *British Journal of Cancer*, 86, 207–212.

Greenacre, M. (1984). *Theory and Applications of Correspondence Analysis*. Academic Press, London.

Greenacre, M. (2010). *Biplots in Practice*. BBVA Foundation, Bilbao.

Greenacre, M. (2016). *Correspondence Analysis in Practice*, 3rd edition. Chapman and Hall/CRC, Boca Raton, Florida.

Greenacre, M. (2018). *Compositional Data Analysis in Practice*. Chapman and Hall/CRC, Boca Raton, Florida.

Greenacre, M. and Blasius, J., eds. (2006). *Multiple Correspondence Analysis and Related Methods*. Chapman and Hall/CRC, Boca Raton, Florida.

Greenwood, M. and Yule, G. U. (1920). An inquiry into the nature of frequency distributions representative of multiple happenings with particular reference to the occurrence of multiple attacks of disease or of repeated accidents. *Journal of the Royal Statistical Society*, 83, 255–279.

Groenen, P. J. F. and van de Velden, M. (2005). Multidimensional scaling. In *Encyclopedia of Statistics in Behavioral Science* (eds. B. S. Everitt and D. C. Howell). John Wiley & Sons, Chichester, U.K.

Groenen, P. J. F. and Borg, I. (2014). Past, present, and future of multidimensional scaling. In *Visualization and Verbalization of Data* (eds. J. Blasius and M. Greenacre). Chapman and Hall/CRC, Boca Raton, Florida.

Groves, R. M., Fowler Jr., F. J., Couper, M. P., Lepkowski, J. M., Singer, E. and Tourangeau, R. (2009). *Survey Methodology*, 2nd edition. John Wiley & Sons, Hoboken, New Jersey.

Haavelmo, T. (1943). The statistical implications of a system of simultaneous equations. *Econometrica*, 11, 1–12.

Hämäläinen, R. P., Jones, R. and Saarinen, E. (2014). *Being Better Better: Living with Systems Intelligence*. Aalto University Publications Crossover 4/2014, http://systemsintelligence.aalto.fi/being_better_better/ (accessed June 28, 2018).

Hand, D. J. (2005). Discriminant analysis, linear. In *Encyclopedia of Biostatistics*, 2nd edition (eds. P. Armitage and T. Colton). John Wiley & Sons, Chichester, U.K.

Hand, D. J. (2008). *Statistics: A Very Short Introduction*. Oxford University Press, Oxford.

Heitjan, D. F. (1997). Bayesian interim analysis of phase II cancer clinical trials. *Statistics in Medicine*, 16, 1791–1802.

Hendrickson, A. E. and White, P. O. (1964). Promax: A quick method for rotation to oblique simple structure. *British Journal of Mathematical and Statistical Psychology*, 17, 65–70.

Heywood, H. B. (1931). On finite sequences of real numbers. *Proceedings of the Royal Statistical Society, Series A*, 134, 486–501.

Hildreth, L. (2013). Residual analysis for structural equation modeling. D.Phil. Thesis. Graduate Theses and Dissertations, Iowa State University. https://lib.dr.iastate.edu/etd/13400 (accessed August 2, 2018).

Hotelling, H. (1933). Analysis of a complex of statistical variables into principal components. *Journal of Educational Psychology*, 24, 417–441.

Hothorn, T. and Everitt, B. S. (2014). *A Handbook of Statistical Analyses Using R*, 3rd edition. Chapman and Hall/CRC, Boca Raton, Florida.

Houghton, J. D. and Jinkerson, D. L. (2007). Constructive thought strategies and job satisfaction: A preliminary examination. *Journal of Business Psychology*, 22, 45–53.

Howell, D. C. (2012). *Statistical Methods for Psychology*, 8th edition. Wadsworth, Belmont, California.

Howell, D. C. and Huessy, H. R. (1981). Hyperkinetic behavior followed from 7 to 21 years of age. In *Intervention Strategies with Hyperactive Children* (eds. M. Gettleman and M. E. Sharp). Armonk, New York.

Howell, D. C. and Huessy, H. R. (1985). A fifteen year follow-up of a behavioral history of attention deficit disorder (ADD). *Pediatrics*, 76, 185–190.

Hsieh, F. Y. (1987). A simple method of sample size calculation for unequal-sample-size designs that use the logrank or t-test. *Statistics in Medicine*, 6, 577–581.

Hu, L. and Bentler, P. M. (1999). Cutoff criteria for fit indexes in covariance structure analysis: Conventional criteria versus new alternatives. *Structural Equation Modeling: A Multidisciplinary Journal*, 6, 1–55.

Huba, G. J., Wingard, J. A. and Bentler, P. M. (1981). A comparison of two latent variable causal models for adolescent drug use. *Journal of Personality and Social Psychology*, 40, 180–193.

Huck, S. W. and Sandler, H. M (1979). *Rival Hypotheses: Alternative Interpretations of Data Based Conclusions.* Harper & Row, New York.

Husson, F., Lê, S. and Pagès, J. (2017). *Exploratory Multivariate Analysis by Example Using R.* Chapman and Hall/CRC, Boca Raton, Florida.

Hutcheson, G. D., Baxter, J. S., Telfer, K. and Warden, D. (1995). Child witness statement quality: Question type and errors of omission. *Law and Human Behavior*, 19, 631–648.

Jackson, D. L., Gillaspy, Jr., J. A. and Purc-Stephenson, R. (2009). Reporting practices in confirmatory factor analysis: An overview and some recommendations. *Psychological Methods*, 14, 6–23.

Jacobson, G. C. and Dimock, M. A. (1994). Checking out: The effects of bank overdrafts on the 1992 House elections. *American Journal of Political Science*, 38, 601–624.

Jennrich, R. I. (2004). Rotation to simple loadings using component loss functions: The orthogonal case. *Psychometrika*, 69, 257–273.

Jennrich, R. I. (2006). Rotation to simple loadings using component loss functions: The oblique case. *Psychometrika*, 71, 173–191.

Jennrich, R. I. (2007). Rotation methods, algorithms, and standard errors. In *Factor Analysis at 100: Historical Developments and Future Directions* (eds. R. Cudeck and R. C. MacCallum). Lawrence Elbaum, Mahwah, New Jersey.

Jennrich, R. I. and Sampson, P. F. (1966). Rotation for simple loadings. *Psychometrika*, 31, 313–323.

Johnson, V. E. and Albert, J. H. (2013). *Ordinal Data Modeling*. Springer, New York.

Jolliffe, I. T. (1970). Redundant variables in multivariate analysis. D.Phil. Thesis, University of Sussex.

Jolliffe, I. T. (1972). Discarding variables in a principal components analysis. I: Artificial data. *Journal of the Royal Statistical Society, Series C (Applied Statistics)*, 21, 160–173.

Jolliffe, I. T. (1973). Discarding variables in a principal components analysis. II: Real data. *Journal of the Royal Statistical Society, Series C (Applied Statistics)*, 22, 21–31.

Jolliffe, I. T. (1989). Rotation of ill-defined components. *Journal of the Royal Statistical Society, Series C (Applied Statistics)*, 38, 139–148.

Jolliffe, I. T. (2002). *Principal Component Analysis*, 2nd edition. Springer, New York.

Jöreskog, K. G. (1970). A general method for analysis of covariance structures. *Biometrika*, 57, 239–251.

Jöreskog, K. G. (1973). A general method for estimating a linear structural equation system. In *Structural Equation Models in the Social Sciences* (eds. A. S. Goldberger and O. D. Duncan). Seminar Press, New York.

Jöreskog, K. G. (1978). Structural analysis of covariance and correlation matrices. *Psychometrika*, 43, 443–477.

Jöreskog, K. G. (2007). Factor analysis and its extensions. In *Factor Analysis at 100: Historical Developments and Future Directions* (eds. R. Cudeck and R. C. MacCallum). Lawrence Elbaum, Mahwah, New Jersey.

Kaiser, H. F. (1958). The varimax criterion for analytic rotation in factor analysis. *Psychometrika*, 23, 187–200.

Kalbfleisch, J. D. and Prentice, R. L. (2002). *The Statistical Analysis of Failure Time Data*, 2nd edition. John Wiley & Sons, Hoboken, New Jersey.

Kaplan, E. L. and Meier, P. (1958). Nonparametric estimation from incomplete observations. *Journal of the American Statistical Association*, 53, 457–481.

Kaufman, L. and Rousseeuw, P. J. (1990). *Finding Groups in Data: An Introduction to Cluster Analysis*. John Wiley & Sons, New York.

Keele, L. (2008). *Semiparametric Regression for the Social Sciences*. John Wiley & Sons, Chichester, U.K.

Kelsey, J. L. and Hardy, R. J. (1975). Driving of motor vehicles as a risk factor for acute herniated lumbar interverteblar disc. *American Journal of Epidemiology*, 102, 63–73.

Kinsey, A. C., Wardell, B. P. and Martin, C. E. (1948). *Sexual Behavior in the Human Male*. W. B. Saunders, Philadelphia.

Kinsey, A. C., Wardell, B. P., Martin, C. E. and Gebhard, P. H. (1953). *Sexual Behavior in the Human Female*. W. B. Saunders, Philadelphia.

Kleinbaum, D. G., Kupper, L. L., Nizam, A. and Rosenberg, E. S. (2013). *Applied Regression Analysis and Other Multivariable Methods*, 5th edition. Cengage Learning, Boston.

Kline, R. B. (2016). *Principles and Practice of Structural Equation Modeling*, 4th edition. Guilford Press, New York.

Kruskal, J. B. (1964a). Multidimensional scaling by optimizing goodness of fit to a nonmetric hypothesis. *Psychometrika*, 29, 1–27.

Kruskal, J. B. (1964b). Nonmetric multidimensional scaling: A numerical method. *Psychometrika*, 29, 115–129.

Kruskal, J. B. and Wish, M. (1978). *Multidimensional Scaling*. Sage University Paper series on Quantitative Application in the Social Sciences, 07-011. Sage, London.

Krzanowski, W. J. (2000). *Principles of Multivariate Analysis: A User's Perspective*, 2nd edition. Oxford University Press, Oxford.

Krzanowski, W. J. and Marriott, F. H. C. (1994). *Multivariate Analysis. Part 1: Distributions, Ordination and Inference*. Edward Arnold, London.

Laaksonen, S. (2018). *Survey Methodology and Missing Data: Tools and Techniques for Practitioners*. Springer International, Cham, Switzerland.

Labovitz, S. (1970). The assignments of numbers to rank order categories. *American Sociological Review*, 35, 515–524.

Lawley, D. N. and Maxwell, A. E. (1971). *Factor Analysis as a Statistical Method*, 2nd edition. Butterworths, London.

Lebart, L., Morineau, A. and Warwick, K. (1984). *Multivariate Descriptive Statistical Analysis: Correspondence Analysis and Related Techniques for Large Matrices*. John Wiley & Sons, Chichester, U.K.

Lee, Y. J. (1984). Quick and simple approximation of sample sizes for comparing two independent binomial distributions: Different-sample-size case. *Biometrics*, 40, 239–241.

Lehman, D., Wortman, C. and Williams, A. (1987). Long term effects of losing a spouse or a child in a motor vehicle crash. *Journal of Personality and Social Psychology*, 52, 218–231.

Lehtonen, R. and Pahkinen, E. (2004). *Practical Methods for Design and Analysis of Complex Surveys*, 2nd edition. John Wiley & Sons, Chichester, U.K.

Liang, K. and Seger, S. L. (1986). Longitudinal data analysis using generalized linear models. *Biometrika*, 73, 13–22.

Little, R. J. A. (2005). Missing data. In *Encyclopedia of Biostatistics*, 2nd edition (eds. P. Armitage and T. Colton). John Wiley & Sons, Chichester, U.K.

Little, R. J. A. and Rubin, D. B. (2002). *Statistical Analysis with Missing Data*, 2nd edition. John Wiley & Sons, New York.

Longford, N. T. (1993). *Random Coefficient Models.* Oxford University Press, Oxford.

Macdonnell, W. R. (1902). On criminal anthropometry and the identification of criminals. *Biometrika*, 1, 177–227.

Magnello, E. and van Loon, B. (2009). *Introducing Statistics: A Graphic Guide*. Icon Books, London.

Manly, B. F. J. (1986). *Multivariate Statistical Methods: A Primer*. Chapman and Hall, London.

Mardia, K. V., Kent, J. T. and Bibby, J. M. (1979). *Multivariate Analysis.* Academic Press, London.

Marriott, F. H. C. (1974). *The Interpretation of Multiple Observations.* Academic Press, London.

Marriott, F. H. C. (1982). Optimization methods of cluster analysis. *Biometrika*, 69, 417–421.

Matthews, D. E. (2005). Multiple linear regression. In *Encyclopedia of Biostatistics*, 2nd edition (eds. P. Armitage and T. Colton). John Wiley & Sons, Chichester, U.K.

Matthews, J. N., Altman, D. G., Campbell, M. J. and Royston, P. (1990). Analysis of serial measurements in medical research. *British Medical Journal*, 300, 230–235.

Maxwell, S. E. and Delaney, H. D. (2003). *Designing Experiments and Analyzing Data: A Model Comparison Perspective*, 2nd edition. Lawrence Erlbaum, Mahwah, New Jersey.

McCullagh, P. and Nelder, J. A. (1989). *Generalized Linear Models*, 2nd edition. Chapman and Hall, London.

McHugh, R. B. and Le, C. T. (1984). Confidence estimation and the size of a clinical trial. *Contemporary Clinical Trials*, 5, 157–163.

McKay, R. J. and Campbell, N. A. (1982a). Variable selection techniques in discriminant analysis. I: Description. *British Journal of Mathematical and Statistical Psychology*, 35, 1–29.

McKay, R. J. and Campbell, N. A. (1982b). Variable selection techniques in discriminant analysis. II: Allocation. *British Journal of Mathematical and Statistical Psychology*, 35, 30–41.

McNeish, D., An, J. and Hancock, G. R. (2018). The thorny relation between measurement quality and fit index cutoffs in latent variable models. *Journal of Personality Assessment*, 100, 43–52.

Miles, J. and Shevlin, M (2001). *Applying Regression and Correlation.* Sage, London.

Morrison, D. F. (1990). *Multivariate Statistical Methods*, 3rd edition. McGraw-Hill, New York.

Morrison, D. F. (2005). Multivariate analysis of variance. In *Encyclopedia of Biostatistics*, 2nd edition (eds. P. Armitage and T. Colton). John Wiley & Sons, Chichester, U.K.

Mulaik, S. A. (2009). *Linear Causal Modeling with Structural Equations*. Chapman and Hall/CRC, Boca Raton, Florida.

Mulaik, S. A. (2010). *Foundations of Factor Analysis*, 2nd edition. Chapman and Hall/CRC, Boca Raton, Florida.

Murdoch, D. J. and Chow, E. D. (1996). A graphical display of large correlation matrices. *The American Statistician*, 50, 178–180.

Murray, G. and Findlay, J. (1988). Correcting for bias caused by dropouts in hypertension trials. *Statistics in Medicine*, 7, 941–946.

Mustonen, S. (1995). *Tilastolliset monimuuttujamenetelmät* [*Statistical Multivariate Methods*, in Finnish]. Survo Systems, Helsinki. https://www.survo.fi/mustonen/monim.pdf (accessed June 17, 2018).

Mustonen, S. (1996). *Survo ja minä* [*Survo and I*, in Finnish]. Survo Systems, Helsinki. https://www.survo.fi/books/1996/SM_kirja.pdf (accessed June 7, 2018).

Nathanson, J. A. (1971). An application of multivariate analysis in astronomy. *Journal of the Royal Statistical Society, Series C (Applied Statistics)*, 20, 239–249.

Needham, R. M. (1967). Automatic classification in linguistics. *Journal of the Royal Statistical Society, Series D (The Statistician)*, 17, 45–54.

Nelder, J. A. (1977). A reformulation of linear models (with discussion). *Journal of the Royal Statistical Society, Series A*, 140, 48–77.

Nelder, J. A. and Wedderburn, R. W. M. (1972). Generalized linear models. *Journal of the Royal Statistical Society, Series A*, 135, 370–384.

Oakes, M. (1986). *Statistical Inference: A Commentary for the Social and Behavioural Sciences*. John Wiley & Sons, Chichester, U.K.

Oldham, P. D. (1962). A note on the analysis of repeated measurements of the same subjects. *Journal of Chronic Diseases*, 15, 969–977.

Palotie, U., Eronen, A. K., Vehkalahti, K. and Vehkalahti, M. M. (2017). Longevity of 2- and 3-surface restorations in posterior teeth of 25- to 30-year-olds attending Public Dental Service—A 13-year observation. *Journal of Dentistry*, 62, 13–17.

Pearl, J. and Mackenzie, D. (2018). *The Book of Why: The New Science of Cause and Effect*. Basic Books, New York.

Pearson, K. (1901). On lines and planes of closest fit to systems of points in space. *Philosophical Magazine*, 2, 559–572.

Pett, M. A., Lackey, N. R. and Sullivan, J. J. (2003). *Making Sense of Factor Analysis: The Use of Factor Analysis for Instrument Development in Health Care Research*. Sage, London.

Piantadosi, S. (1997). *Clinical Trials: A Methodologic Perspective*. John Wiley & Sons, New York.

Pocock, S. J. (1996). Clinical trials: A statistician's perspective. In *Advances in Biometry* (eds. P. Armitage and H. A. David). John Wiley & Sons, Chichester, U.K.

Proudfoot, J., Ryden, C., Everitt, B. S. et al. (2004). Clinical efficacy of computerized cognitive-behavioural therapy for anxiety and depression in parimary care: Randomized controlled trial. *British Journal of Psychiatry*, 185, 46–54.

Puntanen, S., Styan, G. P. H. and Isotalo, J. (2011). *Matrix Tricks for Linear Statistical Models: Our Personal Top Twenty.* Springer, Heidelberg. http://www.sis.uta.fi/tilasto/matrixtricks/ (accessed August 22, 2018).

Puntanen, S., Styan, G. P. H. and Isotalo, J. (2013). *Formulas Useful for Linear Regression Analysis and Related Matrix Theory: It's Only Formulas But We Like Them.* Springer, Heidelberg.

Rabe-Hesketh, S. and Skrondal, A. (2012). *Multilevel and Longitudinal Modeling Using Stata*, 3rd edition. Volume I: Continuous Responses. Volume II: Categorical Responses, Counts, and Survival. Stata Press, College Station, Texas.

Rawlings, J. O., Pantula, S. G. and Dickey, D. A. (1998). *Applied Regression Analysis: A Research Tool*, 2nd edition. Springer, New York.

Rencher, A. C. and Christensen, W. F. (2012). *Methods of Multivariate Analysis*, 3rd edition. John Wiley & Sons, New York.

Rosenbaum, P. R. (2002). *Observational Studies*, 2nd edition. Springer, New York.

Rosenman, R. H., Brand, R. J., Jenkins, C. D., Friedman, M., Straus, R. and Wurm, M. (1975). Coronary heart disease in the Western Collaborative Group study: Final follow-up experience of 8 1/2 years. *The Journal of the American Medical Association*, 233, 872–877.

Rosling, H., Rosling, O. and Rosling Rönnlund, A. (2018). *Factfulness: Ten Reasons We're Wrong About the World—and Why Things Are Better Than You Think.* Sceptre, London.

Rubin, D. B. (1976). Inference and missing data. *Biometrika*, 63, 581–592.

Rubin, D. B. (2004). *Multiple Imputation for Nonresponse in Surveys.* John Wiley & Sons, New York.

Rubin, D. B. and Schenker, N. (1991). Multiple imputation in health-care databases: An overview and some applications. *Statistics in Medicine*, 10, 585–598.

Saarinen, E. and Hämäläinen, R. P. (2004). Systems intelligence: Connecting engineering thinking with human sensitivity. In *Systems Intelligence—Discovering a Hidden Competence in Human Action and Organizational Life* (eds. R. P. Hämäläinen and E. Saarinen). Helsinki University of Technology, Research Reports A88. http://sal.aalto.fi/publications/pdf-files/systemsintelligence2004.pdf (accessed March 28, 2018).

Sarkar, D. (2008). *Lattice: Multivariate Visualization with R.* Springer, New York.

Schafer, J. L. (1997). *Analysis of Incomplete Multivariate Data.* Chapman and Hall, London.

Schafer, J. L. (1999). Multiple imputation: A primer. *Statistical Methods in Medical Research*, 8, 3–15.

Schafer, J. L. and Graham, J. W. (2002). Missing data: Our view of the state of the art. *Psychological Methods*, 7, 147–177.

Schmid, C. F. (1954). *Handbook of Graphic Presentation.* Ronald Press, New York.

Schmidt, U., Evans, K., Tiller, J. and Treasure, J. (1995). Puberty, sexual milestones and abuse: How are they related in eating disorder patients? *Psychological Medicine*, 25, 413–417.

Schoenfeld, D. A. (1983). Sample-size formula for the proportional-hazards regression model. *Biometrics*, 39, 499–503.

Schuman, H. and Kalton, G. (1985). Survey methods. In *Handbook of Social Psychology*, Vol. I (eds. G. Lindzey and E. Aronson). Random House, New York.

Scott, A. J. and Symons, M. J. (1971). Clustering methods based on likelihood ratio criteria. *Biometrics*, 37, 387–398.

Seeber, G. U. H. (2005). Poisson regression. In *Encyclopedia of Biostatistics*, 2nd edition (eds. P. Armitage and T. Colton). John Wiley & Sons, Chichester, U.K.

Senn, S. J. (1997). *Statistical Issues in Drug Development.* John Wiley & Sons, Chichester, U.K.

Shadish, W. R., Cook, T. D. and Campbell, D. T. (2002). *Experimental and Quasi-Experimental Designs for Generalized Causal Inference.* Houghton Mifflin, Boston.

Shepard, R. N. (1962a). The analysis of proximities: Multidimensional scaling with an unknown distance function. I. *Psychometrika*, 27, 125–140.

Shepard, R. N. (1962b). The analysis of proximities: Multidimensional scaling with an unknown distance function. II. *Psychometrika*, 27, 219–246.

Sibson, R. (1979). Studies in the robustness of multidimensional scaling: Perturbational analysis of classical scaling. *Journal of the Royal Statistical Society, Series B*, 41, 217–229.

Siddhartha, R. D., Fowlkes, E. B. and Hoadley, B. (1989). Risk analysis of the space shuttle: Pre-Challenger prediction of failure. *Journal of the American Statistical Association*, 84, 945–957.

Siegfried, T. (2010). “Odds are, it’s wrong: Science fails to face the shortcomings of statistics”. *Science News*, 177, 26.

Simon, R. (1991). A decade of progress in statistical methodology for clinical trials. *Statistics in Medicine*, 10, 1789–1817.

Skrondal, A. and Rabe-Hesketh, S. (2004). *Generalized Latent Variable Modeling: Multilevel, Longitudinal, and Structural Equation Models.* Chapman and Hall/CRC, Boca Raton, Florida.

Smith, D. A. and Patterson, E. B. (1984). Applications and a generalization of MIMIC models to criminological research. *Journal of Research in Crime and Delinquency*, 21, 333–352.

Spear, M. E. (1952). *Charting Statistics.* McGraw-Hill, New York.

Spearman, C. (1904). General intelligence, objectively determined and measured. *American Journal of Psychology*, 15, 201–293.

Spicer, C. C., Lawrence, C. J. and Southall, D. P. (1987). Statistical analysis of heart rates and subsequent victims of sudden infant death syndrome. *Statistics in Medicine*, 6, 159–166.

Steinley, D. (2008). Stability analysis in K-means clustering. *British Journal of Mathematical and Statistical Psychology*, 61, 255–273.

Stigler, S. M. (2016). *The Seven Pillars of Statistical Wisdom.* Harvard University Press, Cambridge, Massachusetts.

Tarkkonen, L. and Vehkalahti, K. (2005). Measurement errors in multivariate measurement scales. *Journal of Multivariate Analysis*, 96, 172–189.

Thall, P. F. and Vail, S. C. (1990). Some covariance models for longitudinal count data with overdispersion. *Biometrics*, 46, 657–671.

Therneau, T. M. and Grambsch, P. M. (2000). *Modeling Survival Data: Extending the Cox Model.* Springer, New York.

Thomsen, O. Ø., Wulff, H. R., Martin, A. and Springer, P. A. (1993). What do gastroenterologists in Europe tell cancer patients? *The Lancet*, 341, 473–476.

Thurstone, L. L. (1931). Multiple factor analysis. *Psychological Review*, 39, 406–427.

Thurstone, L. L. (1935). *Vectors of Mind.* The University of Chicago Press, Chicago.

Thurstone, L. L. (1947). *Multiple-Factor Analysis.* The University of Chicago Press, Chicago.

Timm, N. H. (2002). *Applied Multivariate Analysis.* Springer, New York.

Torgerson, W. S. (1952). Multidimensional scaling: I. Theory and method. *Psychometrika*, 17, 401–419.

Torgerson, W. S. (1958). *Theory and Methods of Scaling.* John Wiley & Sons, New York.

Törmänen, J., Hämäläinen, R. P. and Saarinen, E. (2016). Systems Intelligence inventory. *The Learning Organization*, 23, 218–231.

Tourangeau, R., Rips, L. J. and Rasinski, K. (2000). *The Psychology of Survey Response.* Cambridge University Press, New York.

Tufte, E. R. (1983). *The Visual Display of Quantitative Information.* Graphics Press, Cheshire, Connecticut.

Tukey, J. W. (1977). *Exploratory Data Analysis.* Addison Wesley, Reading, Massachusetts.

United Nations (2016). *Demographic Yearbook.* United Nations, New York. https://unstats.un.org/unsd/demographic-social/products/dyb/ (accessed June 3, 2018).

van Buuren, S. (2018). *Flexible Imputation of Missing Data*, 2nd edition. Chapman and Hall/CRC, Boca Raton, Florida.

Vehkalahti, K., Koponen, J. and Kuusi, H. (2018). From Russia with love to *infovis*: Graphic train schedules reflect the history of Finland. *CHANCE*, 31, 46–53.

Vehkalahti, K., Puntanen, S. and Tarkkonen, L. (2007). Effects of measurement errors in predictor selection of linear regression model. *Computational Statistics & Data Analysis*, 52, 1183–1195.

Velleman, P. F. and Wilkinson, L. (1993). Nominal, ordinal, interval, and ratio typologies are misleading. *The American Statistician*, 47, 65–72.

Vetter, B. M. (1980). Working women scientists and engineers. *Science*, 207, 28–34.

Wainer, H. (1997). *Visual Revelations.* Springer, New York.

Wasserstein, R. L. and Lazar, N. A. (2016). The ASA's statement on *p*-values: Context, process, and purpose. *The American Statistician*, 70, 129–133.

Watkins, E. and Williams, R. M. (1998). The efficacy of cognitive-behavioural therapy. In *The Management of Depression* (ed. S. Checkley). Blackwell Science, Oxford.

White, I. R., Royston, P. and Wood, A. M. (2011). Multiple imputation using chained equations: Issues and guidance for practice. *Statistics in Medicine*, 30, 377-399.

Widaman, K. F. (2007). Common factors versus components: Principals and principles, errors and misconceptions. In *Factor Analysis at 100: Historical Developments and Future Directions* (eds. R. Cudeck and R. C. MacCallum). Lawrence Elbaum, Mahwah, New Jersey.

Wilkinson, L. (1992). Graphical displays. *Statistical Methods in Medical Research*, 1, 3–25.

Willerman, L., Schultz, R., Rutledge, J. N. and Bigler, E. D. (1991). In vivo brain size and intelligence. *Intelligence*, 15, 223–228.

Wittes, J. and Wallenstein, S. (1987). The power of the Mantel–Haenszel test. *Journal of the American Statistical Association*, 82, 1104–1109.

Wright, S. (1921). Correlation and causation. *Journal of Agricultural Research*, 20, 557–585.

Wright, S. (1934). The method of path coefficients. *The Annals of Mathematical Statistics*, 5, 161–215.

Yarkoni, T. and Westfall, J. (2017). Choosing prediction over explanation in psychology: Lessons from machine learning. *Perspectives on Psychological Science*, 12, 1100–1122.

Yates, F. (1982). Regression models for repeated measurements. *Biometrics*, 38, 850–853.

Young, G. and Householder, A. S. (1938). Discussion of a set of points in terms of their mutual distances. *Psychometrika*, 3, 19–22.

Yule, W., Berger, M., Butler, S., Newham, V. and Tizard, J. (1969). The WPPSI: An empirical evaluation with a British sample. *British Journal of Educational Psychology*, 39, 1–13.