

Statistics for Biology and Health

Daniel Zelterman

Applied Multivariate Statistics with R

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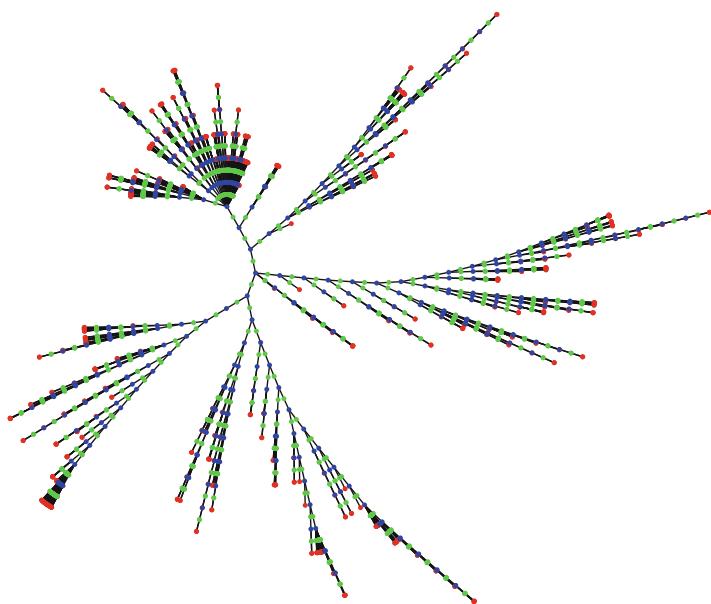
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Applied Multivariate Statistics with R



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Barry H Margolin
1943–2009
Teacher, mentor, and friend

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Public domain data in Table 1.4 was obtained from the U.S. Cancer Statistics Working Group. *United States Cancer Statistics: 1999–2007 Incidence and Mortality Web-based Report*. Atlanta: U.S. Department of Health and Human Services, Centers for Disease Control and Prevention and National Cancer Institute; 2010. Available online at www.cdc.gov/uscs.

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<http://www.thedailybeast.com/galleries/2010/06/17/40-unhealthiest-burgers.html>.

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The data in Table 8.3 was reported by the National Vital Statistics System (NVSS):

<http://www.cdc.gov/nchs/deaths.htm>.

The data in Table 9.3 was generated as part of the Medicare Current Beneficiary Survey: <http://www.cms.gov/mcbs/> and available on the cdc.gov website.

The data in Table 9.4 was collected by the United States Department of Labor, Mine Safety and Health Administration. This data is available online at

<http://www.msha.gov/stats/centurystats/coalstats.asp>.

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In Addition

Several data sets referenced and used as examples were obtained from the UCI Machine Learning Repository [<http://archive.ics.uci.edu/ml>]. Irvine, CA: University of California, School of Information and Computer Science (Bache and Lichman 2013).

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Preface

MULTIVARIATE STATISTICS is a mature field with many different methods. Many of these are mathematical. Fortunately, these methods have been programmed so you should be able to run these on your computer without much difficulty.

This book is targeted to a graduate-level practitioner who may need to use these methods but does not necessarily know about the mathematical derivations. For example, we use the sample average of the multivariate distribution to estimate the population mean but do not need to prove optimal properties of such an estimator when sampled from a normal parent population. Readers may want to analyze their data, motivated by discipline-specific questions. They will discover ways to get at some important results without a degree in statistics. Similarly, those well trained in statistics will likely be familiar with many of the univariate topics covered here, but now can learn about new methods.

The reader should have taken at least one course in statistics previously and have some familiarity with such topics as t-test, degrees of freedom (df), p-values, statistical significance, and the chi-squared test of independence in a 2×2 table. He or she should also know the basic rules of probability such as independence and conditional probability. The reader should have some basic computing skills including data editing. It is not necessary to have experience with R or with programming languages although these are good skills to develop.

We will assume that the reader has a rudimentary acquaintance of the univariate normal distribution. We begin a discussion of multivariate models with an introduction of the bivariate normal distribution in Chap. 6. These are used to make the leap from the scalar notation to the use of vectors and matrices used in Chap. 7 on the multivariate normal distribution. A brief review of linear algebra appears in Chap. 4, including the corresponding computations in R. Other multivariate distributions include models for extremes, described in Sect. 13.3.

We frequently include the necessary software to run the programs in R because we need to be able to perform these methods with real data. In some cases we need to manipulate the data in order to get it to fit into the proper format. Readers may want to produce some of the graphical displays

given in Chap. 3 for their own data. For these readers, the full programs to produce the figures are listed in that chapter.

The field of statistics has developed many useful methods for analyzing data, and many of these methods are already programmed for you and readily available in R. What's more, R is free, widely available, open source, flexible, and the current fashion in statistical computing. Authors of new statistical methods are regularly contributing to the many libraries in R so many new results are included as well.

As befitting the Springer series in Life Sciences, Medicine & Health, a large portion of the examples given here are health related or biologically oriented. There are also a large number of examples from other disciplines. There are several reasons for this, including the abundance of good examples that are available. Examples from other disciplines do a good job of illustrating the method without a great deal of background knowledge of the data.

For example, Chap. 9 on multivariable linear regression methods begins with an example of data for different car models. Because the measurements on the cars are readily understood by the reader with little or no additional explanation, we can concentrate on the statistical methods rather than spending time on the example details. In contrast, the second example, presented in Sect. 9.3, is about a large health survey and requires a longer introduction for the reader to appreciate the data. But at that point in Chap. 9, we are already familiar with the statistical tools and can address issues raised by the survey data.

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The APL computer language and TW Anderson's book (Anderson 2003)¹ on multivariate statistics provided me with the foundation for writing this book as a graduate student in the 1970s. I watched Frank Anscombe² working on his book (Anscombe 1981) and was both inspired and awed by the amount of effort involved.

¹Theodore Wilbur Anderson (1918–). American mathematician and statistician.

²Francis John Anscombe (1918–2001). British statistician. Founded the Statistics Department at Yale.

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Chapter 1

Introduction

WE ARE SURROUNDED by data. How is multivariate data analysis different from more familiar univariate methods? This chapter provides a summary of most of the major topics covered in this book. We also want to provide advocacy for the multivariate methods developed.

This chapter introduces some useful data sets and uses them to motivate the topics and basic principles and ideas of multivariate analysis. Why do we need multivariate methods? What are the shortcomings of the marginal approach, that is, looking at variable measurements one at a time? In many scientific investigations, there are several variables of interest. Can they be examined one at a time? What can be lost by performing such univariate analysis?

1.1 Goals of Multivariate Statistical Techniques

Let us summarize the types of problems to be addressed in this book and briefly describe some of the methods to be introduced in subsequent chapters. As an example, consider the data given in Table 1.1. This table lists each of the 50 US states (plus DC) and several indications of the costs associated with living there. For each state, this table shows the population, average gross income, cost of living index relative to the US as a whole, median monthly apartment rentals, and then median housing price. Because the cost of living index is calculated on estimates of prices including housing costs, we quickly see that there may be a strong relationship between measures in this table.

Table 1.1: Costs of living in each of the 50 states

State	Median apartment rent in \$	Median home value in \$1000	Cost of living index	2009 population in 1000s	Average gross income in \$1000
AK	949	237.8	133.2	698.47	68.60
AL	631	121.5	93.3	4708.71	36.11
AR	606	105.7	90.4	2889.45	34.03
⋮	⋮	⋮	⋮	⋮	⋮
WV	528	95.9	95.0	1819.78	33.88
WY	636	188.2	99.6	544.27	64.88

Source: US Census, 2007 and 2009 data

As an example of a multivariate statistical analysis, let us create a 95 % joint (simultaneous) confidence interval of both the mean rent and housing prices.¹ In Fig. 1.1 we present both the marginal confidence intervals and the joint, bivariate confidence ellipsoid that is described more fully in Sect. 6.3.

The marginal confidence intervals treat each variable individually, and the resulting 95 % confidence interval for the two means is pictured as a rectangle. The bivariate confidence ellipsoid takes into account the correlation between rents and housing prices resulting in an elongated elliptical shape oriented to reflect the positive correlation between these two prices.

The elliptical area and the rectangle overlap. There are also areas included in one figure but not the other. More importantly, notice the area of the ellipse is smaller than that of the rectangle. This difference in area illustrates the benefit of using multivariate methods over the marginal approach. If we were using univariate methods and obtaining confidence intervals for each variable individually, then the resulting confidence region is larger than the region that takes the bivariate relationship of rents and housing costs into account. This figure provides a graphical illustration of the benefits of using multivariate methods over the use of a series of univariate analyses.

¹The thoughtful reader might argue this exercise does not make sense because there are only 50 states and this *census* represents the values of the complete population. In other words, there is no uncertainty associated with this data because there is no larger population of states for us to sample from.

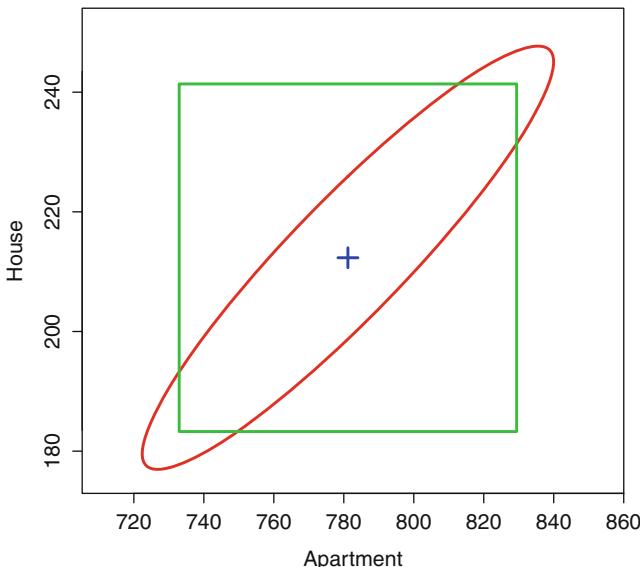


Figure 1.1: Joint 95 % confidence ellipsoid for housing prices and monthly apartment rents. The box is formed from the marginal 95 % confidence intervals. The sample averages are indicated in the *center*

1.2 Data Reduction or Structural Simplification

Which variables should be recorded when constructing a multivariate data set? We certainly want to include everything that might eventually turn out to be relevant, useful, and/or important. Much of these decisions require knowledge of the specific subject matter and cannot be adequately covered in a book on statistics. There is a trade-off between the fear of leaving out some information that later proves to be critical. Similarly, it may be next to impossible to go back to record data that was not recoded earlier.

Hopefully the subject matter experts have collected the most useful sets of measurements (with or without the aid of a statistician). The first task for the data analyst is to sort through it and determine those variables that are worthy of our attention. Similarly, much of the data collected may be redundant. A goal of data analysis is to sift through the data and identify what should be kept for further examination and what can safely be discarded.

Let us consider the data in Table 1.2 on the outcome of a standardized test of students taken in different countries (or economies) in 2009. The Program for International Student Assessment (PISA) is a triennial survey of

Table 1.2: Reading and other academic scores from OECD nations

Nation	Overall reading	Reading subscales					
		Access retrieve	Integrate interpret	Reflect eval.	Continuous	Noncontin.	Math
China:							
Shanghai	556	549	558	557	564	539	600
Korea	539	542	541	542	538	542	546
Finland	536	532	538	536	535	535	54
Hong Kong	533	530	530	540	538	522	555
:	:	:	:	:	:	:	:
Peru	370	364	371	368	374	356	365
Azerbaijan	362	361	373	335	362	351	431
Kyrgyzstan	314	299	327	300	319	293	331

Source: OECD PISA 2009 database

academic achievements of 15-year-old students in each of 70 different countries.² The US is #17 on this list behind homogeneous populations of Finland, Korea, Hong Kong.

The overall reading score is broken down into five different subscales measuring specific skills. Mathematics and science are listed separately. How much is gained by providing the different subscales for reading? Is it possible to remove or combine some of these with little loss of detail?

More specifically, Fig. 1.2 is a matrix scatterplot of the eight different academic scores from Table 1.2. The matrix scatterplot plots every pair of measurements against each other twice, with the axes reversed above and below the diagonal.

The immediate impression we get from this figure is how highly correlated all of the measurements are with each other. There are a few outliers and some pairs of measurements are more tightly correlated, of course, but it is clear that any one academic measurement in the data could stand as a good representation for most of the others. There is a large amount of data simplification that can be performed for this data without significant loss of information.

1.3 Grouping and Classifying Observations

In 2006, Pluto was demoted from the family of planets in our solar system and it is now classified as just one of many objects orbiting the sun. Part of the argument for Pluto's reassignment consists of the large number of smaller and larger additional objects orbiting the sun at about the same distance. One group of these is referred to as the Kuiper Belt³ extending from the orbit of Neptune at about 30 AU out to about 55 AU. (One astronomical unit (AU) is the distance to the earth from the sun.) The Kuiper Belt contains more than a thousand known objects, and there are estimates of many tens of thousands more yet to be discovered. Data on several of the largest of these appears in Table 1.3.

Albedo refers to the percentage of light that is reflected rather than absorbed. Snow, for example, appears very bright and has a high albedo. The absolute magnitude is a measure of apparent brightness, corrected for the distance of the object, measured on a logarithmic scale. Higher absolute magnitude refers to dimmer objects. The semimajor axis is the orbit's greatest distance from the sun, measured in AU. Many of the values in this table are, at best, rough estimates for these distant, poorly understood objects.

²This survey is funded by The Organisation for Economic Co-operation and Development (OECD).

³Named for Dutch astronomer Gerard Peter Kuiper (rhymes with viper) 1905–1973.

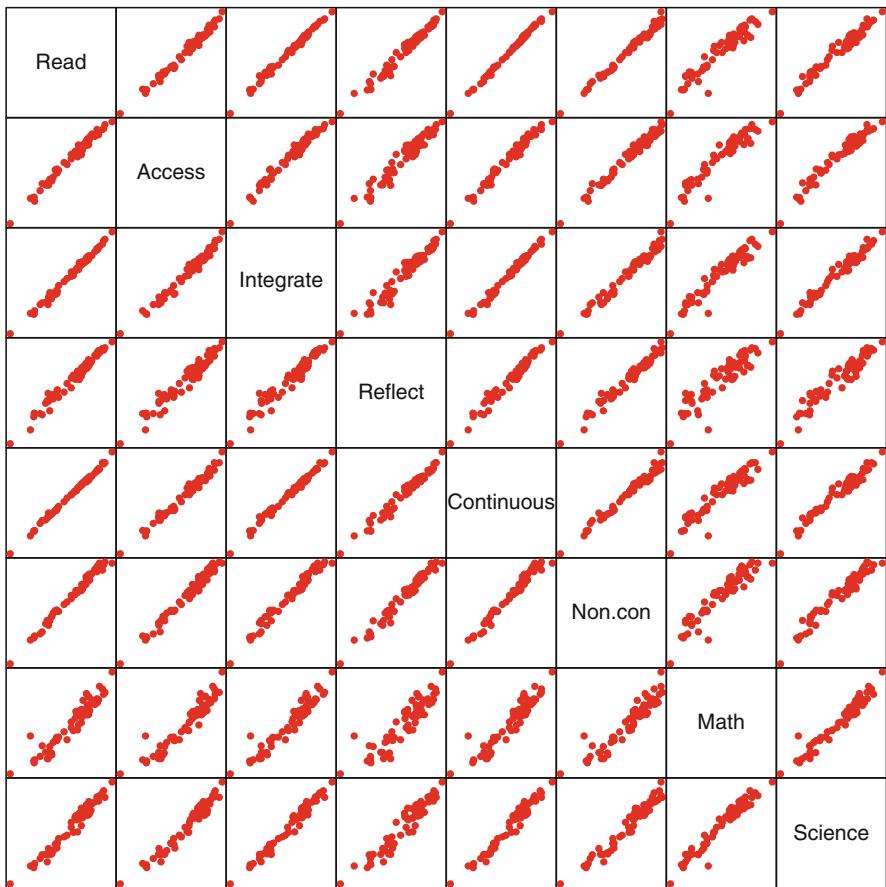


Figure 1.2: Matrix scatterplot of reading and academic scores of 15-year-old students in 2009 in OECT nations

Is Pluto a real standout object among the items in this list, or does it appear similar in character to the others? Does Pluto deserve to regain its former planet status or is it just one member of a larger club? In Sect. 8.1 we look at this data and see if there is a way to simplify it. Can this multivariate data be summarized in a way that retains much of the useful information? Where does Pluto fall in this larger schema of things?

A comparison of the cancer rates in each of 50 states is another example to illustrate grouping. The data in Table 1.4 lists overall 2007 cancer rates for each of the 50 US states as well as for several of the most common cancers. These rates are reported as cases per 100,000 persons. Each state has a slightly different distribution of ages within its populations so these rates are *age adjusted*, as well.

Table 1.3: Several Kuiper Belt objects

Designation	Absolute magnitude	Albedo (%)	Equatorial diameter (km)	Semimajor axis (AU)	Year of discovery
Permanent	Provisional				
Pluto	-1.00	60.0	2320.0	39.4	1930
Makemake	2005 FY9	-0.30	80.0	1500.0	45.7
Haumea	2003 EL61	0.10	84.0	1150.0	43.3
Charon	S/1978 P 1	1.00	40.0	1205.0	39.4
Orcus	2004 DW	2.30	19.7	946.3	39.4
Quaoar	2002 LM60	2.60	19.9	844.0	43.5
Ixion	2001 KX76	3.20	12.0	650.0	39.6
55636	2002 TX300	3.30	10.0	800.0	43.1
55565	2002 AW197	3.30	11.7	734.6	47.4
55637	2002 UX25	3.60	11.5	681.2	42.5
Varuna	2000 WR106	3.70	16.0	500.0	43.0
2002 MS4		3.80	8.4	726.2	41.8
2003 AZ84		3.90	12.3	685.8	39.6

Source: Wikipedia

Table 1.4: Age-adjusted cancer rates per 100,000 persons, combined for sexes and all races

	All	Mel-	Female	Pan-	Leu-	Cer-	Pro-				
State	cancers	Lung	Colon	anoma	breast	creas	kemia	Ovary	vix	state	Liver
CT	584.1	54.4	52.4	27.9	133.9	16.2	13.7	12.1	6.5	172.8	9.8
ME	598.9	70.4	53.6	24.6	128.9	13.1	20.7	11.8	7.5	165.7	6.2
MA	571.0	62.6	50.7	26.0	131.7	13.3	16.0	11.8	5.3	166.9	10.9

OR	508.8	59.1	46.1	28.7	129.6	12.2	13.5	12.7	7.9	145.2	8.5
WA	525.3	56.6	45.9	27.5	124.0	13.0	17.1	12.5	5.9	155.1	10.1
US	535.3	65.2	52.7	23.5	120.4	13.2	15.0	12.2	7.9	156.9	9.9

Source: US Centers for Disease Control

Is a high rate of one cancer associated with an increase in other cancers? If so, which cancer rates tend to move together in lock step? Which appear to be unrelated to others? Lung cancers, for example, are frequently associated with environmental causes and colon cancers sometimes have a dietary origin. We might want to know how different cancer types cluster into similar patterns.

We can also ask about states clustering. Which states are comparable in their various rates? Do neighboring states have similar rates? Do the southern states group together with comparable cancer rates? How do Southern states differ from the Western states?

Perhaps the best summary is just group all of the data together. As an example, the “All cancers” rate is a sum of all cancer types, including the many diseases not listed here. Is this rate a reasonable summary of the rates for each state? Do the states that cluster together also have comparable rates of their “all cancers”? Instead of a simple sum of all individual rates, would it be better to construct a weighted average, where some cancers receive more emphasis than others? Should rarer cancers (liver and cervix, for examples) be given more or less weight than more common cancers?

Methods to answer these questions are described in Chaps. 10 and 11. Discrimination and classification are used to identify characteristics of groups of individuals, when group membership is known. Clustering assumes that there are groups of individuals but their group membership is not known.

1.4 Examination of Dependence Among Variables

Table 1.5 lists a survey of the recommended investment allocations from major financial management firms as of early 2011. The numbers represent percent allocations for their “model portfolios” but they would usually make specific recommendations for individual circumstances. Stocks and bonds are broken into three categories: US, non-US industrialized countries, and developing nations. Alternative investments include leases, oil and gas partnerships, real estate property, precious metals, and similar investments. Cash includes short-term investments such as money market, bank deposits, and certificates of deposit.

At the time this table was created, the US was pulling out of a deep recession. It was generally felt that US stocks and bonds were the appropriate investments at the time, so these two columns represent the largest entries in the table. Interest rates on cash equivalents were very low so only small allocations appear in that column.

The numbers add up to 100% for each advisory firm. We should expect a small overall negative mutual correlation of all of the percentages within each row because of this restriction on these percentages. (The totals may be off by a small amount due to rounding.)

Each of the investment firms hears the same economic news and reads each other’s published recommendations, so we should expect a small correlation between the different rows of this data. As befits the conservative nature of this business, no firm wants to be known for a consistently deviant recommendation, so there probably is an attenuation of extreme opinions present as well. Within each firm’s recommendations, there are certain percentages allocated to traditional stocks and bonds. Each of these is further broken down by firms that specialize in domestic and foreign companies.

Another example of the data we might encounter appears in the nutritional data in Table 1.6. This a collection of some of the highest calorie hamburgers served in chain restaurants collected on the website fatsecret.com. Nutrition is an intrinsically multivariate concept. We cannot talk about calories alone when discussing nutrition but also need to include data on how much of the caloric value is derived from fat. Amounts of sodium (salt) and protein are not part of calorie count and provide different qualities to the total nutritional content.

The nutritional content was obtained from the individual restaurant’s websites. Each burger lists its calories and calories from fat, fat, saturated fat, sodium, carbohydrates, and protein content. The nutritional content of each menu item is not a single measurement but expressed as these seven separate components. The seven values are related to each other and must be taken as a whole. This is the fundamental concept of multivariate data: each individual item is characterized by a set of several related measurements on each.

The seven nutritional values are mutually correlated. Saturated fat and carbohydrates are related to the calories. Sodium is different from the other six. Perhaps we want to create a “health index” that is constructed as a weighted average of the components of each burger, thereby reducing the seven-dimensional data into a single number for each. This is the aim of some multivariate methods such as factor analysis, described in Chap. 8. Another goal might be to creatively display all nutritional components simultaneously such as in Fig. 3.15 or 3.20.

1.5 Describing Relationships Between Groups of Variables

Let us go back to the data given in Table 1.1. How can we describe the differences in costs associated with living in each of the states? There are three measures of costs (rents, home prices, and cost of living index), and these three are mutually correlated. Each of these measures of costs might separately be explained by populations and incomes. Perhaps more people living there, with higher incomes, would drive up the prices relative to sparsely populated states with lower average incomes.

The three measures of costs are themselves related but the use of three separate regressions would lose these relationships. How much of the cost of living index can be explained by population and income, for example, and after correcting for these, how much of these differences across states can be attributed to housing costs? Chapter 9 covers the topic of multivariable regression and in Exercise 9.1 we will examine this example in detail.

1.6 Hypothesis Formulation and Testing

Interesting data sets are generated by a wide range of disciplines as new discoveries increasingly rely on statistical methods. Massive amounts of data are collected in genetics and astronomy, for example, where hypotheses are generated from within the discipline as well as on the basis of statistical analyses of the data.

Let us illustrate some data from astrostatistics, a relatively new field bringing together astronomy and statistics. In Fig. 1.3 we plot the visual magnitude of 3858 galaxies in a portion of the sky. Locations in the sky are addressed in polar coordinates much as we identify places on the earth: right ascension is similar to longitude and declination is similar to latitude.

Table 1.5: Recommended investment allocations (in %) by financial management firms at the beginning of 2011

Manager	Stocks			Bonds			Alter-	
	US	Non-US	Dev.	US	Non-US	Dev.	native	Cash
Alliance Bernstein	45	3	17	35	0	0	0	0
Atlantic Trust	28	6	9	30	3	0	24	0
Bank of America	53	9	3	28	1	1	0	5
BNY Mellon	26	9	10	30	0	0	25	0
Bessemer	19	9	3	20	4	5	34	6
Brown Advisory	29	13	12	19	3	0	20	4
Citi Private Bank	18	27	3	18	16	1	17	0
Constellation	20	10	10	25	5	0	30	0
Deutsche Bank	29	14	6	29	2	4	17	2
Fidelity	40	14	4	35	2	0	6	0
Fiduciary Trust	40	10	13	31	0	0	5	2
Fifth Third Bank	28	9	7	36	0	0	15	5
GenSpring	13	8	5	18	8	0	45	5
Glenmede	35	12	5	18	2	3	23	2
Harris Private Bank	54	10	4	18	0	0	15	0
Highmount Capital	25	5	10	40	5	0	15	0
Janney Montgomery	47	4	4	26	4	5	10	0
JPMorgan	20	9	5	22	3	0	38	3
Legg Mason	55	3	7	17	0	0	15	3
Northern Trust	24	8	5	31	0	0	32	0
PNC Asset Mgmt	40	8	2	30	0	0	20	0
Charles Schwab	29	20	5	29	1	0	11	5
SunTrust	26	6	3	25	7	0	30	3
UBS	32	10	7	27	6	0	17	2
US Bank	43	16	7	21	3	0	10	0
Wells Fargo	27	13	5	21	4	2	28	0
Wilmington Trust	27	11	4	31	1	0	27	0
Averages	32.3	10.2	6.5	26.3	3.0	0.8	19.6	1.7

Used with permission S&P, Dow Jones

Table 1.6: Some of the highest calorie hamburgers served in chain restaurants

Rest- aurant Name of burger		Calories	Fat	Sat. fat (g)	Sodium (mg)	Carbs. (g)	Protein (g)
	From fat	Total	(g)				
Chili's Bacon Burger	612	1050	68	21	1750	53	55
Chili's Big Mouth Bites	1197	2120	133	38	4200	139	65
Chili's Southern Bacon	963	1610	107	36	4150	81	53
⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮
Sonic Cheese w/ Mayo	573	999	64	24	1591	62	46
Sonic Dbl Cheeseburger	730	1160	81	33	1580	44	63

Source: www.fatsecret.com. Used with permission

Magnitude is visual brightness measured on an inverted log scale: larger numbers are dimmer. Every increase in one unit is about 2.5 times dimmer. A magnitude of 6 is about the limit of the human eye; this is extended to about 10 with binoculars. Magnitude 27 is the approximate limit of the largest earth-bound telescopes, and the Hubble Space Telescope can detect to magnitude 32. In Fig. 1.3, the brighter (and generally closer) galaxies are in red and dimmer ones are in blue.

The brighter galaxies in red appear to be distributed uniformly across this field, but the dimmer ones in blue seem to cluster in the upper left of this figure. It is well known in astronomy that galaxies are not uniformly distributed across the universe, but, rather, clustered much like the surface of bubbles, on curved walls, centered around vast, seemingly empty spaces.

Of course, this figure can only plot the objects that are known at the time the data was collected. Dimmer, as yet undetected galaxies are missing. There are many more objects that would be plotted in blue in this figure at a future date as our technology improves.

1.7 Multivariate Graphics and Distributions

R offers strong graphical methods. These are illustrated in Chap. 3. You may want to thumb through this chapter before reading any further. Most of these examples require some knowledge of R in order to format the data appropriately. If you have no familiarity with R, then you can learn about its basic functions in Chap. 2.

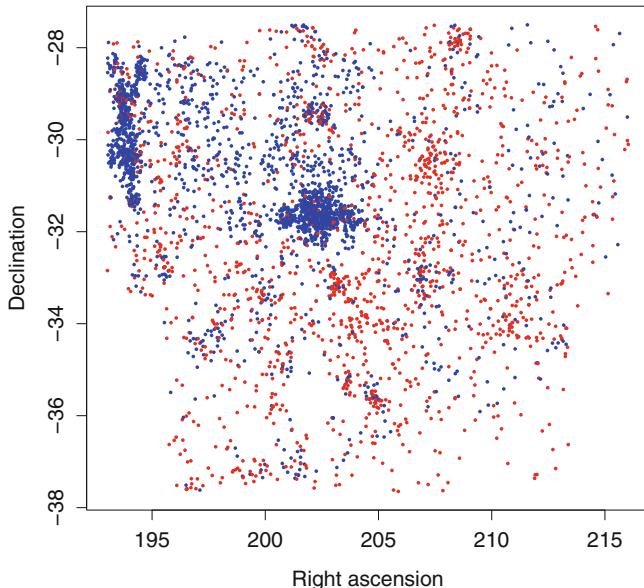


Figure 1.3: Visual magnitudes of 3858 galaxies in a portion of the sky. Brighter objects are plotted in red

1.8 Why R?

Finally, a word about the choice of R for the present book. There are a number of high-quality software packages available to the data analyst today. As with any type of tool, some are better suited for the task at hand than others. Understanding the strengths and limitations will help determine which is appropriate for your needs. It is better to decide this early, rather than investing a lot of time on a major project, only to be disappointed later.

Let us begin with a side-by-side comparison of SAS⁴ and R, two popular languages regularly in use by the statistical community today. The most glaring differences between these packages are the capability to handle huge databases and the capability to provide a certification for the validity of the results. SAS is the standard package for many applications such as in pharmaceuticals and financials because it can handle massive data sets and provide third-party certification. In contrast, R is more suited for quick and nimble analyses of smaller data sets. There is no independent review of R and errors can continue, uncorrected, for years.

SAS is also more suitable for sharing programs and data, as in a business setting. SAS encourages the development of large programs through the use

⁴SAS is copyright © SAS Institute, Cary, NC.

of its powerful *macro*⁵ language. The macro writes code that is expanded before the interpreter actually reads the code that is converted into instructions. In contrast, R has limited macro capabilities.

R was chosen as the software tool for the present book because of its extensive libraries to perform the relevant analyses and more flexible graphics capability. The author also teaches, regularly uses, and has written books using SAS. R is widely available as a free download from the Internet.⁶ Follow the instructions: It should not be too difficult to download R and install it on your computer. R is open source, meaning that in many cases, you can examine the source code and see exactly what action is being performed. Further, if you don't like the way it performs a task, then you can rewrite the code to have it do what *you* want it to do. Of course, this is a dangerous capability if you are just a novice, but it does point out a more useful property: Anybody can contribute to it. As a result there are hundreds of user-written packages available to you. These include specialized programs for different analyses, both statistical and discipline specific, as well as collections of data. Table 1.7 summarizes the differences between SAS and R.

The learning curve for R is not terribly steep. Most users are up and running quickly, performing many useful actions. R provides a nice graphical interface that encourages visual displays of information as well as mathematical calculation. Once you get comfortable with R, you will probably want to learn more.

It is highly recommended that all users of R work in Rstudio, an interface that provides both assistance for novices as well as productivity tools for experienced users. The Rstudio opens four windows: one for editing code, a window for the console to execute R code, one track to the variables that are defined in the workspace, and the fourth to display graphical images.

1.9 Additional Readings

There are many excellent introductory books on the capabilities of R, multivariate statistics, and the intersection of these two subjects.

An excellent introduction to R is Krause and Olson (1997). This book describes S and S-PLUS, the predecessors of R, and is light on statistical methods. Everitt and Hothorn (2011) also has a limited number of statistical topics and is more about R computing than statistical inference. Kabacoff (2011) describes R and statistical diagnostics but less statistical methodology. Venables and Ripley (2010) has a mix of statistical theory and R. Johnson and Wichern (2007) is more theoretical and does not incorporate software. Izenman (2008) is also theoretical, addresses current issues of mining large databases, references many relevant data sets, but does not emphasize computing. Anderson (2003) has the most theory of the books listed here.

⁵Briefly, a macro is a program that writes a program.

⁶<http://cran.r-project.org/>.

Table 1.7: A side-by-side comparison of SAS and R

SAS	R
Good for examining huge data sets	Not suitable for massive data sets
Good for shared projects	Better for individual work
Limited graphical presentation	Strong and flexible graphics
Difficult for custom analyses	Encourages customized analysis
Few independently written modules	Large 3rd party software library
“Black box” code is hidden	Often open source
Iterative Matrix Language (IML)	Facilitates matrix operations
Powerful macro facility	Limited macro capabilities
Difficult to write new functions	Easy to write new functions
Point and click analyses	No hand-holding
Certified and verified	No promises made
Easy to produce tables with labels	More difficult to produce tables
Expensive for non-academics	Free
Fewer independently written references	Many independent reference books

Chapter 2

Elements of R

THE SOFTWARE PACKAGE “R” has become very popular over the past decade for good reason. It has *open source*, meaning you can examine exactly what steps the program is performing. Compare this to the “black box” approach adopted by so many other software packages that hope you will just push the `Enter` button and accept the results that appear. Another feature of open software is that if you identify a problem, you can fix it, or, at least, publicize the error until it gets fixed. Finally, once you become proficient at R you can contribute to it. One of the great features of R is the availability of packages of programs written by R users for other R users. Best of all, R is free for the asking and easy to install on your computer.

On the downside, there is no certifying authority verifying that the answers that R gives you are actually correct. Errors are only judged in the court of popular opinion and may remain uncorrected for years. *Caveat emptor*.

Because R is so widely used, there are a number of good introductory books about its capabilities. While we can’t go over everything that can be done in R here, we can cover enough material to get started with the computing needed to perform the statistical analyses described in this book. Despite its many strengths, R does lack the capability to produce a nicely formatted output for a report. If your goal is to produce a formatted document then you will need to learn how to copy the output from R into a word processing program. That is how this book was produced.

At the time of this writing, the R source can be found at

<http://cran.r-project.org/>.

Simply follow the instructions on downloading the most recent package from any of the many mirror sites. There are versions of R for Mac, Linux, and Windows, so there should be a version for almost everybody.

2.1 Getting Started in R

R is interactive. You type something, and the computer types something in response. Try out the examples illustrated here, as they have been designed to ease your introduction to R.

2.1.1 R as a Calculator

Let's give R a try. Click on the R icon. It will open a window, and print some introductory text. Finally, you will see a line with a greater sign: > meaning that you can now type something.

A typical session might go like this:

```
> 3 + 4
[1] 7
> 2 * 6
[1] 12
> 2 ^ 4
[1] 16
>
```

Information you enter appears on the lines that begin with >. For many operations, R produces lines that begin with a number in braces, (e.g., [1]). The numbers in braces will help find locations when there is a lot of output. This brief example shows that R can be used as a calculator, but of course, it is much more than that.

We can assign a value to a name using the paired symbols <-.

```
> radius <- 3
> radius
[1] 3
> circum <- 2 * pi * radius
> circum
[1] 18.84956
```

In this brief dialog we assign the value 3 to the variable called `radius`. Typing the name displays its value. We can then combine arithmetic with this named variable. We assign the result of a mathematical computation to yet another variable called `circum` but don't see the result unless we specifically ask for it.

The name `pi` has the value of $\pi = 3.14159\dots$ and it would be a good idea not to change this. Another good idea is to use variable names that have meaning to us rather than a name such as `x` that conveys little information concerning its use. If you lose track of the variables used and their names, the `ls()` or `objects()` commands will provide a list of everything in the workspace.

You quit R with the `q()` command. You will be prompted if you want to save the workspace. It is a good idea to always check the YES button to save your results for a later session. If you end the R session in this manner, the variables `radius` and `circum` are still available after you close R, turn off your computer, and then restart it at a later time.

A variable, once created, is always available until you specifically ask for it to be deleted. To explicitly remove a variable, we use the `rm()` command as in

```
> radius
[1] 3
> rm(radius)
> radius
Error: object 'radius' not found
```

As you work in R, your workspace will soon become cluttered with a large number of intermediate results and data from various projects. You should make generous use of the `rm` function in order to keep your workspace free of litter. There is also a way to break up your R activities into different workspaces. These are described in Sect. 2.8.

2.1.2 Vectors in R

Vectors are a natural feature of R and can be constructed using the `c` (concatenate) function:

```
> evens <- c(2, 4, 6, 8, 10)
> evens
[1] 2 4 6 8 10
```

and then multiply the vector by a scalar:

```
> 2 * evens
[1] 4 8 12 16 20
```

The `rep(,)` function takes two arguments and is used to make multiple copies of the first argument. The first argument may be either a vector or a scalar. The `each =` option makes copies of individual elements of the list. Here are examples of its use:

```
> c(1, rep(2, 3), 4)
[1] 1 2 2 2 4
> rep( c(1, 2), 4)
[1] 1 2 1 2 1 2 1 2
> rep( c(3, 5), each = 4)
[1] 3 3 3 3 5 5 5 5
```

The colon (`:`) operator produces an increasing or decreasing sequence of integers as in these two examples:

```
> 3 : 10
[1] 3 4 5 6 7 8 9 10
> 12 : 5
[1] 12 11 10 9 8 7 6 5
```

These can be combined in arithmetical expressions giving

```
> 4 : 8 / 4
[1] 1.00 1.25 1.50 1.75 2.00
```

so that we are not restricted to working only with integer sequences.

In this last example, we see that the sequence operation is given precedence over the division. That is, the sequence operator in `4:8 / 4` is evaluated first, then the division. You should use parentheses to force the order if you are uncertain about which operation takes precedence.

We can combine arithmetic operations, sequences, and concatenation as in

```
> evens
[1] 2 4 6 8 10
> (evens <- c(evens, 2 * (6 : 10)))
[1] 2 4 6 8 10 12 14 16 18 20
```

Here we see an example where the name `evens` appears on both sides of the `<-` operation. It is better to think of the `<-` operation as *replacing* an existing value rather than *assigning* a value. In the last line here, we see that an assignment contained in parenthesis will also print the resulting value for us.

Another good habit is to leave a *space* before and after the `<-` symbols. This will avoid any ambiguity (e.g., if you meant to write `x < -3` instead of `x <- 3`). This habit also makes your R code easier to read. It is generally a good idea to leave spaces before and after *any* operation symbols. We also leave a space after the coma in lists, as in `c(1, 2, 3)`. A larger set of operators is given in Table 2.1.

It is possible to address individual elements in a vector using square brackets `[]`. As examples, we have

```
> evens
[1] 2 4 6 8 10 12 14 16 18 20
> evens[4 : 7]
[1] 8 10 12 14
> evens[ c(1, 5, 6) ]
[1] 2 10 12
```

A negative subscript omits that element. If we want to omit the third element of a vector, for example, we can write

```
> evens
[1] 2 4 6 8 10 12 14 16 18 20
> evens[-3]
[1] 2 4 8 10 12 14 16 18 20
```

When subscripts are out of range or invalid, R is defined in an unintuitive manner. See Exercise 2.12 for some examples of these.

The `length()` function tells us the length of a vector:

```
> evens
[1] 2 4 6 8 10 12 14 16 18 20
> length(evens)
[1] 10
```

Suppose we wanted a subset of only those vector elements with values larger than 9. To accomplish this, we combine logical (true/false) values with a subscript as in the following:

Table 2.1: A list of logical operators in R

<code>==</code>	Equal to	<code>!</code>	Not, negate
<code>&&</code>	And, element-wise	<code>&</code>	And, pairwise
<code> </code>	Or, element-wise	<code> </code>	Or, pairwise
<code>></code>	Greater than	<code><</code>	Less than
<code>>=</code>	Greater than or equal to	<code><=</code>	Less than or equal to

```

> evens > 9

[1] FALSE FALSE FALSE FALSE  TRUE  TRUE  TRUE  TRUE  TRUE
> evens[evens > 9]
[1] 10 12 14 16 18 20

```

The `evens > 9` script yields a list of logical TRUE and FALSE values indicating whether or not the corresponding vector element is greater than 9. If we use this list of logical values in the subscript brackets, then only values associated with TRUE are selected. A list of logical operators in R is given in Table 2.1. Finally, we can assign TRUE and FALSE as values to variables and abbreviate these as T and F.

Sometimes we want to find a member in a list of items. The `%in%` operator returns a logical value indicating whether or not an item is in the list. Here are examples:

```

> 3 %in% ( 1 : 5 )
[1] TRUE
> 8 %in% ( 1 : 5 )
[1] FALSE

```

The `match()` function allows us to find the location of specific elements in a vector. The `match()` function takes two arguments and finds the index of occurrences of the first argument in the second. So

```

> match( 3 : 4,  2 : 12)
[1] 2 3

```

shows that the numbers 3 and 4 are located at positions 2 and 3 of the sequence `2 : 12`. The `match` function is used in the production of Fig. 3.10, for example, in order to identify the index of unusual data points.

The `which()` function is similar to `match()` except that it works on logical values. So, for example,

```

> which( ( 2 : 5 ) > 3 )
[1] 3 4

```

2.1.3 Printing in R

The last functions we will describe in this introduction control the output of results. The simplest way to see the value is to type the variable name. We also display the value of a variable using the `print` command. The `digits =` option in `print()` can be used to format the data by controlling the number of significant digits to be printed. Here is an example:

```
> x <- 1 / (6 : 7)
> print(x)
[1] 0.1666667 0.1428571
> print(x, digits = 2)
[1] 0.17 0.14
```

If you try to mix text and numbers in `print`, the whole result is converted into text strings but the result may look awkward. It is better to use the `cat()` function which concatenates the output:

```
> print(c("x is", x))
[1] "x is"           "0.1666666666666667" "0.142857142857143"
> cat(c("x is", x))
x is 0.1666666666666667 0.142857142857143
```

Similar results can be obtained using the `noquote()` command or the `quote = FALSE` option in `print()`. Notice that `cat()` produces output without the leading subscript [1].

The `format()` command can be used with `cat()` to combine text and numbers printed to a specified number of significant digits:

```
> cat(c("x is", format(x, digits = 3)))
x is 0.167 0.143
```

To end this section, let us point out the extensive help available to the user of R. The help is most useful if you have a reasonably good idea of the procedure you want to perform and want to learn more.

If you have a general idea about what you want, the help button in the console window will open a set of R manuals. Many of these have search options that allow you to look for functions that perform the task you want. A search for *variance*, for example, returns a large number of operations that contain this keyword in their help file including the `var()` function. If you want to know more about the `var()` function, typing `help(var)` will open a web page with a complete reference on that function. The web page will contain complete details about this function, examples of its use in R, along with names of several closely related functions, and some references on the relevant subjects. This web page also describes how missing values are treated, how a weighted variance estimate could be obtained, links to functions that calculate tests and confidence intervals for variances, as well as nonparametric procedures for these methods. Keep in mind that R is user supported, so not every help entry will be this extensive, complete, useful, or even correct. Sometimes the R function may have been written as part of a published book, and the help entry will be minimal in an attempt to boost sales for those who want to learn more.

2.2 Simulation and Simple Statistics

R allows us to generate random data. Statistical scientists will frequently use this important capability to test theories and to learn about properties of procedures when the behavior of the data is known.

The `rnorm()` function generates observations from a standard normal distribution with mean zero and unit variance:

```
> rnorm(3)
[1] 0.3645054 1.1591904 1.7222996
> rnorm(4)
[1] 0.4007988 -0.6369772 0.8908059 0.2781956
```

Notice how the values are different every time this function is called. Your values will also be different from these when you try it. Let us illustrate this feature in a brief example of a *simulation*. We frequently perform a computer simulation to answer difficult questions that might not otherwise be answerable. The following question has a simple solution, and knowledge of the exact answer allows us to confirm the simulation method is working correctly.

Question: Suppose X is a standard normal variate. What is the probability that X^2 is between 0.5 and 1.2?

Table 2.2: Some continuous distributions and related functions available in R

Distribution	Density function	Cumulative distribution	Quantile function	Generate random variables
Normal	<code>dnorm</code>	<code>pnorm</code>	<code>qnorm</code>	<code>rnorm</code>
Uniform	<code>dunif</code>	<code>runif</code>	<code>qunif</code>	<code>runif</code>
Student's t	<code>dt</code>	<code>pt</code>	<code>qt</code>	<code>rt</code>
Central and noncentral				
chi-squared	<code>dchisq</code>	<code>pchisq</code>	<code>qchisq</code>	<code>rchisq</code>
Gamma	<code>dgamma</code>	<code>pgamma</code>	<code>qgamma</code>	<code>rgamma</code>
Multivariate normal	<code>dmvnorm</code>	<code>pmvnorm</code>		<code>rmvnorm</code>
Multivariate Student's t	<code>dmvt</code>	<code>pmvt</code>	<code>qmvt</code>	<code>rmvt</code>
Exponential	<code>dexp</code>	<code>pexp</code>	<code>qexp</code>	<code>rexp</code>
Cauchy	<code>dcauchy</code>	<code>pcauchy</code>	<code>qcauchy</code>	<code>rcauchy</code>
Wishart	<code>dwish</code>			<code>rwish</code>

These are found in the MASS, MCMCpack, and mvtnorm libraries

To simulate a solution to this question in R, we can write

```
> nsim <- 500
> x <- rnorm(nsim)
> x <- x ^ 2
> sum(.5 < x & x < 1.2) / nsim
[1] 0.192
```

In the first line of this set of code, we define the number of replicates so that it will be easier to change if we want to perform this simulation again later with a different sample size. In the next two lines of this sequence of R commands, we use `rnorm` to generate 500 standard normal values and then square these. The expression `(x > 0.5 & x < 1.2)` returns a set of 500 TRUE and FALSE values depending on whether these conditions are met for each of the components of `x`. We can sum over these logical values (`TRUE` is 1 and `FALSE` is 0) to see how many of the 500 values meet our criteria. Keep in mind that your result will be slightly different every time you repeat this simulation. The exact answer is 0.206 so this simulation is not too far off the mark. A random sample much larger than 500 would likely produce a closer

estimate to the true value, of course. See Exercise 2.4 for more information. In Sect. 2.5 we perform a larger simulation to describe the behavior of the correlation coefficient.

There are many continuous statistical distributions already programmed in R. A brief list of these is given in Table 2.2. The general pattern for the names of these functions is that density functions begin with a `d`, cumulative distributions with a `p`, the quantile function begins with a `q`, and the random number generator with an `r`.

As an example of several simple statistical functions that might be useful in data analysis, we generate ten uniform variates, sort these, find their minimum, maximum, mean, standard deviation, and variance:

```
> x <- runif(10)
> x
[1] 0.5330116 0.2722369 0.5743971 0.3922796 0.2738410
    0.1701639

[7] 0.8477313 0.5537144 0.1998406 0.7271472
> sort(x)
[1] 0.1701639 0.1998406 0.2722369 0.2738410 0.3922796
    0.5330116

[7] 0.5537144 0.5743971 0.7271472 0.8477313
> min(x)
[1] 0.1701639
> max(x)
[1] 0.8477313
> mean(x)
[1] 0.4544364
> sd(x)
[1] 0.2296803
> var(x)
[1] 0.05275305
```

In each of these operations we see that the arguments for the R functions are vectors of arbitrary length. Such *vector-valued arguments* for functions are convenient for us. The `mean` function returns a scalar-valued average of the vector values, but the `sort` function returns a sorted vector of the same length. Notice that the original values are not replaced by their sorted values unless we assign these, as in `x <- sort(x)`.

Another useful R function is `hist()`, a function that opens a graphical window and produces a histogram. As an example, `hist(rnorm(75))` produces Fig. 2.1.

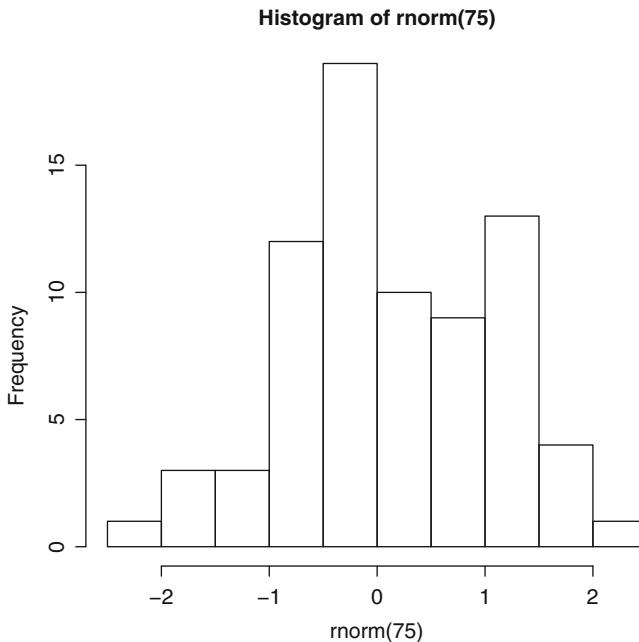


Figure 2.1: Histogram of randomly distributed normal variates

This figure will be a little different from yours, of course, and will also differ every time you run it. When the graphical window opens, you can click on the **Windows** tab in the R screen and then use the **Tile Vertically** option to produce a pair of side-by-side windows: one for typing R commands and another for viewing the resulting graphics. We will discuss other graphical methods in the following chapter.

Now that we have covered some examples of basic arithmetic, simple statistics, and random number generation in R, let us move on to importing and manipulating data from external files. In Chap. 3 we describe the `hist()` command again, along with many other graphical presentations of multivariate data.

2.3 Handling Data Sets

This section covers two topics: bringing your data into R from files and then constructing `data.frames`. You don't want to type in a large data set using only the `c()` command. We need an easy way to get your data into R. Once it is in R, the `data.frame` is a convenient way to structure it in a useful format with handy labels identifying the columns and/or rows. If you are familiar with other data processing languages such as SAS then you will already be comfortable with this data format.

The easiest way to get your data into R is to prepare a file whose contents follow a pattern such as this:

	Apartment	House
AK	949	237.8
AL	631	121.5
AR	606	105.7
AZ	866	229.2
. . .		
WI	704	173.3
WV	528	95.9
WY	636	188.2

This file, `housing.txt`, appears on this book's website. It contains the average apartment rents and house prices in each of the 50 states.

Such a table is relatively easy to create if your data is already arranged as rows and columns in a spreadsheet program. Beginning with the data in Table 1.1, for example, we can select the columns we want, copy these to a separate worksheet, then save it as a file or perhaps copy and paste the result into a word processing language to clean it up further.

The headings and labels clarify the meanings of the numerical values in the various rows and columns. In this example, the rows have labels for each of the states, and the columns for apartment rents and housing prices are clearly marked. These labels are a very helpful feature when you put R aside for a few days and forget what the columns of data values represent. Similarly, try to avoid headings with names like `x` that convey no meaning.

The `read.table()` function is very useful for reading such formatted data into R. This function can be used to read data sets along with row and column labels. As an example, we can read the data from the `housing.txt` file using

```
>housing <- read.table("housing.txt", header = TRUE,
  row.names = 1)
>housing
```

	Apartment	House
AK	949	237.8
AL	631	121.5
AR	606	105.7
AZ	866	229.2
. . .		

```
WA      874 308.1
WI      704 173.3
WV      528 95.9
WY      636 188.2
```

The result of the `read.table()` is assigned to a variable called `housing` and printed here. The name of the external file (in the appropriate working directory) is listed in quotes. This directory may be different on your computer. Working directories are discussed in Sect. 2.8.

The `header` option in `read.table` indicates that column headings are present. The `row.names=` value indicates which column contains the labels for each row. In this case, the abbreviations for the state names appear in the first column of the data.

In this example, the `read.table` function builds what is called a *data frame* in R. Individual columns of data can be referenced from the data frame using either of two methods illustrated here:

```
> housing$Apartment

[1]  949  631  606  866 1135  848  970 1011  917  947  787 1298  607
[14]  690  811  670  654  578  698  991 1074  702  706  734  657  638
[27]  631  694  534  626  914 1068  668 1011  953  667  614  780  726
[40]  850  675  569  660  768  784  934  797  874  704  528  636

> housing[1]

  Apartment
AK      949
AL      631
AR      606
AZ      866

. . .

WI      704
WV      528
WY      636
```

In the first method, `housing$Apartment` refers to the column of apartment rents which are given as a vector of values without labels. In the second method, `housing[1]` is listed as the rent values along with their corresponding state labels.

We can also exploit the property that R also treats the `data.frame` as a matrix, with two subscripts separated by commas. The first subscript addresses rows, as in this example:

```
> housing[1 : 4, ]
```

	Apartment	House
AK	949	237.8
AL	631	121.5
AR	606	105.7
AZ	866	229.2

listing the first four rows.

The second subscript addresses columns, as in

```
housing[,1]
```

```
[1] 949 631 606 866 1135 848 970 1011 917 947 787 1298 607 690 811
[16] 670 654 578 698 991 1074 702 706 734 657 638 631 694 534 626
[31] 914 1068 668 1011 953 667 614 780 726 850 675 569 660 768 784
[46] 934 797 874 704 528 636
```

We can use this property to subset the data as in this example

```
housing[ housing$Apartment > 1000 , ]
```

	Apartment	House
CA	1135	467.0
DC	1011	474.1
HI	1298	560.2
MD	1074	341.2
NJ	1068	364.1
NV	1011	271.5

in which we select only those observations whose average monthly apartment rents exceed \$1000.

We can also create subsets of subsets as in

```
> housing[ housing$Apartment > 1000, ] [-3,]
```

	Apartment	House
CA	1135	467.0
DC	1011	474.1
MD	1074	341.2
NJ	1068	364.1
NV	1011	271.5

using a -3 in a second set of subscripts to omit the third item (HI) from the list.

R recognizes the labels as such so it is valid to take log of these values as either

```
> log( housing[1] )
```

```

      Apartment
AK 6.855409
AL 6.447306
AR 6.406880
.
.
```

or else as

```

> log(housing$Apartment)
[1] 6.855409 6.447306 6.406880 6.763885 7.034388 6.742881 6.877296 6.918695
.
.
```

with no confusion about accidentally trying to take the logarithm of character values. Notice how R includes row labels in the first example, but not the second.

If you get tired of writing `housing$Apartment` and just want to refer to the data by the column names, the `attach()` command allows R to understand that you are always referring to data frame of interest:

```

> attach(housing)
> Apartment
[1] 949 631 606 866 1135 848 970 1011 917 947 787 1298 607 690
[15] 811 670 654 578 698 991 1074 702 706 734 657 638 631 694
[29] 534 626 914 1068 668 1011 953 667 614 780 726 850 675 569
[43] 660 768 784 934 797 874 704 528 636

```

The `cbind()` command works to add columns to data frames the way the `c()` command works to append to vectors. So the example

```

> lh <- cbind( housing, log(housing[1]) )
> lh[1 : 5, ]
      Apartment House Apartment
AK        949 237.8 6.855409
AL        631 121.5 6.447306
AR        606 105.7 6.406880
AZ        866 229.2 6.763885
CA       1135 467.0 7.034388

```

appends log of apartment rents as another column onto the housing data frame.

We can fix the column heading using `colnames()` command. This command can either be used to print the column names, as in

```

> colnames(lh)
[1] "Apartment" "House"      "Apartment"

```

or else be used to assign a value, as in this example

```
> colnames (lh) [3] <- "Log Apt"
> lh[1 : 5, ]
  Apartment House  Log Apt
  AK      949 237.8 6.855409
  AL      631 121.5 6.447306
  AR      606 105.7 6.406880
  AZ      866 229.2 6.763885
  CA     1135 467.0 7.034388
```

There is a similar command called `rbind()` that adds rows to a `data.frame` and `row.names()` can be used to both query and manipulate the row names of a data frame.

There are several other R commands to read more diverse types of data in different formats. The `scan` function is very general and can be used to read numerical values from external files. The values read using `scan()` will appear as a single vector in R. You will need to format these appropriately into rows and columns using `matrix()` function and possibly use `t()` to transpose the matrix. The `data.frame()` command creates a data frame from a matrix and subsequently allows you to add row and column titles.

For reading different types of files, the `foreign` library contains R programs that allow you to read files from other data analysis programs such as SAS, S, Minitab, dBase, and Stata, to name a few. Programs such as Excel can export files where columns are separated by tab characters. In this case you might have to use instructions such as

```
housing <- read.table("housing.txt", sep="\t", header=TRUE, row.names=1)
```

to indicate that the separators (`sep=`) between columns are tab characters.

You can also use `read.table` to read from the *clipboard*. The familiar `copy` and `paste` operation involves highlighting a block of numbers or text in Excel or a word processing language. The `copy` operation is performed using a `Ctrl-C` command, which copies the highlighted material into a file called the `clipboard`. This material can be retrieved in R with the command

```
mydata <- read.table(file = "clipboard")
```

as though the `clipboard` were an actual file. This approach for reading data into R is best suited for small amounts of data.

2.4 Basic Data Manipulation and Statistics

R will sort your data. We sort a vector or a column in a `data.frame` using the `sort()` command:

```
> sort(housing$Apartment)
[1] 528 534 569 578 606 607 614 626 631 631 636 638 654 657
[15] 660 667 668 670 675 690 694 698 702 704 706 726 734 768
[29] 780 784 787 797 811 848 850 866 874 914 917 934 947 949
[43] 953 970 991 1011 1011 1068 1074 1135 1298
```

R can also rank the values:

```
> order(housing$Apartment)
[1] 50 29 42 18 3 13 37 30 2 27 51 26 17 25 43 36 33 16 41 14 28 19 22
[24] 49 23 39 24 44 38 45 11 47 15 6 40 4 48 31 9 46 10 1 35 7 20 8
[47] 34 32 21 5 12
```

In a `data.frame` we can sort on one column of data values and apply this ordering to all of the rows. Then

```
> housing [ order(housing$Apartment), ]
  Apartment House
WV      528 95.9
ND      534 112.5
SD      569 126.2
KY      578 118.4
.
.
.
NJ      1068 364.1
MD      1074 341.2
CA      1135 467.0
HI      1298 560.2
```

rearranges all of the rows so that the values in `Apartment` column are increasing.

For values decreasing in this column, we can sort on the *negative values*:

```
> housing [ order( -housing$Apartment), ]
  Apartment House
HI      1298 560.2
CA      1135 467.0
.
.
.
ND      534 112.5
WV      528 95.9
```

and this provides the ordering from largest to smallest.

To calculate simple statistics on a `data.frame`, we can write

```
> colMeans(housing)
```

```
Apartment      House
781.1765  212.3255
```

and this provides sample averages and column names for each of the columns.

The variance/covariance matrix is obtained

```
> var(housing)
          Apartment      House
Apartment  29391.83 16349.12
House      16349.12 10668.70
```

and the correlation matrix is

```
> cor(housing)
          Apartment      House
Apartment  1.000000 0.923263
House      0.923263 1.000000
```

Functions such as the mean and standard deviation are best applied to the columns of the `data.frame` using the `sapply` function. Examples of these are

```
> sapply(housing, mean)
          Apartment      House
Apartment  781.1765 212.3255
> sapply(housing, sd)
          Apartment      House
Apartment  171.4405 103.2894
```

R provides the capacity to *merge* data from two different data.frames. When working with large data sets, we frequently find that the data is spread across more than one physical file. A merge is a process that combines the files into one, by matching individual rows on the values in a specified column.

Let us illustrate the merge capabilities in R with a simple example. Suppose we have a data.frame with names and ages:

```
> first <- data.frame(
+   name = c("Charles", "Bill", "Amy", "Fred"),
+   age  = c(15, 25, NA, 22))
> first
  name age
1 Charles 15
2 Bill 25
3 Amy NA
4 Fred 22
```

(Notice how R produces a + prompt because the unbalanced parenthesis expect a resolution in a subsequent line rather than another R command.)

Suppose a second data.frame containing names and heights:

```
> second <- data.frame(
+   handle = c("Charles", "George", "Amy", "Bill"),
+   height = c(61, 65, 60, 67))
> second
  handle height
1 Charles     61
2 George     65
3 Amy       60
4 Bill       67
```

There are a number of problems that immediately appear. Specifically, there are names in one data.frame that are absent from the other, and, further, the names that do occur in both data.frames appear in different orders. Nevertheless, we want to produce a single file containing names, ages, and heights. Even so, there is some ambiguity as to how this should be accomplished, in light of the missing data.

In one version of the `merge` command, we can combine the two data.frames

```
> m1 <- merge(first, second, by.x = "name", by.y = "handle")
> m1
  name age height
1 Amy  NA    60
2 Bill 25    67
3 Charles 15    61
```

and recover only those names that appear in both data.frames.

The `merge` command in this example creates a new data.frame with the combined attributes (age and height) from the two separate data.frames. The `by.x=` and `by.y=` options specify the columns containing the data values we wish to merge on.

We can also combine all names, regardless of whether these appear in only one or both lists:

```
> m2 <- merge(first, second, by.x = "name", by.y = "handle", all=TRUE)
> m2
  name age height
1 Amy  NA    60
2 Bill 25    67
3 Charles 15    61
4 Fred 22    NA
5 George  NA    65
```

using the `all=TRUE` option.

In this last example, notice how the `merge` function fills in the missing values with NAs when the corresponding values are absent in the one of the merged data.frames.

It is possible to clean your data and remove any records with missing values. This is especially useful for those procedures in R which will not perform analyses on missing (NA) values. These records need to be deleted for the procedure to work properly.

The easiest way to delete incomplete rows of data is through the `complete.cases` function. The `complete.cases` function identifies rows in a data.frame with no missing values. So, in the case of the merged data.frame `m2`, we have

```
> complete.cases(m2)
[1] FALSE  TRUE  TRUE FALSE FALSE
```

showing that only lines 2 and 3 have no missing data values.

We can then build a data.frame with no missing data using

```
> m2[complete.cases(m2), ]
      name age height
2    Bill  25     67
3 Charles  15     61
```

After performing a merge, there may be several duplicated records. These can be identified using the `duplicated` function, which works on vectors as well as on `data.frames`.

As an example of its use,

```
> list <- c(1, 2, 5, 4, 2, 4, 5, 3)
> duplicated(list)
[1] FALSE FALSE FALSE FALSE  TRUE  TRUE  TRUE FALSE
> list[ !duplicated(list) ]
[1] 1 2 5 4 3
```

the duplicated items in this list are removed. Table 2.1 shows the exclamation symbol (!) negates a logical operation.

2.5 Programming and Writing Functions in R

A powerful feature of R is the capability to program your own functions, adding new and useful functionality within your work. We regularly use a number of R library functions, such as the square root (`sqrt()`). It is useful to write your own functions if you have some you use frequently or if you need to create long sequences of R commands. You can break these up into short procedures that can be written and tested separately. This is especially useful when you want to tackle a large task. Break the task into component units that can be sequentially built upon smaller segments.

To write a function in R, assign a variable the name `function`, followed by the arguments and then the definition. As an example, consider the function

```
> addA <- function(x) x + A
```

that returns the sum of the argument (`x`) and the variable `A`.

To test it out we have

```
> A <- 4
> addA(5)
[1] 9
> A <- 6
> addA(2)
[1] 8
```

Typing the name of the function, without an argument, will print the definition:

```
> addA
function(x) x + A
```

If the function definition takes more than one line, put it in curved brackets `{}`. A function can return more than one value if these are put into a vector. Results are returned when they are at the end of the function definition, as though we were printing the values in the interactive mode. We can also use the `return` statement.

As an example of a function that spans several lines and returns more than one value, we have

```
> addTwo <- function(x)
+ {
+   first <- x + A
+   second <- 2 * x
```

```

+   c( first, second)
+ }
> A <- 5
> addTwo(6)

[1] 11 12

> first

Error: object 'first' not found

```

As we work with functions, the *scope* limits where data values can be accessed. In the two examples given, notice that the value of *A* is “known” inside the definition of the function. In the second example, we are unable to access the values *first* and *second* because these are considered local and only exist inside the definition of the function.

Here’s another example of writing a larger function in R. Suppose we want to look at the statistical properties of *spacings*. Spacings are the differences between adjacent ordered data values. We might use a large number of small adjacent spacings as statistical evidence of an area of high density of observations, for example.

As a numerical example of spacings, suppose we start with the data values {8, 14, 3, 16}. Then the sorted data values are

3 8 14 16

and the corresponding set of spacings are

5 6 2 .

Notice that the spacings themselves are not sorted, and there is one fewer spacing than data value.

Here is a function in R to calculate spacings of any vector:

```

spacing <- function(x)
# Calculate spacings in vector x
{
  n <- length(x)
  if(n <= 1) return(NA)  # undefined if x is empty or
                         # scalar
  sortx <- sort(x)       # sorted values of x
  sortx[ -1 ]-sortx[ -n ] # return spacings
}

```

A value of `NA` is returned if we ask for the spacings of a scalar, whose length is 1. The `NA` symbol is a special value in R. It stands for “not available” and is useful to indicate a missing value. “Not a number” or `NaN` may be the result of an invalid computation resulting in an ambiguous or erroneous value such as division by zero. See Exercise 2.10 for more on these special codes for invalid numerical values.

We exit the function in the middle of the function’s definition and return some value at that point using the `return()` statement. In the present example, the `return()` statement is used to return `NA` to indicate that invalid data was entered and an error has occurred. As a good programming habit, anticipate any errors that a user might make and catch these before they cause unpredictable results. We can also write `spacing` in a much simpler fashion (see Exercise 2.11), but the present form illustrates useful features of functions in R.

In this function to calculate spacings, notice how we *document* or explain to the human reader what is going on. Anything written on a line in R following a pound sign (#) is treated as a comment by R and ignored. Such comments are extremely useful when you look at your program after a time and do not want to forget what the role of the program code. If you share your program with others, then documentation is even more essential.

Don’t try to write more than a few lines of R code directly in the console. It is much better to use the text editor in `Rstudio`. You could also use your favorite word processor and then copy and paste the code into the R window.

Let us generate some data and run the `spacing` program. For example,

```
> z <- sample(25,5)
> z
[1] 3 18 12 22 15
> spacing(z)
[1] 9 3 3 4
```

The `sample(25,5)` function generates five random integers between 1 and 25. Then the `spacing` program returns the four spacings of the five data values that `sample(25,5)` sent to it, as required.

When writing your own program, you should check all of the various branches and paths it might take to ensure these are all working properly. In our `spacing` program, we should also verify that

```
> spacing(5)
[1] NA
```

to see that the error processing works correctly as well.

In the next section, we use these function writing techniques to perform a larger simulation study than the one presented in Sect. 2.2.

2.6 A Larger Simulation

A small simulation was introduced in Sect. 2.2. Let us next consider a more complicated example of a simulation in R. Suppose we want a program that will help address the following:

Question: How can we describe the distribution of the correlation coefficient calculated from normally distributed samples?

We will need to generate several sets of (possibly correlated) paired normal random values and find the sample correlation of each set. In this way, we will have a random sample of correlation coefficients produced under specified conditions. Then we can draw a histogram of these correlations and calculate summary statistics, as well. This is the essence of a simulation study: Produce randomly distributed quantities (such as normals) whose behavior is well understood in order to study functions of these (such as the correlations) whose distributions are less well known to us.

We will also look at the correlation coefficient under the model of sampled independent normals as well as under a model in which the samples of the underlying paired normals are correlated. There are approximations to the behavior of the correlation coefficient (see Sect. 6.3), but in this simulation study, we do not want to use any approximations.

This process is an example of a simulation experiment. Statistical scientists frequently perform experiments on the computer in order to test theories about the behaviors of random processes.

To begin, we will generate correlated, normal random variables with the program `rmmvnorm` in the `mvtnorm` library. For example,

```
> library(mvtnorm)
> rmvnorm(5, mean = c(0, 0), sigma = matrix(c(1,.8, .8, 1), 2, 2))
      [,1]      [,2]
[1,]  1.03550508  0.06044561
[2,]  0.53386104  1.03063539
[3,] -0.06674766 -0.41792785
[4,] -0.59569721 -0.54805093
[5,]  0.96581969  0.61702999
```

This example generates five pairs of bivariate, random normals as a 5×2 matrix. The `mean=` option specifies the means of these pairs. The correlation measures association independently of location, so we can assume that the population means are both zero.

The variance matrix is specified using `sigma=`. In the present example, the 2×2 matrix

```
> matrix(c(1,-.8, -.8, 1), 2, 2)
      [,1] [,2]
[1,]  1.0 -0.8
[2,] -0.8  1.0
```

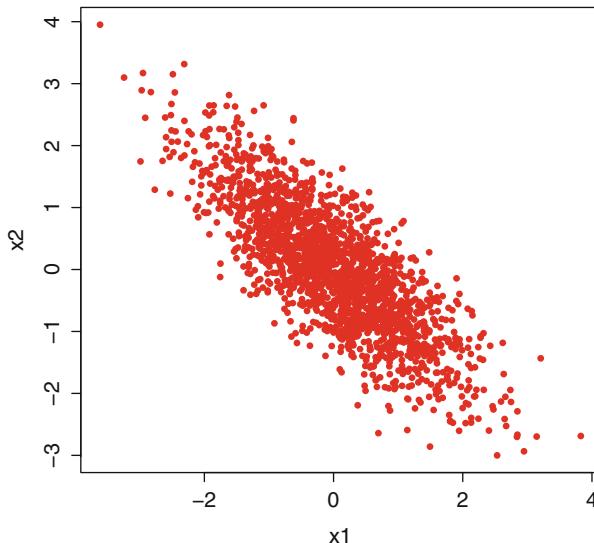


Figure 2.2: Simulated bivariate normals

specifies unit marginal variances for each of the two components and a correlation (and covariance) of -0.8 . (We will discuss the covariance matrix again, in Chap. 7.)

Using the `rmvnorm` program, we can provide a visual check that everything is working correctly. The code

```
plot(rmvnorm(2000, mean = c(0,0),
             sigma = matrix(c(1, -.8, -.8, 1), 2,2)),
      xlab="x1", ylab="x2", pch = 16, col = "red")
```

generates 2000 pairs of random bivariate normals and produces Fig. 2.2 giving us good visual evidence that `rmvnorm` works as described. Many of the options in the `plot` function are described in Chap. 3.

Now that we are able to generate bivariate, correlated normally distributed random values, we need to calculate the correlation of these pairs. The `cor()` function produces a matrix of correlation coefficients when its argument is a matrix, as is the case with the output of `rmvnorm`. In the case of paired data, the output of `cor` is a 2×2 matrix:

```
> z <- rmvnorm(5, mean=c(0,0), sigma = matrix(c(1,.8, .8, 1), 2,2))
> z
      [,1]      [,2]
[1,]  0.5400575 -0.1341743
[2,] -0.5003746 -0.3225571
[3,]  0.0657274  0.4185394
[4,] -1.7284671 -2.0219641
[5,]  0.3055753  0.6599834
```

```
> cor(z)

[,1]      [,2]
[1,] 1.000000 0.903586
[2,] 0.903586 1.000000
```

We can address the specific matrix element

```
> cor(z) [1,2]

[1] 0.903586
```

in order to select the (scalar) value we want.

Now that we have the tools to generate bivariate, correlated random normals and obtain their correlation, what parameters do we want to vary in our experiment? First, we need to decide how many correlation coefficients we want to generate. In the end, we will probably want to draw a histogram of their values in order to describe their distribution, so it makes sense to let this number vary in our program.

Let us denote the number of random correlation coefficients to be generated in our program by `ncor`. Each of these correlations will be based on a number of normally distributed pairs. Let us call the number of these pairs `nnor` in our program. In both of these parameters, let us use variables instead of fixed values. These variables will allow us greater flexibility. In both parameters, we choose names for the variables that convey meaning to their purpose.

Finally, we need a way to model the widest possible range of independence and dependence. We will examine a variety of correlated populations, so let us call this parameter `rho`.

The program called `simcor` to simulate the correlation is given in Output 2.1. Let us review several features of this program before we actually run it. A good feature of any program is to anticipate errors before these occur. Specifically, notice how the program checks the validity of the arguments `ncor`, `nnor`, and `rho` and will return NAs if these are not in the correct range. (Recall similar error checking in the program to calculate spacings, considered earlier in the previous section.)

We would not get an error message from R if `ncor` was a negative number, but it would be awkward for us to interpret the result. (See Exercise 2.6 for a discussion of this.) It is not clear how a negative value of `nnor` would be defined. The correlation coefficient needs at least two pairs of observed values in order to be defined. For this reason, we checked against these possibilities early in the program before R caught them, leading to unexpected results. To complete the error checking, notice how the program also checks that the values of `rho` are in the valid range between -1 and $+1$.

The second feature of the `simcor` program is the use of the `if()` statement along with the corresponding `else`. The `if()` statement breaks up the

Output 2.1: R function to generate random correlation coefficients

```

simcor <- function(ncor, nnor, rho)

# Simulate ncor random correlation coefficients based on nnor
# pairs of bivariate normals with population correlation rho.
{

# Check validity of arguments:
if( ncor < 1 || nnor < 2 || rho < -1 || rho > 1 )return(NA)
library(mvtnorm)           # access library

vm <- matrix(c(1, rho, rho, 1),
              2, 2)           # variance matrix
simcor <- NULL            # start a list of values
for (i in 1 : ncor)        # For every simulated correlation:
{
  norv <- rmvnorm(nnor,   # generate normal pairs
                  mean = c(0,0), sigma = vm )
  sc <- cor(norv)[1, 2]  # correlation of these pairs
  simcor <- c(simcor, sc) # add to list of values
}
simcor                      # Done
}

```

order of instructions depending on whether or not the logical condition in the parenthesis is met. The statement following the `else` is executed if the logical condition evaluates to `FALSE`. See Table 2.1 for a list of comparisons that result in logical `TRUE` or `FALSE` conditions.

If the logical condition in the `if()` is met, the next statement is executed. If the condition is not met, the program flows to the statement following the `else`. If we want several statements to be executed when the condition is met, then we can place those statements inside curly brackets.

The third feature of this program is called a *loop*. The loop is a powerful feature in programming that gets the computer to repeat a series of instructions any number of times. All of the commands inside the code

```

for (i in 1:ncor)           # loop on the number of correlations
{
  ...
}                           # code lines to be repeated

```

will be repeated `ncor` times.

Inside this loop, the value of `i` will successively take on the values 1, 2, ..., `ncor`. Within each repeat of this loop, the program generates `nnor` pairs of correlated normal values and then finds their correlation, denoted by `sc`.

These randomly generated correlation coefficients are accumulated in a vector with the same name as that of the function, `simcor`. These are returned at the completion of the function. It is not necessary to use the same name as the function for the returned values, but it can make it easier to remember.

The loop then repeats the process `ncor` times generating one random correlation coefficient with each repeat of the loop. We sometimes refer to each repeat as an *iteration*. Another habit that good programmers have is to indent successive levels of brackets {}, making it easier to see the scope of the loop and where it begins and ends. Those with programming experience will already be familiar with the looping construct and the `if` and `else` conditional branching.

Let's try our new program. First verify the checks and error processing for invalid values of `ncor`, `nnor`, and `rho`, respectively,

```
> simcor(ncor = -1, nnor = 10, rho = 0)
[1] NA
> simcor(ncor = 10, nnor = -1, rho = 0)
[1] NA
> simcor(ncor = 5, nnor = 15, rho = 1.8)
[1] NA
> simcor(ncor = 6, nnor = 12, rho = -1.2)
[1] NA
```

so the error checking appears to be working correctly.

Next, let's try the program using legitimate parameter values

```
> simcor(ncor = 5, nnor = 15, rho = -.8)
[1] -0.7392940 -0.7368622 -0.8276200 -0.7509294 -0.8466513
```

using R to generate a set of `ncor`=5 simulated correlation coefficients, each from `nnor` pairs of normal variates. It is not necessary to identify the arguments (`ncor`, `nnor`, `rho`) by name, but including these names when invoking the function makes it easier to remember the roles of the three parameters, as opposed to having to recall their order in the list.

Now we can try the program at full strength with a large number of replicates

```
> sim <- simcor(ncor = 2500, nnor = 15, rho = .8)
> mean(sim)
> hist(sim, main = " ", col = "red")
[1] 0.7866204
```

generating 2500 correlations, finding their mean, and producing the histogram given in Fig. 2.3.

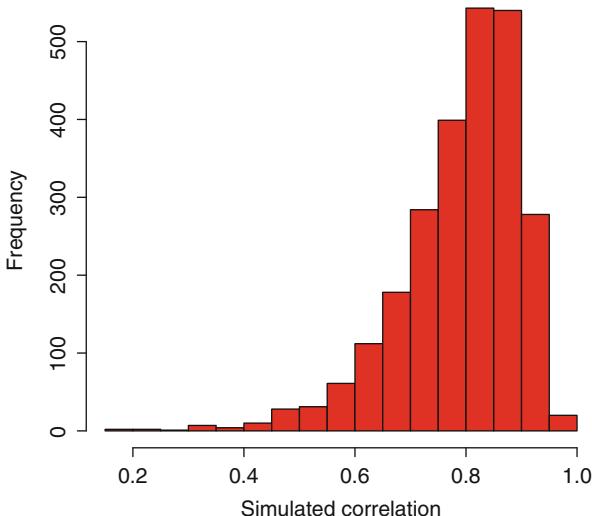


Figure 2.3: Histogram of 2500 simulated correlation coefficients

The average of these values is reasonably close to the population value of 0.8. This provides some additional confirmation that the program is doing what we expected it to do.

The histogram of these 2500 values produced by `simcor` appears in Fig. 2.3. This histogram shows that the distribution of the sample correlation coefficient is skewed with a longer tail to the left, as we would expect. The mean of these values is also reasonably close to where we expected it to be. Now that we have the program to simulate correlation coefficients, we can use it for other purposes such as estimating statistical significance levels and approximating power for estimating the sample sizes of experiments. See Exercise 2.6 for an example of these uses.

Let us review the process to write the simulation program `simcor` and run it. We began with a clearly stated goal: To examine the behavior of the correlation coefficient. Then we identified the tools to generate bivariate normals and their correlations: `mvnorm`, `matrix`, `cor`. Next, we determined what variables we wanted to vary in the program: `ncor`, `nnor`, `rho`.

In programming as well as simulation experiments, we need to go over similar steps: Define the task, then decide which factors are fixed and which will vary. This planning will save you trouble later if you need to make revisions.

Be generous in placing comments inside your program. Experienced programmers will tell you that there should be about one line of comments for every line of code. Such comments will help you if you put this project aside for a while and later come back to it. Sharing code with a colleague makes this documentation even more indispensable. Finally, avoid using abstract variable names such as `x` that convey no information about their role.

2.7 Advanced Numerical Operations

R allows for the numerical maximization and minimization of specified functions. Beginning in Sect. 5.7, we see that this process is an important tool in estimating model parameters. Sometimes we can use calculus (and brute, mathematical force) to find the maximum. But it is often easier to let the `nlm` (non linear minimization) program in R do this heavy lifting for us. This program requires that we write the objective function and provide reasonably good starting values for the estimate of the location of the minimum. In functions of many parameters, the choice of starting values can often represent a large challenge, so be prepared to spend time on this.

The `nlm()` program will minimize a specified function of several variables. We need to program the objective function to be minimized and provide a rough idea of where the search for a minimum should begin. The output from `nlm` will include a list of the parameter values that minimize the function and numerical estimates of the first and second derivatives at the place the function is minimized. The first and second derivatives are called the *gradient* and *Hessian*, respectively. These derivatives are also estimated, numerically, by examining the change of the value of the objective function near the optimal parameter values. These estimates also help `nlm` in locating the minimum. Close to the true minimum, the objective function should behave approximately as a quadratic function, and R can numerically solve this equation for the next best place to look for a better estimate of the location of the minimum.

Unfortunately, `nlm` can get confused along the way. It can “wander off” and look for the minimum very far from where the minimum is located. In addition, it can give errors by looking in illegal or undefined places. This occurs when some parameter values are only defined for positive values, as a normal variance, for example. These problems will be illustrated in Sect. 5.7 and are often avoided by using good starting values. See Exercise 2.9 as an example.

We can also numerically evaluate integrals in R. This topic is often referred to as *numerical quadrature*. The `integrate` function will numerically approximate a one-dimensional integral, with possibly infinite endpoints. Of course, if you are evaluating a function such as a cumulative distribution, then it is much better to use the specific function in R designed for that purpose, if available. There are routines in R that approximate multi-dimensional integrals as well, such as `adaptIntegrate` in the `cubature` library.

Finally, a wide variety of other mathematical computations can be obtained in R related to matrix and linear algebra. These include determinants, solutions to linear equations, and eigenvectors, just to name a few. These are discussed in Chap. 4.

2.8 Housekeeping

In this section we illustrate several additional R features worth knowing. Working directories allow you to better organize your workspace. Workspaces help organize your R work into separate folders for different projects. There is also a way to “take out the garbage” when it is time to clean up unused data within each project after these have outlived their usefulness. Finally, we show how to install new packages that allow you to take advantage of the many optional libraries of programs that are available.

After working with R for a while, your workspace can start to look like a very cluttered desk, containing many data sets from a variety of different projects. When you use the `ls()` or `objects()` commands to list all of the things in your workspace, you will see a huge number of variables (and maybe some programs) from a variety of different projects. The best way to organize your desk is to create a new *working directory* for each project.

Use `getwd()` to find the name of the current working directory and `setwd()` to change it. Don’t forget to include the two parentheses on the `getwd()` command with no additional arguments. Typing `getwd()` on your computer might give

```
> getwd()  
[1] "C:/Users/My Name/Desktop/"
```

This working directory probably points to some high-level place on your computer. It would be much better to have a separate working directory that is specific to each project. In this case we could change the working directory by typing something like

```
> setwd("C:/Users/My Name/Desktop/Projects/multivariate/data")
```

that is particular to your computer.

Changing the working directory will also be useful for reading data sets into R because a shorter address can be used. Specifically, commands such as `read.table()` and `scan()` will look for files in the current working directory. After we quit R, there will be an icon for the R program written into the working directory. Later, you can click on this icon from the directory and not have to change it again with a `setwd()` command. This process can be repeated, resulting in an R icon in each of the directories of each of your different projects. Each icon will open the R in that directory. Finally, notice the address of the directory is delimited with a forward-leaning slash (/) and not the more commonly used backslash used in directory addresses.

As a final note on organizing your workspace, consider generous use of the `rm()` command to remove unused variables. A cluttered workspace will make it difficult to find important things at some future date, often with names that may have been forgotten.

A great feature of R is the huge amount of software written by other users. A list of the libraries used in this book is given in the Appendix. To take advantage of the many libraries available, you will need to install these packages on your computer. First you will need to learn the name of the specific package you want to install. (More on this below.)

Let's say that you want to install the `TeachingDemos` package which contains introductory tutorials in R. The R command to install packages is

```
install.packages("TeachingDemos")
```

This command will be followed by a prompt for you to select a mirror site¹ from which the packages are to be downloaded to your computer. After choosing a mirror site, you will be prompted for the name of the package. After a few seconds, you will receive a message when the package finishes loading. This command only needs to be done once for all of your working directories. The command `installed.packages()` provides a complete list of all packages installed, including many that came as part of your original download of R to your computer.

To access the package in each working directory, interchangeably use either the `library` or `require` command, as in

```
library(TeachingDemos)
```

or else as

```
require(TeachingDemos)
```

without the quote marks. Either of these is needed every time you begin a session in R to access the installed package.

After installing and loading the package, you can then type `help(TeachingDemos)` to learn more about the package and its contents.

How can you learn about the various packages and their contents? One approach is through R itself. The R help file frequently describes features available in packages that may not already be installed on your computer. You will see help file entries with a notation of the form

```
faces{TeachingDemos}
```

indicating the name of the function and the package containing it.

¹There is some debate on how to choose a mirror site. There is a cloud option that picks a site for you. Picking a site geographically close to you will reduce web traffic. Conversely, a very distant site may offer faster service because most people on that side of the earth are asleep.

A second way to learn about packages for R is on the web through your favorite search engine. There are a huge number of packages available, and the authors of these will frequently create websites publicizing their capabilities. There are packages written for specialized statistical methods as well as areas of application such as genetics, chemistry, psychology, and economics. Some packages complement a book, in which case the `help` may be minimal to encourage you to buy the book to learn more.

This completes an introduction to the important elements of R. Additional features will be introduced in subsequent chapters as needed. As with piano playing, the best way to learn R is not just by reading the book but by sitting at the keyboard, trying the exercises, and engaging in some creative experimentation.

2.9 Exercises

- 2.1 The `seq` command in R is similar to the colon `:` operator but allows for non-integer sequences. It takes three arguments: the starting value, final value, and (optionally) the incremental value. Here are two examples of its use:

```
> seq(5, 9)
[1] 5 6 7 8 9
> seq(9.1, 8.3, -.1)
[1] 9.1 9.0 8.9 8.8 8.7 8.6 8.5 8.4 8.3
```

Use the `seq` and `c` functions to create a single vector of values from zero to one by 0.1 and then from 1 to 10 by 1. Be careful that the value 1 is not included twice.

- 2.2 Write a program in R that is a function of a positive integer `j` and produces a vector of the form

1, 1, 2, 1, 2, 3, 1, 2, 3, 4, 1, 2, 3, 4, 5, ..., 1, 2, ..., `j`.

- 2.3 The mean absolute deviation of a set of values x_1, x_2, \dots, x_n is the average absolute difference between the observations and their mean. Mathematically,

$$\text{mean absolute deviation}(\mathbf{x}) = n^{-1} \sum_{i=1}^n |x_i - \bar{x}|$$

where \bar{x} is the sample average of the xs . It is sometimes used instead of the standard deviation as a *robust* measure of variability of the data values. Robust methods are insensitive to outliers that may be present in the data.

- (a) Write a function in R that computes the mean absolute deviation of a vector of values. You may find the `mean()` and `abs()` functions useful in writing this program.
- (b) Discuss the pros and cons of using the median, as opposed to the mean \bar{x} in this definition. Similarly, consider the median absolute deviation about the median value as a measure of variability in a sample.
- (c) One way we describe robust properties of a statistical estimator is to introduce seemingly outlandish outliers into the data to see how these affect the final result. Perform a small experiment comparing the change in the standard deviation with that of the mean absolute deviation for a sample of observations with increasingly distorted outliers. Which statistic is more robust?
- 2.4 If X behaves as a standard normal, then X^2 behaves as chi-squared with 1 df. The cumulative chi-squared distribution can be found in R using the function `pchisq(y, d)` where y is the ordinate and d is the degrees of freedom. Use this function to find the probability of a 1 df chi-squared variate taking values between 0.5 and 1.2.
- 2.5 Look at the academic score data in Table 1.2. The various scores that went into this table have been standardized across countries to adjust for cultural differences.
- (a) Are the standard deviations of the different scores comparable? Consider using the `bartlett.test()` test for equality of variances. Other tests of equality of variances available in R are `var.test()`, `fligner.test()`, `ansari.test()`, and `mood.test()`. Use the `help()` file to read about these tests.
- (b) Examine the correlation matrix of this data using the `cor` function. Describe what you see. See also Exercise 8.7.
- 2.6 Explore properties of the `simcor` program to simulate statistical significance of the correlation coefficient.
- (a) What would happen if we allowed the `ncor` parameter to be negative? Remove the error check for this condition and explain how the new program behaves for $ncor < 0$.
- (b) Generate a large sample (m) of correlation coefficients from pairs of normal variates for a specified sample size and zero correlation. Estimate the 95 % confidence interval that would cover these, for a fixed size of the (normal) sample n . Do this by sorting the many simulated correlations and finding their 2.5 and 97.5 percentiles.
- (c) Propose a more efficient method for estimating the 95 % confidence interval of the correlation coefficient using the symmetry of the distribution.

(d) One of the most important questions asked of statisticians concerns the sample size (n) necessary to conduct a research project. Write a program with iterations and a convergence criteria to achieve a small 95 % confidence interval of the correlation coefficient. How fast does the size of this interval shrink as a function of the sample size n ? Draw a graph of this relationship.

(e) Suppose the data is sampled from a population with a correlation coefficient of ρ . Use the `simcor` program to estimate the value of ρ needed so that 80 % of the sampled correlations are not included in the interval you found in part b. This sample size (n) will have 80 % power to detect this value of ρ at statistical significance 0.05.

2.7 How useful is the histogram to detect normally distributed data?

(a) Use `runif(50)` to generate a set of 50 random values, distributed uniformly between zero and one. Draw the histogram of these using `hist()`. Do these look normally distributed?

(b) Generate 50 random values, each the sum of 3 uniforms and plot the histogram. Do these look normally distributed? Suppose we looked at the histogram of the sum of 20 uniforms. How many uniform random values do we need to add together to produce a “normal-looking” histogram?

(c) As a comparison, look at a histogram of 50 normal random values generated using `rnorm()`. How normal does this histogram appear?

2.8 Consider the function

$$f(x) = \frac{1}{2 + \sin(5\pi x)}$$

for values of $0 \leq x \leq 1$.

(a) Plot the function f in R. (See Sect. 3.1 for an example of how to do this.)

(b) Find the area under this curve using numerical quadrature with `integrate()`.

(c) Identify maximums and minimums of this function in R using `nlm()`. Show how the results depend on the starting values.

2.9 Use `nlm` to find the minimum of the function:

$$f(x, y, z) = 100 - \sum_{i=1}^5 \exp\{-5(x - i)^2\}/i + \exp\{-5(y - i)^2\}/i + \exp\{-5(z - i)^2\}/i$$

The true minimum of f occurs at $x = y = z = 1$ but there are several other local minimums. Show that by varying the starting values for `nlm`, we can converge on any of these other local minimums.

Table 2.3: Nonnumeric, symbolic values in R

Symbol	Description	R test
NULL	No value	<code>is.null()</code>
NA	Not available, missing	<code>is.na()</code>
NaN	Not a number	<code>is.nan()</code>
Inf	+Infinity	<code>is.infinite()</code>
-inf	-Infinity	<code>is.infinite()</code>

- 2.10 As you work in R, you will notice a variety of symbolic values in addition to numerical values. A list of these and tests for their values is given in Table 2.3.

- (a) What happens when we use `Inf` in arithmetical statements? For example,

```
> x <- Inf
> is.infinite(x)

[1] TRUE
```

will assign and test an infinite value. How does R define $-x$? What is the result when we multiply x by -1 or by zero? Can we test $-Inf < 0$?

- (b) How does R work with `NULL` in arithmetic? How does `NULL` differ from `NaN`? For example, suppose we assign

```
x <- c( 1, 2, NULL, 4)
```

What is the `length` of x ? What is the `sum` of x ?

Similarly, suppose we assign

```
y <- c(1, 2, NaN, 4) ?
```

What is the length and sum of y ?

- (c) Give examples of arithmetic operations that yield `NaN` and `Inf`. How are these results different? Which are accompanied with an error message?

- (d) Build a table of the resulting symbols when two of these symbols are used in arithmetic operations. For examples, what does the sum of `NA` and `NaN` yield? What is the product of zero and `NULL`?

2.11 (a) Can we access the values of `sortx` outside the `spacing` function given in Sect. 2.5? Explain.

(b) Write a one line `function` in R to calculate the spacings of any set of numbers using the `diff()` function. The `diff(x)` function calculates the difference of adjacent observations in a vector `x`.

2.12 What does R do when we try to access subscripts that are out of range? Suppose we start with

```
> x <- 1:3
```

(a) A negative subscript such as `x[-2]` will omit the second element of the vector. What does `x[-5]` yield in this example?

(b) What does `x[0]` give us? Can you explain this outcome?

(c) Suppose we try to assign a value to an invalid element of the vector, such as in `x[7] <- 9`. What does this produce?

(d) Is an empty subscript `x[]` different from `x` with no subscript at all? As an example, how is `x[] <- 3` different from `x <- 3`?

Chapter 3

Graphical Displays

You can observe a lot by just watching.

Yogi Berra

THERE ARE MANY GRAPHICAL METHODS that can be demonstrated with little or no explanation. You are likely familiar with histograms and scatterplots. Many options in R have improved on these in interesting and useful ways. The ability to produce statistical graphics is a clear strength of R. Graphics commands can produce files of a variety of file formats. All of the figures in this book were produced in this manner, for example. We begin with a discussion of the basics. Later sections of this chapter demonstrate a variety of more complex procedures available to us.

3.1 Graphics in R

The `plot` function is a general purpose routine with many options. The basic form is `plot(x, y)` which produces a scatterplot of the values in `x` and `y`. The `plot` function sets the frame and limits of the axes for you. There are many options including printing titles along the axes and changing colors. These will be illustrated in this chapter.

Let us illustrate the use of the `plot` function in drawing the densities of the chi-squared distribution. A very basic figure can be drawn using

```
x <- (0 : 120) / 10
plot (x, dchisq(x, 4), type = "l")
lines(x, dchisq(x, 5))
lines(x, dchisq(x, 6))
```

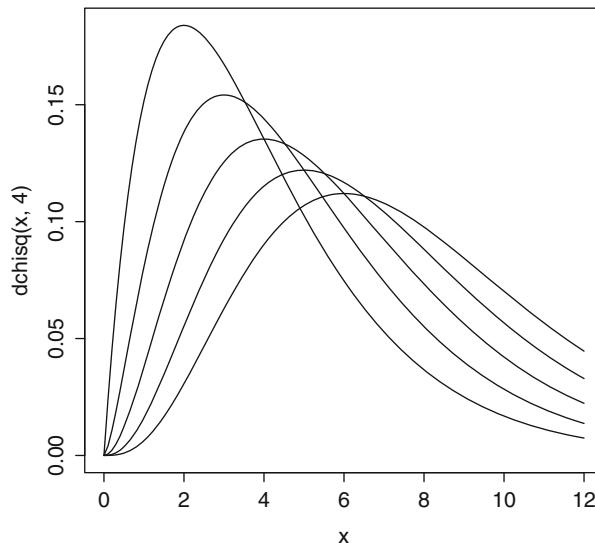


Figure 3.1: Basic chi-squared density plots

```
lines(x, dchisq(x, 7))
lines(x, dchisq(x, 8))
```

which produces Fig. 3.1 in a graphics window.

The R code begins by creating 121 evenly spaced values for x of 0, 0.1, 0.2, ..., 12. The `dchisq(x, 4)` evaluates the chi-squared density function with 4 df at each value of x . The `plot` statement opens the graphics window and sets the limits of the horizontal and vertical axes. The `type="l"` option specifies that lines will be used to connect adjacent points. Omitting this option would produce a series of disconnected dots. The labels of the plot axes are copied from those of the `plot` statement. We will show how to replace these with more useful labels in the next example. (As a helpful hint introduced in Sect. 2.5, whenever we have several lines of code to enter into R, it is best to write these out in a word processor first and then copy them into the R command window.)

The `lines` command is like the `plot` except that it produces lines between observations and plots these on top of the existing plot. These do not adjust for values that run outside the bounds set earlier by the `plot` command. It is best to plan ahead and use the `plot` command first with the widest and tallest of values that your figure is going to contain. It is possible to specify these limits manually, as we will see in the following section.

We can spruce up this figure and make it more presentable for publication. Figure 3.2 adds labels and prints a useful y -axis. This figure was produced using the code

```
pdf(file = "chisquared2.pdf")
x <- (0 : 120) / 10
plot(x, dchisq(x, 4), type = "l",
```

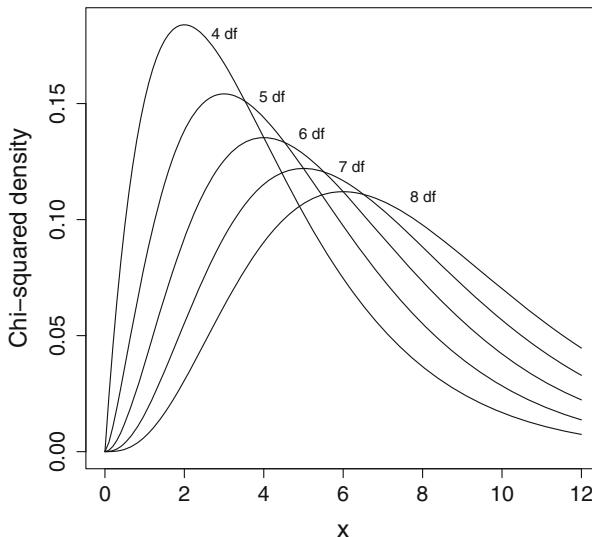


Figure 3.2: Chi-squared density functions for 4–8 df

```

ylab = "Chi-squared density")
lines(x, dchisq(x, 5))
lines(x, dchisq(x, 6))
lines(x, dchisq(x, 7))
lines(x, dchisq(x, 8))

text( c(3, 4.2, 5.2, 6.2, 8), c(.18, .153, .137, .123, .11),
      labels = c("4 df", "5 df", "6 df", "7 df", "8 df"))
dev.off()

```

The placement of the labels inside the figure is done using the `text` statement. This statement lists the desired x -coordinates followed by those for the y -coordinates. The exact positioning is not tricky but usually takes a little trial and error in order to position these correctly.

The `pdf(file= ...)` statement is optional and is used to direct graphic images to external PDF files. These can later be incorporated in other documents. Unless addressed otherwise in the `pdf()` statement, these files will appear in the current working directory. Working directories are described in Sect. 2.8. The images will not appear on the screen while the output is directed elsewhere, so you should make sure that the figure is correct before saving it to an external file. The `dev.off()` closes the graphics file at completion of the image.

Other examples appear in the following sections of this chapter. We demonstrate additional options including how to add text and manipulate other graphical parameters such as colors, plotted characters, and size.

3.2 Displays for Univariate Data

We are all familiar with histograms. These are the simple display for one-dimensional data. The basic command in R is `hist(x)` to obtain a histogram of the values in `x`. Let us introduce some other methods as well.

Consider data on the CD4 counts in HIV+ patients enrolled in a clinical trial. The beneficial CD4 cells are a critical part of our immune system, and lower counts are an indication of disease progression. These cells are attacked and destroyed by the HIV virus. The `cd4` data set in the `boot` library presents the baseline counts of CD4 cells of patients at the time of enrollment in the clinical trial and again after 1 year of treatment. The CD4 values are given in 100s. The critical value of 200 (or lower) is an AIDS-defining event.

A useful univariate display for small amounts of data is the *stem and leaf plot*. The stem and leaf plot is a useful improvement over the usual histogram because the data values are used as plotting characters, rather than the same character for every observation as used in the histogram.

As an example, the baseline CD4 counts are obtained

```
> require(boot)
Loading required package: boot
> cd4
  baseline oneyear
 1      2.12     2.47
 2      4.35     4.61
  .
  .
  .
19      2.66     4.37
20      3.00     2.40
```

The corresponding stem and leaf plot is

```
> stem(cd4$baseline)
The decimal point is at the |

 1 | 9
 2 | 15567
 3 | 000444468
 4 | 0123
 5 | 1
```

The stem and leaf displays the actual data values, and we can recover the original data from the histogram. The vertical line `|` serves as the decimal point so we can read the data values directly from this plot as 1.9, 2.1, 2.5, 2.5, and so on. The originators of this display method saw the vertical line as the stem of a plant and the numbers to the right as leaves, hence the name.

Output 3.1: Back-to-back stem and leaf plots

```

> library(aplpack)
> stem.leaf.backback ( cd4$baseline,
                           cd4$oneyear )

-----+
1 | 2: represents 1.2, leaf unit:
cd4$baseline      0.1 cd4$oneyear
-----+
          | 1* |
1       8| 1. |
3       41| 2* |44      2
7       9655| 2. |58      4
(6)   333300| 3* |022      7
      75| 3. |89      9
      3110| 4* |0233     (4)
          | 4. |678      7
1       1| 5* |2      4
          | 5. |59      3
          | 6* |3      1
          | 6. |
          | 7* |
-----+
n:      20      20
-----+

```

There is also a back-to-back stem and leaf display in the `aplpack` library that allows us to compare two sets of data values. An example appears in Output 3.1. The frequency of the median category is identified in parenthesis. In this display, we can see that the population of 1-year CD4 values are larger and more variable than the baseline values.

The stem and leaf uses the actual data values to display the data. This may not be a useful method if the data set is very large. At the other extreme from the stem and leaf plot is the *boxplot* which reduces the histogram to a few summary statistics and then plots these.

The boxplots of the CD4 counts are given in Fig. 3.3. The dark central horizontal line is the location of the median, and the box identifies the quartiles. (The quartiles are located 25 % in from both ends of the observed values.) The *whiskers* extend out from the central box. Sometimes extreme outliers are also identified by the boxplot. The pair of boxplots in Fig. 3.3 is easier to compare than the raw data values also given in this figure. Unlike a

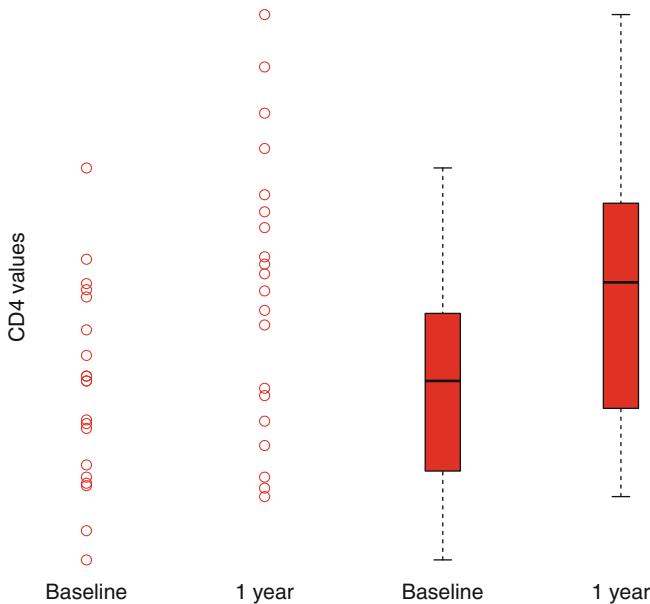


Figure 3.3: Univariate scatterplots and boxplots of CD4 counts

stem and leaf plot of the raw data, the boxplot does not become overwhelming when the sample size is large.

The R code that draws Fig. 3.3 is

```
library(boot)
data(cd4)
n <- length(cd4$baseline) # sample size
pdf(file = "boxplot.pdf")
op <- par(mfrow = c(1, 4), cex.lab = 1.5) # four plots, large labels
plot(rep(.5, n), cd4$baseline, axes = FALSE, xlab = "Baseline",
      xlim = c(0, 1), ylim = range(cd4), col = "red",
      ylab = "CD4 values", cex.lab = 1.5, cex = 2)
plot(rep(.5, n), cd4$oneyear, axes = FALSE, xlab = "1 year",
      xlim = c(0, 1), ylim = range(cd4), col = "red",
      yaxt = "n", ylab = "", cex.lab = 1.5, cex = 2)
text(c(0, 1), c(0, 0),
      c(boxplot(cd4$baseline, xlab = "Baseline", col = "red",
                 ylim = range(cd4), axes = FALSE),
        boxplot(cd4$oneyear, xlab = "1 year", col = "red",
                 ylim = range(cd4), axes = FALSE)))
par(op)
dev.off()
```

The `par()` statement specifies that there will be four figures, side-by-side, in the graphics window and increases the font size of the labels in the margins. The `par(op)` statement resets this back to one figure in the window. Parameters with `cex =` and `cex.lab =` specify character expansions

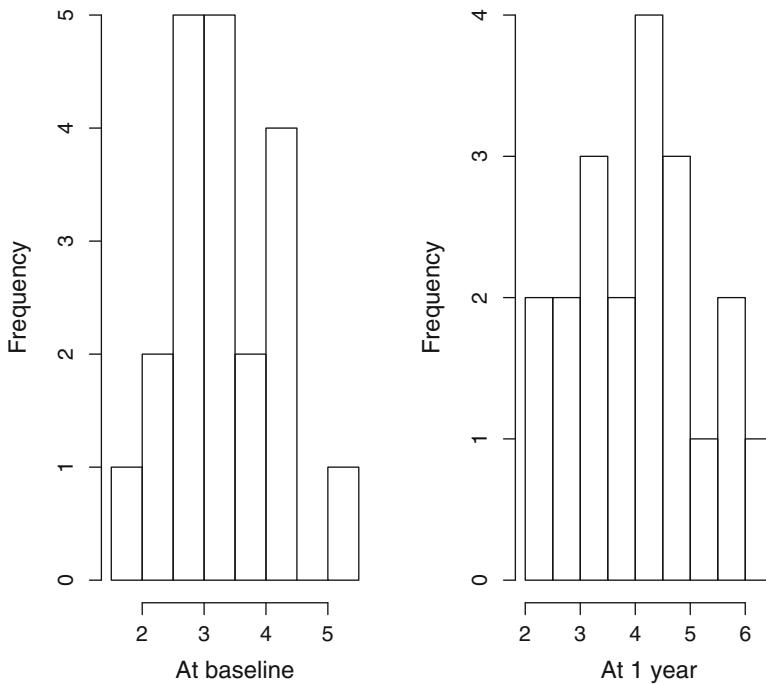


Figure 3.4: Histograms of CD4 counts, values in 100s

to increase font sizes. There are more sophisticated versions on the boxplot called *violin plots*. These are described in Exercise 3.4.

Let us return to the histogram as the display tool. The R code

```
library(boot)                      # the data is in this library
op <- par(mfrow = c(1, 2))        # side by side plots on one
                                   # page
hist(cd4$baseline, main = "", xlab = "At baseline")
hist(cd4$oneyear, main = "", xlab = "At 1 year")
par(op)                           # reset graphical parameters
```

produces the side-by-side histograms in Fig. 3.4.

The `hist()` statements produce the separate histograms with titles along the x -axes. A direct comparison of these two graphs in Fig. 3.4 is difficult. We cannot easily tell, for example, if the 1-year CD4 values are generally larger or smaller than those at baseline. It is not clear which of these two sets of values has a wider range. This figure would be adequate if we were only interested in number of values below the 200 threshold after 1 year.

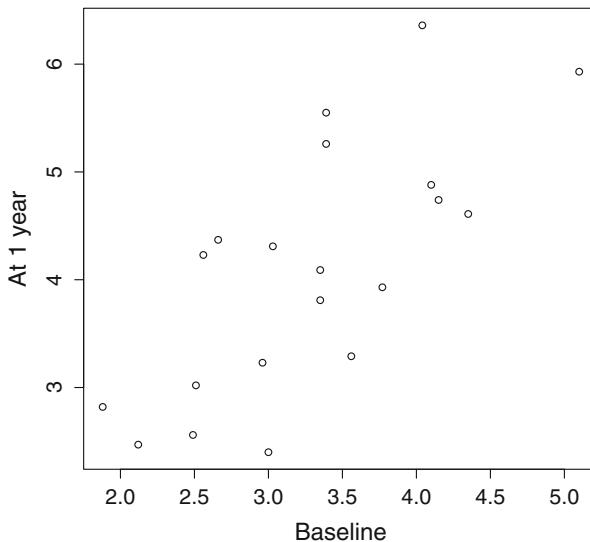


Figure 3.5: Basic scatterplot of CD4 counts

We need to look at these two groups in a manner that allows a quick comparison. The `plot(x,y)` command plots a scatterplot of x - y values. We can plot the baseline and 1-year values and then we can see a correlation between the two values of each subject.

That is, the R command

```
plot(cd4$baseline, cd4$oneyear, xlab = "Baseline", ylab =
    "At 1 year")
```

produces the plot that appears in Fig. 3.5.

This figure demonstrates that baseline and 1-year values are positively correlated within individuals but still does not allow a direct before-and-after comparison.

In order to compare the values, we need other graphical methods. These appear in Fig. 3.6. The membership variable `group` is discrete and a plot of this along the x -axis results in two vertical stripes in the left-most plot in Fig. 3.6.

It is sometimes better to add a small amount of random noise to scatter these values just enough to see the underlying distribution. These *jittered* values are plotted in the center of the three plots. A number of observations will often occlude others in a plot such as this, even with a modest sample size. The `jitter(group)` command takes the group values and adds a small amount of random noise.

Output 3.2: R code to produce Fig. 3.6

```

library(boot)                      # contains the cd4 dataset
n <- length(cd4$baseline)          # sample size
join <- c(cd4$baseline,cd4$oneyear) # concatenate all CD4 values
group <- rep(c(0, 1), each = n)    # assign group membership
par(mfrow = c(1, 3))              # three side by side plots on one page
plot(group, join,                 # 1st plot with simple X axis
      ylab = "CD4 counts", xlab = "", axes = FALSE,
      ylim = c(0, max(join)), xlim = c(-.25,1.25))
text(c(0,1), c(1,1), labels = c("Baseline", "1 year"))

plot(jitter(group), join,         # 2nd plot with jittered X-axis
      ylab = "", xlab = "", axes = FALSE,
      ylim = c(0, max(join)), xlim = c(-.25, 1.25))
text(c(0,1), c(1,1), labels = c("Baseline", "1 year"))

plot(group, join,                # 3rd plot: spaghetti
      ylab = "", xlab = "", axes = FALSE,
      ylim = c(0, max(join)), xlim = c(-.25, 1.25))
text(c(0,1), c(1,1), labels = c("Baseline", "1 year"))
for (i in 1:n)                  # draw individual connecting lines
  lines(c(0,1), c(cd4$baseline[i], cd4$oneyear[i]))

```

The program that produces Fig. 3.6 is given in Output 3.2. In Fig. 3.6 we can see that the 1-year values are more variable than the baseline values. This comparison is easier to make with the jittered grouping values.

The *spaghetti plot* links every individual's paired values. From the spaghetti plot we can see if subjects with high baseline values are associated with high 1-year values. A few individual's values decrease, but clearly there is an overall trend of increasing values among the scattered lines.

3.3 Displays for Bivariate Data

Let's have a look at the well-known scatterplot. Consider the data given in Table 1.1 for the values of apartment rents and house prices for each state. The values are contained in a `data.frame` called `housing` in R so we have

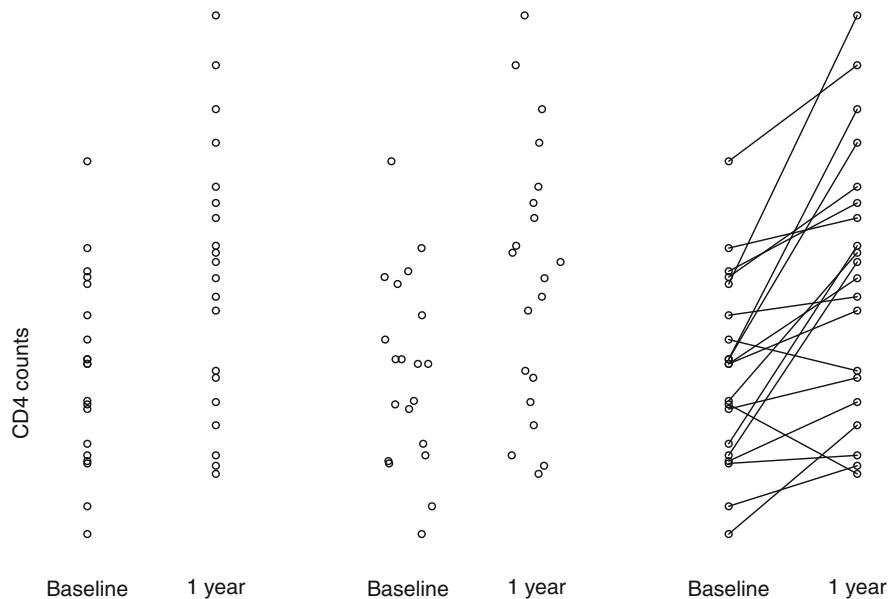


Figure 3.6: CD4 counts by group, with jittering, and as spaghetti

> **housing**

	Apartment	House
AK	949	237.8
AL	631	121.5
AR	606	105.7
...
WI	704	173.3
WV	528	95.9
WY	636	188.2

A simple command

> **plot(housing)**

produces the scatterplot in a familiar format, given in Fig. 3.7.

The figure contains labels for the two axes because they are defined as column names in the **data.frame**. This figure conveys the basic information: The prices of houses are correlated with apartment rents and the values are skewed towards the high ends of both. Let's try to improve upon this basic figure.

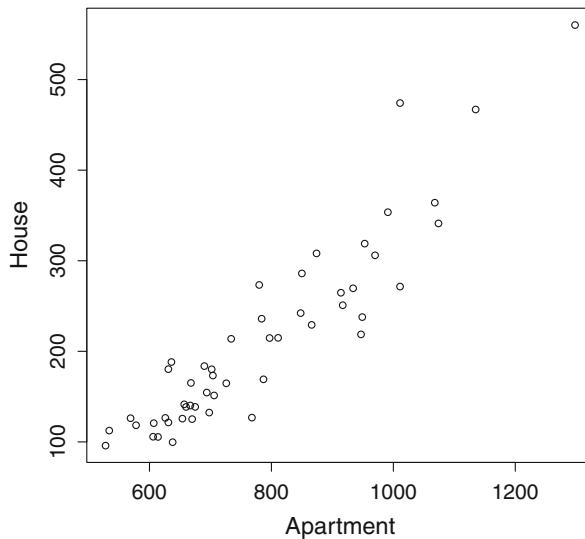


Figure 3.7: Basic scatterplot of housing data

Any serious discussion of statistical graphics would be amiss if it failed to mention the series of books by E Tufte. Tufte (2001) recommends eliminating the *chart junk* or non-essential graphical items in order to draw our attention to the patterns in the data.

Specifically, in Fig. 3.7, the box containing the figure is purely decorative. Further, the numbers and tick marks along the two axes convey only a small amount of information about the range of values.

Tufte (2001) would urge us to maximize the *data to ink ratio*. The point of drawing a scatterplot is to examine the bivariate relationship between the variables of interest, in this case housing prices and apartment rents. A greater amount of “ink” should be dedicated to presenting the data instead of framing the picture with decorative axes. This brings us to the plot in Fig. 3.8 with no numbers in the axes, bold symbols emphasizing the data, and “rug fringes” displaying the two marginal distributions.

Figure 3.8 was produced using

```

require(graphics)                                     # library for rug program
attach(housing)
boundA <- range(Apartment) * c(.95, 1)      # find bounds for plot area
boundH <- range(House) * c(.8, 1)

plot(housing, xlim = boundA, ylim = boundH, # Plot data with bounds
      axes = FALSE,                         # Omit the usual axes
      cex = 1.5, pch = 16,                   # Plot large solid circles
      col = "red")                         # Select color of points
rug(Apartment, side = 1)                      # Add rug fringes
rug(House, side = 2)

```

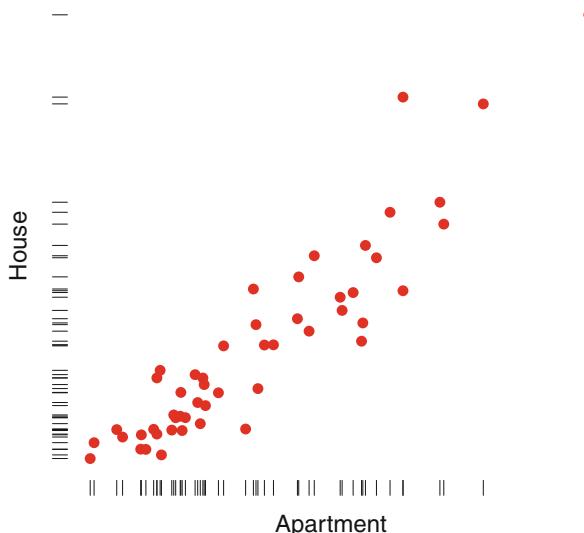


Figure 3.8: Plot with minimal chart junk and a high data to ink ratio

where `rug` adds “fringes” corresponding to a univariate scatterplot of the marginal distributions. Tufte (2001) refers to the style of Fig. 3.8 as a *dot-dashplot*. One problem with the graph in Fig. 3.8 is that our eyes can get distracted and wander away from the figure because it lacks a bounding box to frame the figure and focus our attention.

3.3.1 Plot Options, Colors, and Characters

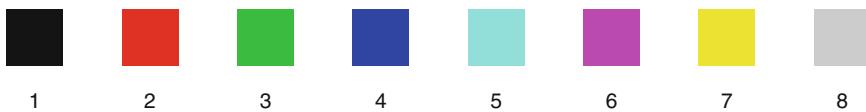
Let us describe some of the many options available when using the `plot` function in R.

The bounds of the original `plot()` statement, used to produce Fig. 3.8, are modified to move the rug fringes a little away from the bivariate data points. This is done using the `xlim=` and `ylim=` options. This last example illustrates the use of the `cex=` option to magnify or shrink the size of the plotted characters. The `axes=FALSE` suppresses the usual axes and their numerical values.

The `plot` statement in this last example uses the `pch=` option to choose the plotting character. The most commonly used `pch=` options are

□	○	△	+	×	◊	▽	▣	*	◊	⊕	⊖	⊗	■	▣	□	■	●	▲	◆	●	●
0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	

Colors may also be used using the `col=` option. The colors can be addressed by name or by number. Eight colors can be addressed by number:



A complete spectrum of colors is also available. See the `help` file on `rainbow` and `palette`. The `rainbow(n)[i]` function divides the visible spectrum into `n` shades and `[i]` picks the `i`th of these.

As an example of the `rainbow` function, the R code

```
plot( c(0,1), c(0,1), type="n", xlab=" ", ylab=" ", axes=FALSE)
n <- 125
for (i in 1:n)
{
  lines(rep(i/(n+1), 2), c(0,1), lwd=4,
        col=rainbow(n)[i])
}
```

produces Fig. 3.9.

The sizes of plotted objects can be changed. The `cex=2` option, for example, will double the size of plotted characters. Similarly, `cex=.5` will shrink characters by half. The `cex.lab=` option is used to change the size of the font used on the axes.

3.3.2 More Graphics for Bivariate Data

In contrast to Fig. 3.8, let us consider a scatterplot with a lot of processing and detail attached. The *bivariate boxplot* is described by Goldberg and Iglewicz (1992) and programmed by Everitt and Hothorn (2011).

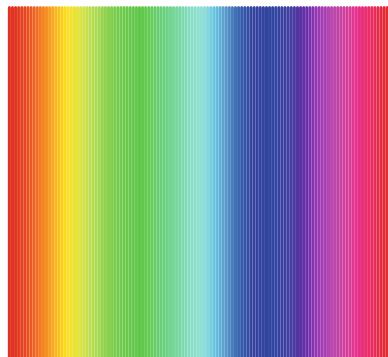


Figure 3.9: An example of the `rainbow()` function

The scatterplot of the housing data in Fig. 3.10 illustrates the bivariate boxplot using the program `bvbox` in the `MVA` library. Instead of the central box containing 50 % of the univariate data as in a univariate boxplot of Fig. 3.3,

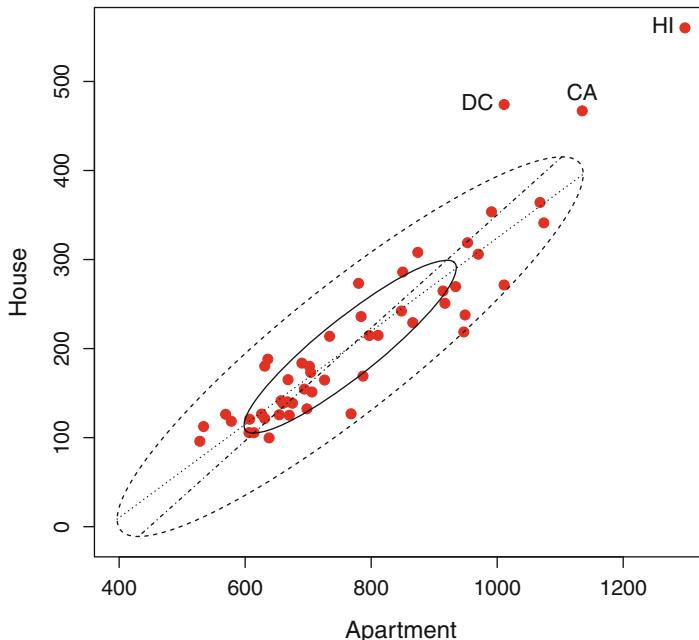


Figure 3.10: Bivariate boxplot of housing data

the bivariate boxplot includes a pair of estimated ellipses, the inner one containing approximately 50 % of the data and the outer one containing about 95 %. For ease of interpretation, we have added `text` to the figure allowing us to identify the three outliers: California, Hawaii, and Washington, DC.

The R code that produces Fig. 3.10 is

```
library(MVA)                                     # library for bvbox
extreme <- c( "DC", "HI", "CA")               # Three extreme states
exst <- match(extreme, rownames(housing)) # identify index in data

bvbox(housing, xlab = "Apartment", ylab = "House",
      pch = 19, cex = 1.25, col = "red")
text(housing$Apartment[exst], housing$House[exst],
     labels = extreme, cex = .8,                 # label names, small font
     pos = c(2,2,3))                           # position labels: L,L, top
```

See Exercise 3.6 on modifying the graphical options in the `bvplot` routine.

The `match()` statement is discussed in Sect. 2.1.2 and is used to identify the subscript (index or observation number) associated with each of the named three extreme states. In this example, `match()` is used to identify the index of each of the three names of extreme values among the `rownames` of the `data.frame`.

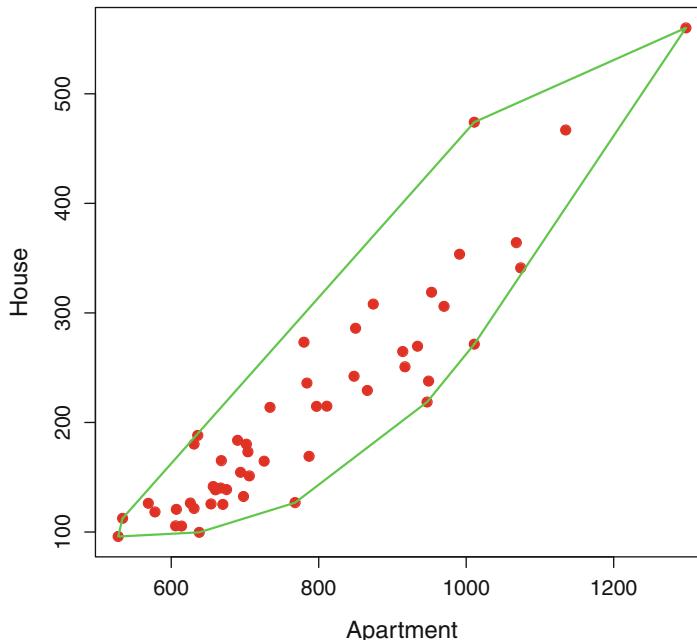


Figure 3.11: Convex hull of the housing data

The two lines inside the ellipses of Fig. 3.10 are estimates of the regression line. The darker line is the usual least squares line using all of the observations. The lighter line is a more robust estimate that reduces the influence of any extreme outlying data values. See Chap. 9 for a full discussion of linear regression. See also Exercise 13.1 for an examination of the most extreme values in this data and whether these can be considered as outliers.

Let us end this section on two-dimensional plots with a discussion of the *convex hull*. The convex hull is a lot like wrapping an irregularly shaped object with the smallest amount of gift paper: The most extreme points in any direction will define the ultimate shape of the package. Mathematically, the convex hull is the smallest convex polygon containing all of the data. In R, the `chull` function returns the indices of the data points that are most extreme in each direction:

```
> chull(housing)
[1] 34 10 44 26 50 29 8 12
```

We can redraw the housing data from Fig. 3.7 and identify those points that are on the convex hull. The program

```

ch <- chull(housing)      # find the indices of the convex hull
ch <- c(ch, ch[1])        # loop back to the beginning
plot(housing, pch = 19, col = 2,
     cex = 1.25)            # plot the original data
lines(housing$Apartment[ch], housing$House[ch],
      type = "l", col = 3, lwd = 2) # bold, green lines

```

draws Fig. 3.11.

The `lines` command adds lines to the figure with the `type="l"` option. The lines that are drawn also need to return back to the beginning, so the list of indices `ch` from the convex hull program `chull` must repeat the first observation at the end of this list in order to complete the polygon. In this example, the `lwd=` option in `lines` controls the width of the lines.

The convex hull in Fig. 3.11 identifies the extremes in the data. Some might argue that not all of these observations should be considered outliers. If there are outliers, the convex hull will pick some of these out. If there are several outliers, as identified in Fig. 3.10, then they might hide behind the largest of these. California is an outlier but is dwarfed by the larger outlier of Hawaii. Such a problem is called *masking*, where one extreme outlier obscures others in the data.

Suppose we omitted the observations on the convex hull and looked at what remains. This would remove the most extreme values to reveal those less extreme. We might then draw the convex hull of those remaining observations. It is also useful to repeat this process several times. The net effect is much like peeling an onion, successively removing the outermost layers, one at a time. This repeated process will give a better idea about the underlying shape of the data.

The program lines

```

library(aplpack)
nlev <- 5                  # Number of levels
colors <- heat.colors(9)[3:(nlev+2)]
plot(housing, n.hull = nlev, col.hull = colors,
     xlab = "Apartment", ylab = "House",
     lty.hull = 1:nlev, density = NA, col = 0, main = " ")
points(housing, pch = 16, cex = 1, col = "blue")

```

draw and then peel away five successive convex hulls to produce Fig. 3.12. Each successive layer is plotted in a different color by `plot.hulls`.

The best way to look at Fig. 3.12 is as a five-layer wedding cake. Layers on the inside are stacked higher and on top of those further out. The smaller and higher cake layers represent areas with a greater density of observations. The baker might be accused of being sloppy, but notice the convex hull has no bias about what these data layers should look like. Compare Fig. 3.12 with Fig. 3.10. In Fig. 3.10 we see layers that are perfect and parallel ellipses, regardless of what the data might suggest. The convex hull peeling in Fig. 3.12 is the nonparametric approach that makes no assumptions about the form of

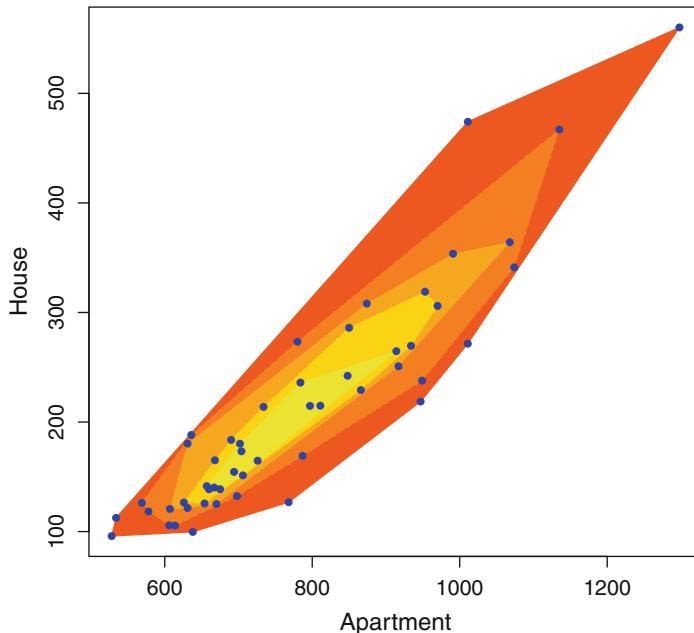


Figure 3.12: Five peeling convex hulls and color fill for the housing data

the underlying data. We can see that these nested convex hulls are almost ellipses, so the best summary of this data may lie somewhere in between Figs. 3.10 and 3.12. See also Exercise 3.7 on drawing convex hulls of data.

3.4 Displays for Three-Dimensional Data

Table 3.1 lists January maximum temperature data in each of many US cities. Along with the city, we also have latitude (degrees north), longitude (degrees east), and altitude in feet above sea level.

The size of the circle or bubble represents values of the third variable. In this example, we plot US cities on the XY-axis as a conventional map in terms of their latitude and longitude. The size of the bubble represents altitude. Cities at the corners of Fig. 3.13 have been identified by state to help orient the reader.

The bubble sizes show that cities on the east and west coasts are all at sea level. Midwest cities are situated at slightly higher altitudes. The highest altitude cities are in the Rocky Mountains in the west. The program that produces this figure is given in Output 3.3.

Longitude is measured as distance from Greenwich, England, and needs to be reversed in order to have this map display east and west in their familiar

Table 3.1: Maximum January temperature (T, in degrees Fahrenheit), latitude, longitude, and altitude in feet above sea level, for some of the largest US cities

T	Lat	Long	Alt	Name	T	Lat	Long	Alt	Name
61	30	88	5	Mobile, AL	59	32	86	160	Montgomery, AL
30	58	134	50	Juneau, AK	64	33	112	1090	Phoenix, AZ
51	34	92	286	Little Rock, AR	65	34	118	340	Los Angeles, CA
55	37	122	65	San Francisco	42	39	104	5280	Denver, CO
37	41	72	40	New Haven, CT	41	39	75	135	Wilmington, DE
44	38	77	25	Washington, DC	67	30	81	20	Jacksonville, FL
74	24	81	5	Key West, FL	76	25	80	10	Miami, FL
52	33	84	1050	Atlanta, GA	79	21	157	21	Honolulu, HI
36	43	116	2704	Boise, ID	33	41	87	595	Chicago, IL
37	39	86	710	Indianapolis, IN	29	41	93	805	Des Moines, IA
27	42	90	620	Dubuque, IA	42	37	97	1290	Wichita, KS
44	38	85	450	Louisville, KY	64	29	90	5	New Orleans, LA
32	43	70	25	Portland, ME	44	39	76	20	Baltimore, MD
37	42	71	21	Boston, MA	33	42	83	585	Detroit, MI
23	46	84	650	Sault Ste Marie	22	44	93	815	Minneapolis, MN
40	38	90	455	St Louis, MO	29	46	112	4155	Helena, MT
32	41	95	1040	Omaha, NE	32	43	71	290	Concord, NH
43	39	74	10	Atlantic City, NJ	46	35	106	4945	Albuquerque, NM
31	42	73	20	Albany, NY	40	40	73	55	New York, NY
51	35	80	720	Charlotte, NC	52	35	78	365	Raleigh, NC
20	46	100	1674	Bismark, ND	41	39	84	550	Cincinnati, OH
35	41	81	660	Cleveland, OH	46	35	97	1195	Oklahoma City
44	45	122	77	Portland, OR	39	40	76	365	Harrisburg, PA
40	39	75	100	Philadelphia, PA	61	32	79	9	Charleston, SC
34	44	103	3230	Rapid City, SD	49	36	86	450	Nashville, TN
50	35	101	3685	Amarillo, TX	61	29	94	5	Galveston, TX
37	40	111	4390	Salt Lake City	25	44	73	110	Burlington, VT
50	36	76	10	Norfolk, VA	44	47	122	10	Seattle, WA
31	47	117	1890	Spokane, WA	26	43	89	860	Madison, WI
28	43	87	635	Milwaukee, WI	37	41	104	6100	Cheyenne, WY
81	18	66	35	San Juan, PR					

Source: Mosteller and Tukey (1977; pp. 73–74), with corrections

right/left orientation. Puerto Rico and the three states Alaska, Hawaii, and Massachusetts are identified to help the reader.

The `with()` and `text()` commands are used to add symbols and labels to this plot. The `symbols` command sets the size of the circles proportional to the `altitude`. Options in the `symbols` command include `inches=` to scale the sizes of the circles, `fg=` to set the color, and `lwd=` to create thick or thin lines.

Another useful display for three dimensions is based on *kriging*. Kriging is named after Daniel Krige¹ who was examining the grades of gold taken from several small exploratory mine shafts. He developed kriging, a smooth mathematical function that summarizes the underlying concentration of gold.

¹Daniel Gerhardus Krige, (1919–2013). South African mining engineer.

Output 3.3: Program to create the bubbleplot in Fig. 3.13

```

JanTemp <- read.table(file="JanTemp.txt", header=TRUE)
require(MASS)
attach(JanTemp)
longe <- 180 - long                                     # Reverse East and West

plot(longe,lat, pch = 16, cex = .7,                   # Plot dots at cities
     xlab="Longitude, east", ylab = "Latitude", col = "red")
with(JanTemp,symbols(longe,lat,circles = alt, # Altitude sized circles
                     inches = .3, add = TRUE, lwd = 3, fg = "green"))
landmarks <- c( "AK", "HI", "MA", "PR")           # Four landmark states
lmi <- match(landmarks, state) # identify landmark's indexes in data
text(longe[lmi],lat[lmi],labels = landmarks, # Identify landmarks
     pos=c(1,1,4,3), col = "blue")

```

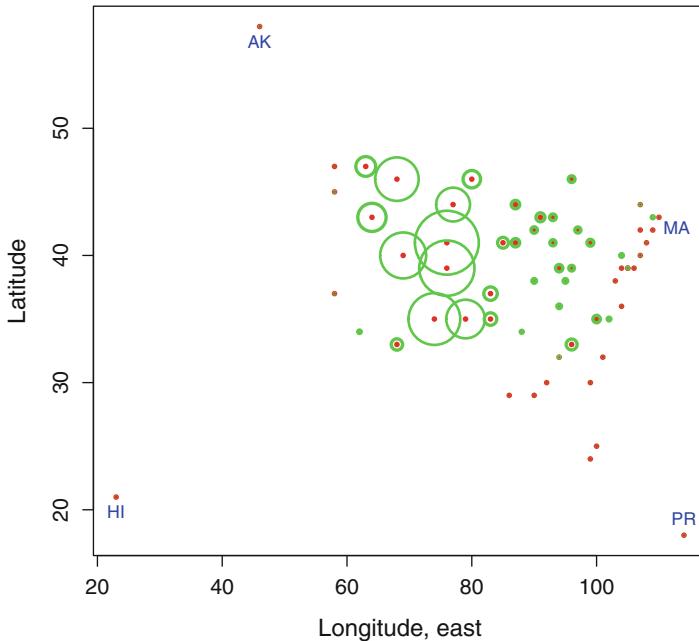


Figure 3.13: Bubble plot of altitudes of US cities

He used this method for interpolating between the data values observed in the mines. We can perform the same process to model the altitude data examined in Fig. 3.13.

Figure 3.14 should look familiar to us as a weather map. Small local deviations are smoothed out, and a simplified version of reality is presented. The map clearly identifies sea-level cities on the coasts and the high-altitude

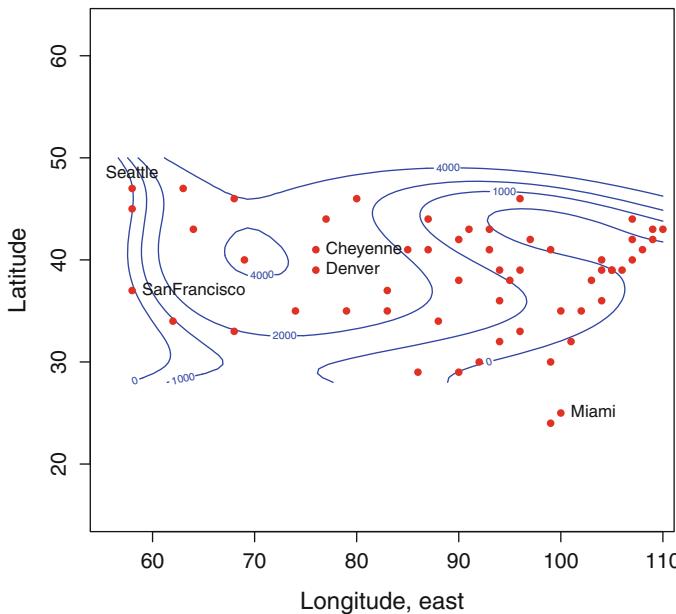


Figure 3.14: Kriging plot of altitudes of US cities

cities in the Rocky Mountains. In this case, the altitude values have been approximated and smoothed. The program that generates this figure appears in Output 3.4.

The `surf.ls(4, ...)` program approximates the altitude values as a 4th degree polynomial in both latitude and longitude. You can try other values: lower polynomial degrees are smoother but may be unrealistic, while large values result in plots that are not very smooth. The actual fitting uses least squares regression to estimate the altitude values. Least squares and other regression methods are described in Chap. 9.

The `eqscplot()` program creates a plotting area in which the x and y axes are presented on the same scale. You may have noticed that the scatterplot US map in Fig. 3.13 (plotted using the `plot` function) appears narrow and tall. The use of `eqscplot` function in this present program sets up and labels the axes, but does no actual plotting because of the `type="n"` option. The remainder of this program plots all of the cities, except the extremes: Juneau, San Juan, and Honolulu. Finally, the program identifies specified individual cities with printed labels using the `text` statement.

 Output 3.4: Program to produce the krig plot in Fig. 3.14

```

library(MASS)
library(spatial)
attach(JanTemp)
longe <- 180 - long          # Longitude, east
alt.kr <- surf.ls(4, longe, lat, alt) # Kriging surface
altsur <- trmat(alt.kr, 55, 110,
                 28, 50, 50)      # Set limits of plot, excluding outliers
eqscplot(altsur, xlab = "Longitude, east", cex.lab = 1.5,
         ylab = "Latitude", type = "n") # plot in equal scale coordinates
contour(altsur, levels = c(0, 1000, 2000, 4000),
        add = TRUE, col = "blue") # specify contour colors and levels
points(longe, lat, pch = 16, col = "red") # add original cities
ex <- c("Miami", "Seattle", "SanFrancisco",
       "Denver", "Cheyenne")           # List of special cities
exi <- match(ex, name)           # index for these cities
text(longe[exi], lat[exi], labels = ex, # label special cities
     pos = c(4, 3, 4, 4, 4), cex = 1)
  
```

3.5 Displays for Higher Dimensional Data

How can we generalize the display of multivariate data with several dimensions? This area is ripe for creative development. Here are a few helpful methods available in R.

3.5.1 Pairs, Bagplot, and Coplot

One straightforward approach is to consider these two at a time and draw all possible bivariate scatterplots. Then we can do it all again, this time, with the axes reversed. An example appears in Fig. 3.15.

The `pairs()` command in R produces a matrix of scatterplots. As an example, the matrix scatterplot of the burger data in Table 1.6 is presented in Fig. 3.15. The names of the variables (calories, fat, sodium, carbohydrates) runs down the diagonal. Every possible pair of these variables is plotted twice with the axes reversed above and below the diagonal.

In this figure we see that carbohydrates and sodium each exhibit a few extreme outliers. Fat and calories from fat are linearly related, but one value seems to be calculated incorrectly. Calories are closely related to fat. Carbohydrates and sodium appear unrelated. This figure was produced using

```

pairs(burger, pch = 16, col = "red")
  
```

We can improve on this basic `pairs()` plot and use some additional options, adding color, different plotting characters, and a smoothed regression line called *loess*. The loess line is a compromise between smoothness and small deviations away from the observed data.

The program that produces Fig. 3.16 is given by

```
pairs(burger, lwd = 3, pch = 16, cex = 1.25, col = "red",
      gap = 0, xaxt = "n", yaxt = "n",
      panel = panel.smooth, col.smooth = "blue")
```

The loess lines help us see nonlinear relationships between carbohydrates and each of the other variables in the upper half of this figure. A number of other options produces a cleaner presentation: `gap=0` removes the spacing between the panels, `xaxt = "n"`, `yaxt = "n"` removes the numbers in the axes, and contrasting colors separate the data from the fitted model.

The *bagplot.pairs* routine combines several features we have covered: the bivariate boxplot, the convex hull, and the pairs scatterplot. The bagplot contains a scatterplot of bivariate data. The outer polygon of each bagplot is a convex hull, excluding extreme outliers. The inner polygon (the “bag”) of the bagplot contains the central 50 % of the data. Data points between the two convex hulls are connected with lines to the central, bivariate median. Figure 3.17 was produced using

```
library(aplpack)
bagplot.pairs(burger[, 4 : 7], gap = 0, col.baghull = "green")
```

The pairwise approach to examining multivariate data reduces the problem back to two dimensions and looks at it as a series of pairs of scatterplots. This simplification overlooks the multivariate character of the data. After all, if there are complex relationships, we need a way to display these simultaneously.

One improvement on the pairwise scatterplot matrix is to look at a series of scatterplots, each representing a view of a slice of a third variable. Chambers (1992) calls this a conditioning plot or *coplot*. In the hamburger data, for example, Fig. 3.15 shows calories and sodium do not have a strong relationship. There is also an outlier with very high values of both sodium and calories. Suppose we want to examine the relationship between calories and sodium across different values of the variable measuring fat content.

The `coplot` function in the R code

```
library(graphics)
coplot(Cal ~ Sodium | Fat, data=burger,
       rows=1, pch=16, cex=1.75, col="red",
       bar.bg = c(num = "blue", fac = gray(0.95)))
```

produces Fig. 3.18.

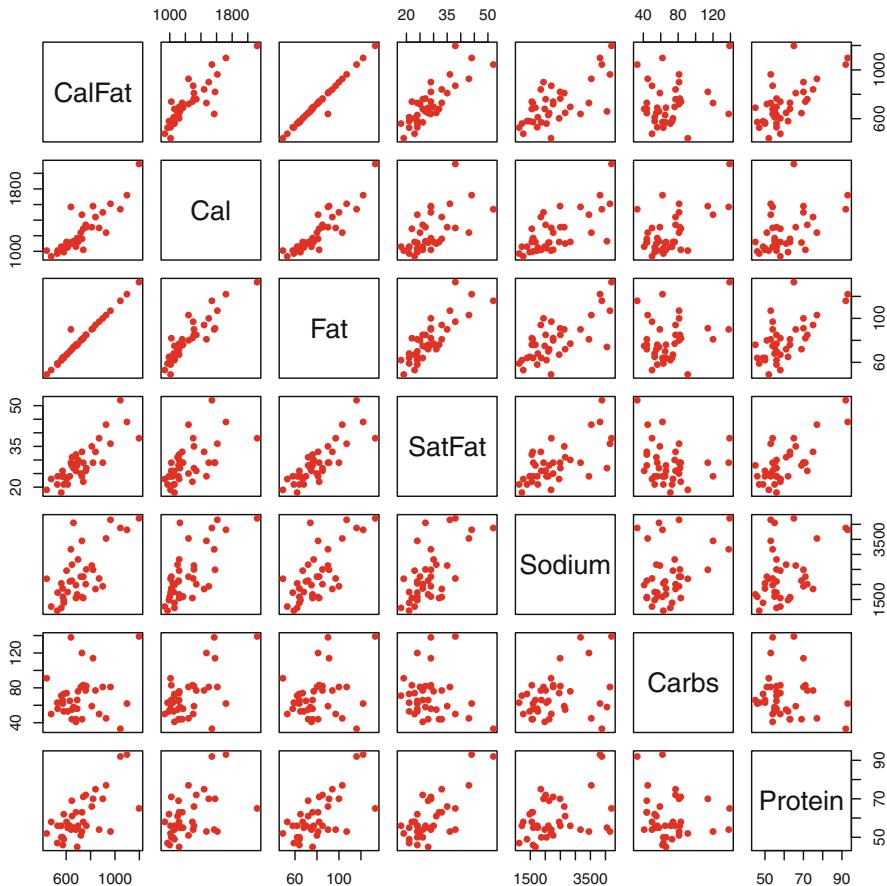


Figure 3.15: Basic matrix scatterplot of hamburger data

The program code `Cal ~ Sodium | Fat` specifies that calories and sodium will be plotted against each other for stratified values of fat. In particular, the top of Fig. 3.18 shows how the coplot program cuts the range of fat values into a series of six overlapping intervals. For each of these intervals of the fat variable, there is a scatterplot of calories plotted against sodium at the bottom half of this figure.

As we look at the scatterplots on the bottom half, from left to right, we see a changing relationship between calories and sodium. For the lowest values of fat, both calories and sodium are small. Larger values of fat are associated with larger values of both calories and sodium. The large outlier between sodium and calories only appears within the highest range of fat. At no value of fat does there appear to be a strong relationship between calories and sodium.

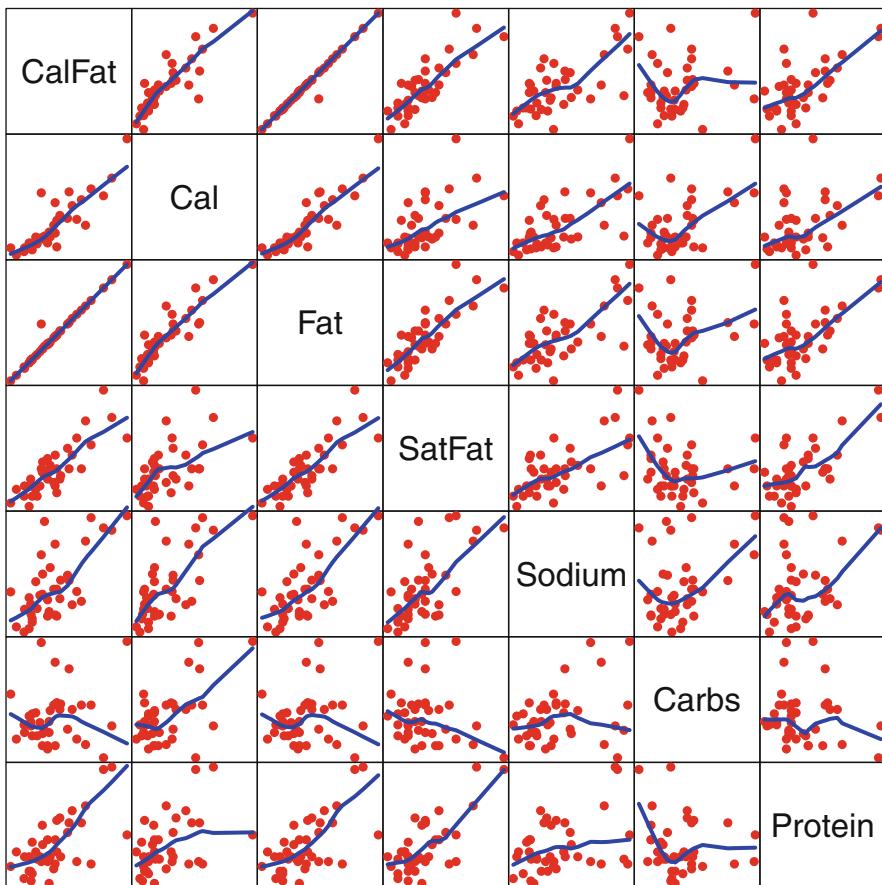


Figure 3.16: Scatterplot of hamburger data with loess smoothing and cleaner presentation

3.5.2 Glyphs: Stars and Faces

The *star plot* summarizes each data item as a circle with different sized wedges. An example for the hamburger data appears in Fig. 3.19. Every star is an individual (row) and every wedge on the star represents a different variable (column) in the data. The radius of each wedge in the star indicates the size of the scaled values for that individual, relative to all other measurements for that variable. These variables are listed in different colors and directions. The key for this is given in the lower right corner of the figure. The radius of each wedge is scaled and can be used to compare the relative magnitude of each variable values across all individuals.

To aid in organization, all burgers have been ordered by their calorie values, in reading order, largest at top, to smallest. We can sort in decreasing

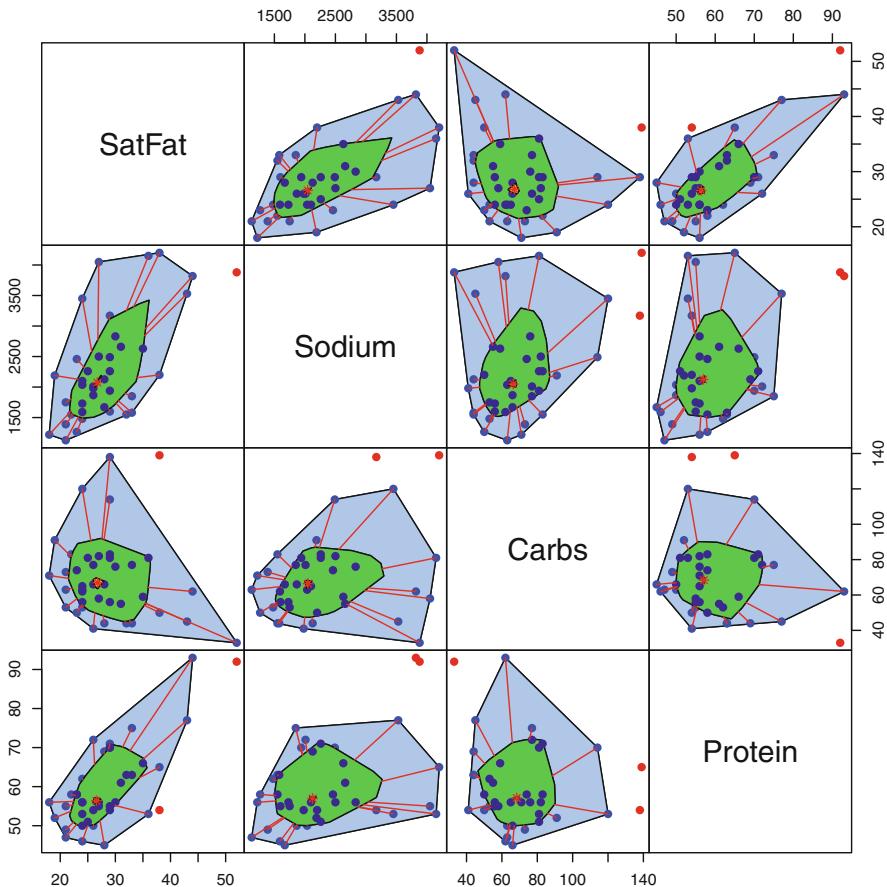


Figure 3.17: Bagplot pairs of hamburger data

order by sorting on the *negative* values, in the code given below. The numbers in the figure refer to the listing order of `row.names` in the `data.frame`. Figure 3.19 was produced using the R commands

```
library(graphics)                      # for the stars program
palette(rainbow(7))                   # set colors
burs <- burger[ order(-burger$Cal), ] # order by Cal, decreasing
stars( burs, len=1, cex=0.5, key.loc=c(12.5, 2),
      labels=row.names(burs), draw.segments=TRUE)
```

which labels each object and provides a useful guide to the directions of the stars in the lower right corner. The help for this command `help(stars)` explains a large number of options available for this graphical display.

In Fig. 3.19, we can see that the burgers in the top two row are simultaneously extreme in most dimensions. The first few burgers are different from

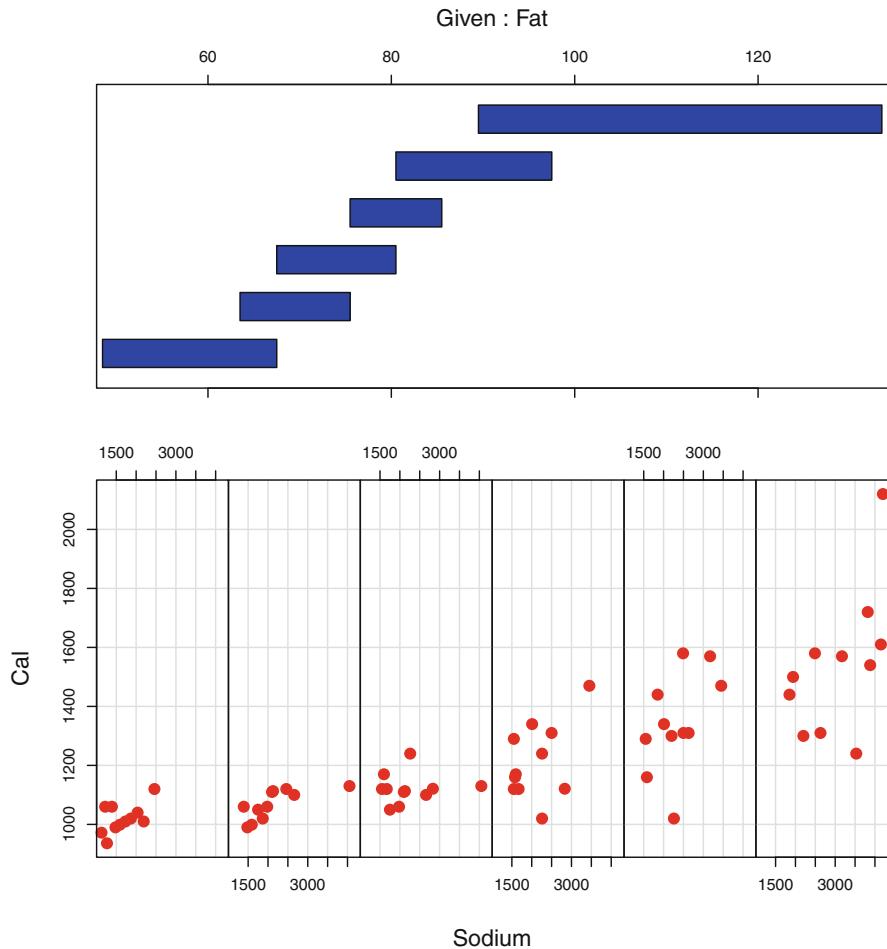


Figure 3.18: Burger coplot of calories and sodium, stratified by fat

the others and extreme in most of the seven dimensions. Outside of the top two rows, the stars for the burgers are not very different from each other and only a few are extreme in more than one dimension.

Stars are an example of a *glyph*. A glyph is a general class of graphics in which the shape of the plotted character is indicative of the multivariate characteristics of the observation. In addition to stars, a simple glyph appears in Fig. 3.13 in which the size of the plotted circle is related to the altitude of the respective city.

Let us examine the most extreme example of a glyph. Chernoff (1973) used cartoon faces as a glyph to demonstrate multivariate information. Each variable can represent some aspect of the face: head size and color, degree of smile or frown, amount and shape of hair, the spacing and size of eyes, and so on.

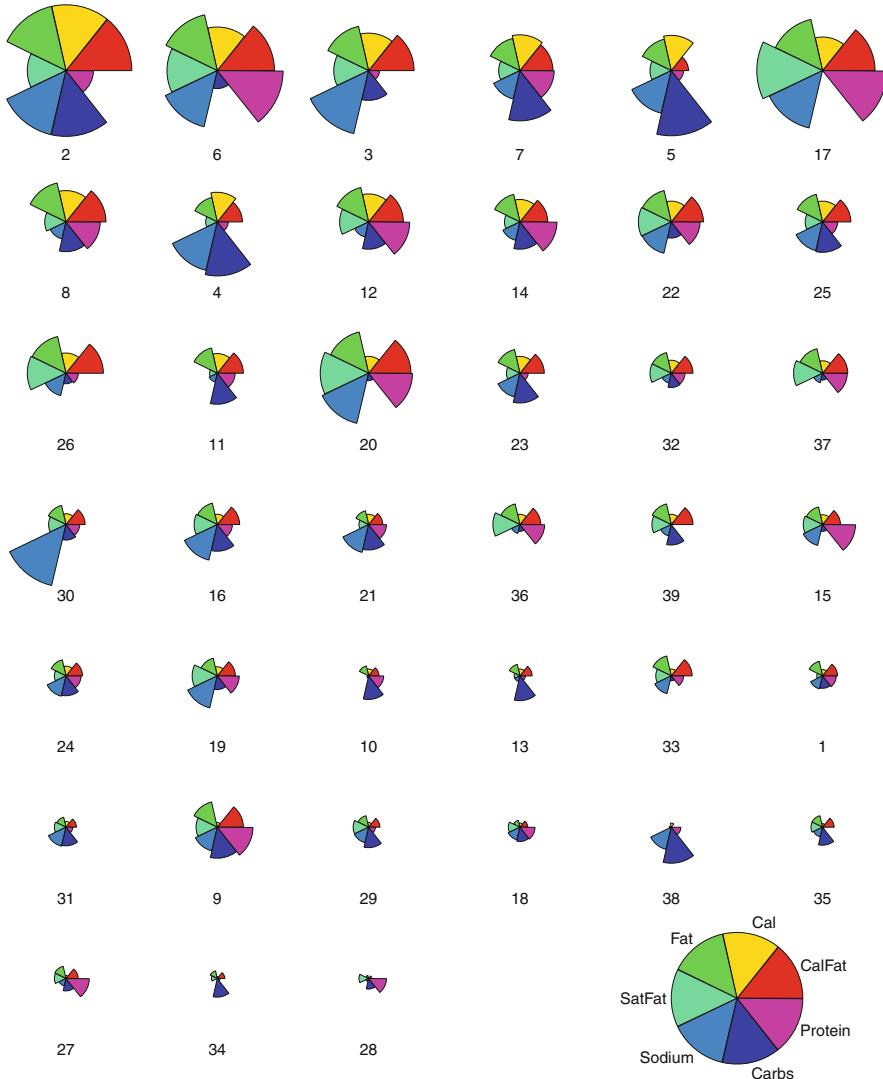


Figure 3.19: Star plot of burgers, ordered by calories, with key

An example of *Chernoff's faces* appears in Fig. 3.20 for the nine highest calorie burgers in Table 1.6. The first three or so of these faces are oversized and outlandish, corresponding to the extreme, high data values. We can see a gradual trend of lower values in the last row of faces in this figure. These correspond to smaller head size, less hair, smaller eyes, and mouths. The faces for the omitted burgers are similar to those of the last row in this figure. The `faces` program that draws these is available in the `aptpack` package.

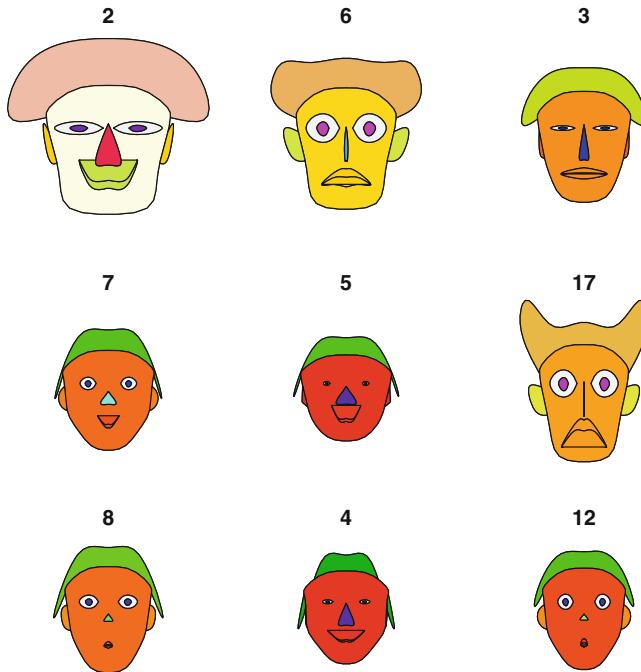


Figure 3.20: Chernoff faces display for the nine highest caloric hamburgers

3.5.3 Parallel Coordinates

Consider multivariate data categorized into a small number of groups. We have several graphical methods that can describe group membership as well as distinguishing characteristics for each group. This is the data examined by RA Fisher² that motivated the initial study of discriminant analysis. (See Sect. 10.3.) In this well-known example of multivariate data, three species of iris flowers are measured in terms of their

- petal length
- petal width
- sepal length
- sepal width

The data is available in the `MASS` library in R. The *parallel coordinate* display (sometimes called the *parallel axes* display) plots the separate coordinate axes parallel to each other, rather than as at right angles to each other, as we often think of in terms of axes.

²Ronald Aylmer Fisher (1890–1962). British geneticist and statistician.

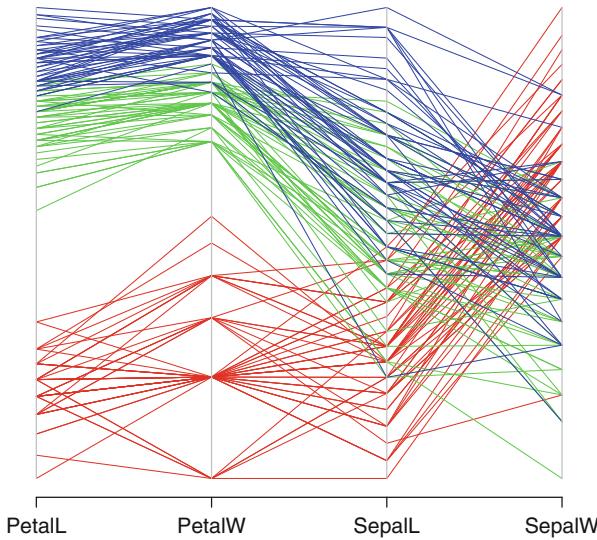


Figure 3.21: Parallel coordinate plot for the iris data

To produce this display, begin by rescaling each of these separate measurements so they are all on the same scale, usually between 0 and 1. The multidimensional values for each item are connected with lines so we can follow these across the different dimensions. In this example, we can also plot each of these series of lines in a different color for each of the iris species. The plot in Fig. 3.21 displays this data, with each species in a different color. Every jagged line traces the four values for one flower across each of the four dimensions.

The R program that produces this figure is

```
library(MASS)
ir <- rbind(iris3[ , , 1], iris3[ , , 2], iris3[ , , 3])
parcoord(log(ir)[ , c(3, 4, 1, 2)], # Order the axes
         col = c(rep("red", 50), rep("green", 50), rep("blue", 50)))
```

In R, the data is listed as a three-dimensional data frame, where the third subscript indicates each of the three separate species. The `rbind` statement creates a `data.frame` called `ir` where the three species are listed one after the other as rows.

The `parcoord` program draws the parallel axes plot given in Fig. 3.21. The data values are scaled on each of the four axes after taking logs of all data. The ordering of the four axes in this plot is specified. You can try other orderings to obtain a more pleasing result. In this case we chose the ordering here so that the three species separate well in the plot. The different colors for each of the species are specified using the `col=` option.

Specifically, the three colors, `col=` values and species, in this figure are as follows:

Color	Species
Red	<i>Setosa</i>
Green	<i>Versicolor</i>
Blue	<i>Virginica</i>

We can see that the *Setosa* (in red) has lowest values of petal length and width. *Setosa* generally also has relatively large values of sepal width. *Virginica* (in blue) and *Versicolor* (in green) have an ordering with larger values of *Virginica* in most cases across all four of the measured variables.

3.6 Additional Reading

The field of statistical graphics is open for new developments. There is so much more left to do. The good news is that the field is so accessible because it does not require an extensive mastery of mathematical and computational expertise before one can make an innovative and lasting contribution. Perhaps the biggest disappointment is that in the twenty-first century we are still limited to two-dimensional paper in a printed book as did publishers since Guttenberg,³ over 500 years ago. Some software packages allow us to slowly rotate a three-dimensional object. This may allow our spatial perception to find patterns, and is usually aided by the inclusion of factor methods, described in Chap. 8.

Innovation in the field of statistical graphics has come at a steady pace with several notable pioneers. Tukey⁴ was ahead of his time. When we look at Tukey (1977) we take many of his ideas for granted because they are now a part of our everyday language. At a time when working at a computer meant waiting for a 110 baud teletype machine to clunk and chug along, Tukey developed a boxplot, the innovative histogram that could be printed in only three lines. He coauthored Chambers et al. (1983) and inspired Cleveland (1993).

The books by Tufte are artistic and passionate contributions to the field. You don't have to have a rigorous background in mathematical statistics to appreciate what is being conveyed. Perhaps a rigorous background in statistics trains us to think in certain rigid ways and this can be a distraction.

Wilkinson (1999) describes a new language that codifies and unifies the whole of statistical graphics. This is a new direction that takes us away from specific examples into a discussion of what is possible, sometimes combining

³Johannes Gutenberg (1398–1468). German, invented movable type. This led to the wide availability of books, which in turn was instrumental in the Renaissance and the scientific advances that followed.

⁴John Wilder Tukey (1915–2000). American statistician and mathematician.

two or more methods of display. An applied version of this in R has been the development of the `ggplot2` function. An introduction to `ggplot2`, and graphics in R more generally, is Chang (2013).

The lattice plot builds on the earlier trellis plot. The `lattice` package is a large suite of useful graphics available in R and more fully described in Sarkar (2008). One example is the violin plot, as part of Exercise 3.4.

Ideally, we should explore data in an interactive environment allowing us to use sliders alongside plots to visualize the effects of different amounts of smoothing. For three-dimensional data, there is no substitute for rotations in a dynamic setting. Some of these tools are available in the `aptpack` library but cannot be adequately appreciated until they are experienced first hand.

3.7 Exercises

- 3.1 Describe the *pie chart*. What type of data is this best suited for? What are its limitations?
- 3.2 How does the sample correlation change when we remove successive layers of convex hulls from our two-dimensional data? Add `cor(x,y)` inside the loop of the program that generates the convex hull peeling in Fig. 3.22. What do you think is the reasons for this change?
- 3.3 Look at the relationship between fat and sodium content for each of the 40 burgers in Fig. 3.15. Sodium values seem to rise quickly for higher levels of fat. Does this look like a linear relationship?
 - (a) Plot fat and sodium using a bivariate boxplot and also as a single convex hull. Do these methods assist or mislead us?
 - (b) In this same data set, calories and fat seem to exhibit an hour-glass shape with greater variability at both the high and low ends. Examine the bivariate boxplot and convex hull of this pair of variables. Are these methods useful in this situation?
- 3.4 In the `lattice` package there is a data set called `singer` which gives the heights of singers in the New York Choral Society, a serious amateur vocal group. Heights are given separately by each of the different voice parts, high to low (soprano, alto, tenor, bass). Each of these is further divided into tiers (1 and 2) for higher and lower voices within each part.
 - (a) In R, explore graphical methods such as jittering and boxplots to show the characteristics and distributions of heights by voice group. The general trend is that taller people have deeper singing voices, but also comment on the shape of the distributions within each vocal group. The documentation for `singer` provides other useful displays of this data.

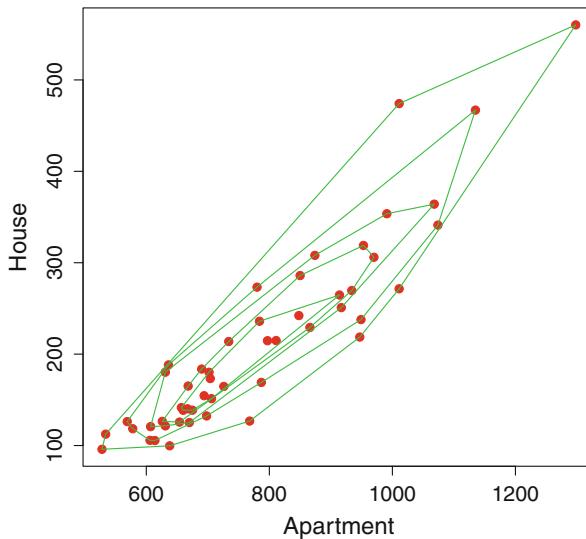


Figure 3.22: Five peeling convex hulls of the housing data

(b) The *violin plot* is an improvement over the boxplot. Read about violin plots in the help file under the name `panel.violin` and examine this data. Explain the various features of these graphical displays and use them to describe additional features of this data.

- 3.5 (a) Consider a set of randomly generated faces:

```
faces(matrix(rnorm(192), 16, 12), main="Random Faces")
```

What is the tendency for us to identify patterns and similar-looking individuals in such a sample? Is this a good feature or a shortcoming of the method?

(b) Similarly, generate randomly distributed data and plot this using `pairs()` with `panel.smooth`. Again, what is the tendency for us to see patterns when there is no reason for these to exist?

- 3.6 The `bvbox` in the `MVA` library produces the bivariate boxplot appearing in Fig. 3.10. Modify this code to create a new program with more options for the graphical output. Copy the program code into a text editor and add options to change the colors, line types, and line widths of the ellipses and the regression lines. See Fig. 6.1 for an example of how the output might look.

- 3.7 Write a program in R that draws and peels away successive convex hulls in bivariate data. As an example, five convex hulls of the housing data

are displayed in Fig. 3.22. Hint: recall that a negative subscript in a list removes that item.

- 3.8 The **anorexia** data set in the MASS library lists the pre- and posttreatment weights of 72 young women with anorexia. There were three different treatments: control or no treatment, behavioral coaching, and family intervention. Find a suitable way to display this data using colors to identify the three different interventions.

Chapter 4

Basic Linear Algebra

MANY OPERATIONS performed on multivariate data are facilitated using vector and matrix notation. In this chapter we introduce the basic operations and properties of these and then show how to perform them in R.

4.1 Apples and Oranges

A single numerical value is called a *scalar*, as in the price of an apple. With multivariate data we like to talk about several different values at the same time. We can combine these as a *2-tuple* (apple, banana), a *3-tuple* (apple, banana, orange), and so on up to the more general *n-tuple*. This collection of information would be referred to as the *vector* of fruit prices. The order of the items in the list matters, of course.

Mathematically, a vector is expressed as a vertical list:

$$\text{fruit price} = \begin{pmatrix} \text{Apple price} \\ \text{Banana price} \\ \text{Orange price} \end{pmatrix}$$

Sometimes it is convenient to express this as a horizontal, rather than a vertical, list. To do this we have the *transpose* operation giving

$$\text{fruit price}' = (\text{Apple price}, \text{Banana price}, \text{Orange price}),$$

where the prime (') exponent indicates the transpose.

Notice how we also use a **bold font** to indicate a vector, to distinguish it from a scalar which appears in a normal font.

Vectors are added component-wise. So, for example, if each fruit has its own tax

$$\text{fruit tax} = \begin{pmatrix} \text{Apple tax} \\ \text{Banana tax} \\ \text{Orange tax} \end{pmatrix}$$

then

$$\text{fruit price} + \text{fruit tax} = \begin{pmatrix} \text{Apple price} + \text{Apple tax} \\ \text{Banana price} + \text{Banana tax} \\ \text{Orange price} + \text{Orange tax} \end{pmatrix}.$$

Suppose we have a shopping list with the quantities of each fruit:

$$\text{fruit quantity} = \begin{pmatrix} \# \text{ of Apples} \\ \# \text{ of Bananas} \\ \# \text{ of Oranges} \end{pmatrix}.$$

The scalar-valued *inner product* of two vectors is defined by

$$\begin{aligned} \text{fruit quantity}' \text{ fruit price} &= \# \text{ of Apples} \times \text{Apple price} \\ &+ \# \text{ of Bananas} \times \text{Banana price} \\ &+ \# \text{ of Oranges} \times \text{Orange price} \end{aligned}$$

which we would interpret as our total price of the fruit.

Notice that the inner product is a linear operator in the sense that

$$\begin{aligned} \text{fruit quantity}'(\text{fruit price} + \text{fruit tax}) &= \text{fruit quantity}' \text{ fruit price} \\ &+ \text{fruit quantity}' \text{ fruit tax} \end{aligned}$$

so that the price we pay for our groceries, including the taxes, can be calculated in either manner.

We can combine all this information about fruit in a matrix:

$$\text{FRUIT} = \begin{pmatrix} \text{Apple price} & \text{Apple tax} & \text{Apple quantity} \\ \text{Banana price} & \text{Banana tax} & \text{Banana quantity} \\ \text{Orange price} & \text{Orange tax} & \text{Orange quantity} \end{pmatrix}.$$

where we interpret the columns as prices, taxes, and quantities, respectively, and the rows correspond to the different fruit.

The notation for a matrix always appears in a **CAPITAL BOLD** font.

The transpose of the **FRUIT** matrix reverses the roles of columns and rows so

$$\mathbf{FRUIT}' = \begin{pmatrix} \text{Apple price} & \text{Banana price} & \text{Orange price} \\ \text{Apple tax} & \text{Banana tax} & \text{Orange tax} \\ \text{Apple quantity} & \text{Banana quantity} & \text{Orange quantity} \end{pmatrix}.$$

Again we use the prime ('') to perform a transpose.

When it comes to multivariate data, it is very handy to talk about the data arranged in columns and rows such as in this example. Data arranged in tables such as in the examples of Chap. 1 will list observed items as rows and attributes or variables measured on each as columns. In matrix notation, we can easily describe arithmetic operations performed in parallel, on the whole data set in a more compact manner.

4.2 Vectors

Let's begin with the basic arithmetic operations for vectors and (in the following section) matrices. In Sect. 4.5 we move on to more advanced matrix properties.

A *scalar* is a single numerical value and a *vector* is a *n-tuple* or collection of numerical values listed in a prescribed order.

We use **bold**, lower case letters to denote vectors. The notation for a vector \mathbf{x} is

$$\mathbf{x} = \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix}$$

and the *transpose* is $\mathbf{x}' = (x_1, x_2, \dots, x_n)$. Two vectors are equal if they have an equal number of components and are equal in each of these components.

A vector \mathbf{x} can be multiplied by a scalar constant c

$$c\mathbf{x} = \begin{pmatrix} cx_1 \\ cx_2 \\ \vdots \\ cx_n \end{pmatrix}.$$

The sum of two vectors \mathbf{x} and $\mathbf{y}' = (y_1, y_2, \dots, y_n)$ is

$$\mathbf{x} + \mathbf{y} = \mathbf{y} + \mathbf{x} = \begin{pmatrix} x_1 + y_1 \\ x_2 + y_2 \\ \vdots \\ x_n + y_n \end{pmatrix}.$$

As with scalar arithmetic, vector addition is commutative so

$$\mathbf{x} + \mathbf{y} = \mathbf{y} + \mathbf{x}.$$

Vector addition is only defined when the vectors have the same length. The *zero vector* $\mathbf{0}' = (0, 0, \dots, 0)$ with all zero components is the additive identity. That is,

$$\mathbf{x} + \mathbf{0} = \mathbf{0} + \mathbf{x} = \mathbf{x}.$$

The number of components in the zero vector is usually not specified, but is assumed, so that the arithmetic operation is defined whenever it appears.

Vector subtraction is similarly defined:

$$\mathbf{x} - \mathbf{y} = \begin{pmatrix} x_1 - y_1 \\ x_2 - y_2 \\ \vdots \\ x_n - y_n \end{pmatrix}$$

and $\mathbf{x} - \mathbf{0} = \mathbf{x}$.

The scalar-valued *inner product* is defined by

$$\mathbf{x}' \mathbf{y} = \sum_{i=1}^n x_i y_i. \quad (4.1)$$

Again, this operation is only defined for vectors of the same length.

The inner product is symmetric in its arguments so that

$$\mathbf{x}' \mathbf{y} = \mathbf{y}' \mathbf{x}$$

and is a linear operator so that

$$\mathbf{x}'(\mathbf{y} + \mathbf{z}) = \mathbf{x}' \mathbf{y} + \mathbf{x}' \mathbf{z}. \quad (4.2)$$

As an example of the operations defined up to this point, suppose

$$\mathbf{x} = \begin{pmatrix} 1 \\ 5 \\ 2 \end{pmatrix} \text{ and } \mathbf{y} = \begin{pmatrix} 3 \\ -1 \\ 6 \end{pmatrix}.$$

Then we have

$$\begin{aligned} \mathbf{x}' &= (1, 5, 2), \\ 3\mathbf{x} &= \begin{pmatrix} 3 \\ 15 \\ 6 \end{pmatrix}, \\ \mathbf{x} + \mathbf{y} &= \begin{pmatrix} 4 \\ 4 \\ 8 \end{pmatrix}, \end{aligned}$$

and

$$\mathbf{x}'\mathbf{y} = (1 \times 3) + (5 \times -1) + (2 \times 6) = 10.$$

Two vectors with an inner product equal to zero are said to be *orthogonal*. The zero vector $\mathbf{0}$ is orthogonal to all other vectors.

A pair of vectors \mathbf{x}_1 and \mathbf{x}_2 are said to be *linearly dependent* if there exists a scalar c such that $\mathbf{x}_1 = c\mathbf{x}_2$.

More generally, a set of vectors $\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n$ are linearly dependent if there exist scalars c_1, c_2, \dots, c_n , not all zero, such that

$$c_1\mathbf{x}_1 + c_2\mathbf{x}_2 + \dots + c_n\mathbf{x}_n = \mathbf{0} \quad (4.3)$$

The implication of linear dependence is that at least one vector can be expressed as a linear combination of the others. Conversely, vectors are said to be *mutually independent* if (4.3) does not hold. That is, if vectors $\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n$ are mutually independent and if (4.3) holds then we must have $c_1 = c_2 = \dots = c_n = 0$. Mutually orthogonal vectors are linearly independent, but linearly independent vectors need not be orthogonal. See Exercise 4.5.

The *Euclidean*¹ *length* (or more simply, the *length*) of a vector is the square root of the inner product with itself:

$$\|\mathbf{x}\| = (\mathbf{x}'\mathbf{x})^{1/2} = \sqrt{x_1^2 + x_2^2 + \dots + x_n^2}. \quad (4.4)$$

¹Euclid, mathematician in ancient Greece, lived around 300 BCE.

In a two-dimensional plane, the Euclidean length is how we interpret distance. As an example, if we travel to a point that is one unit east and two units north away from where we began, then the distance (as the crow flies) is $\sqrt{5}$, just as we would determine using the result of Pythagoras.

4.3 Basic Matrix Arithmetic

A matrix generalizes a vector to an array of values. We use bold **CAPITAL** letters to denote matrices. An $n \times m$ matrix \mathbf{X} having n rows and m columns has elements indexed by two subscripts:

$$\mathbf{X} = \begin{pmatrix} x_{11} & x_{12} & \dots & x_{1m} \\ x_{21} & x_{22} & \dots & x_{2m} \\ \vdots & \vdots & \ddots & \vdots \\ x_{n1} & x_{n2} & \dots & x_{nm} \end{pmatrix}.$$

The transpose \mathbf{X}' of a matrix \mathbf{X} takes its values and turns it on its upper-left and lower-right diagonal. The transpose of an $n \times m$ matrix has dimensions $m \times n$. The transpose has the effect of reversing the subscripts so that

$$\mathbf{X}' = \begin{pmatrix} x_{11} & x_{21} & \dots & x_{n1} \\ x_{12} & x_{22} & \dots & x_{n2} \\ \vdots & \vdots & \ddots & \vdots \\ x_{1m} & x_{2m} & \dots & x_{nm} \end{pmatrix}.$$

A matrix is said to be *symmetric* if it is equal to its transpose, i.e., $\mathbf{X}' = \mathbf{X}$. Only square matrices can be symmetric.

A matrix \mathbf{X} can be multiplied by a scalar c :

$$c\mathbf{X} = \begin{pmatrix} cx_{11} & cx_{12} & \dots & cx_{1m} \\ cx_{21} & cx_{22} & \dots & cx_{2m} \\ \vdots & \vdots & \ddots & \vdots \\ cx_{n1} & cx_{n2} & \dots & cx_{nm} \end{pmatrix}$$

and two matrices with the same dimensions can be added:

$$\mathbf{X} + \mathbf{Y} = \begin{pmatrix} x_{11} + y_{11} & x_{12} + y_{12} & \dots & x_{1m} + y_{1m} \\ x_{21} + y_{21} & x_{22} + y_{22} & \dots & x_{2m} + y_{2m} \\ \vdots & \vdots & \ddots & \vdots \\ x_{n1} + y_{n1} & x_{n2} + y_{n2} & \dots & x_{nm} + y_{nm} \end{pmatrix}.$$

We can also define matrix multiplication. As with the inner product for vectors, the dimensions must be correct for matrix multiplication to be defined. If \mathbf{X} is $n \times m$ and \mathbf{Y} is $m \times p$ then

$$\underset{(n \times p)}{\mathbf{Z}} = \underset{(n \times m)}{\mathbf{X}} \underset{(m \times p)}{\mathbf{Y}}$$

is defined.

Notice that the “middle” dimensions of \mathbf{X} and \mathbf{Y} need to be equal. That is, we can multiply the matrices \mathbf{X} and \mathbf{Y} if the number of columns of \mathbf{X} is equal to the number of rows in \mathbf{Y} . The elements of the resulting matrix product \mathbf{Z} has dimensions $n \times p$. The (ij) th element of \mathbf{Z} is equal to the inner product of the i th row of \mathbf{X} and the j th column of \mathbf{Y} .

As an example of these matrix operations suppose

$$\mathbf{X} = \begin{pmatrix} 5 & -1 & 3 \\ 2 & 4 & 1 \\ 3 & 1 & 2 \\ -2 & 5 & 2 \end{pmatrix}$$

and

$$\mathbf{Y} = \begin{pmatrix} 2 & 3 \\ 4 & 1 \\ 3 & 5 \end{pmatrix}.$$

Then

$$3\mathbf{X} = \begin{pmatrix} 15 & -3 & 9 \\ 6 & 12 & 3 \\ 9 & 3 & 6 \\ -6 & 15 & 6 \end{pmatrix},$$

$$\mathbf{Y}' = \begin{pmatrix} 2 & 4 & 3 \\ 3 & 1 & 5 \end{pmatrix},$$

and

$$\begin{aligned} \mathbf{XY} &= \begin{pmatrix} (5 \times 2) + (-1 \times 4) + (3 \times 3) & (5 \times 3) + (-1 \times 1) + (3 \times 5) \\ (2 \times 2) + (4 \times 4) + (1 \times 3) & (2 \times 3) + (4 \times 1) + (1 \times 5) \\ (3 \times 2) + (1 \times 4) + (2 \times 3) & (3 \times 3) + (1 \times 1) + (2 \times 5) \\ (-2 \times 2) + (5 \times 4) + (2 \times 3) & (-2 \times 3) + (5 \times 1) + (2 \times 5) \end{pmatrix} \\ &= \begin{pmatrix} 15 & 29 \\ 23 & 15 \\ 16 & 20 \\ 22 & 9 \end{pmatrix}. \end{aligned}$$

In this example, we see that matrix multiplication is not *commutative*. That is, \mathbf{XY} is not necessarily equal to \mathbf{YX} nor is \mathbf{YX} necessarily defined. See also Exercise 4.4.

A square *diagonal matrix* has zero entries off the main diagonal:

$$\text{Diag}(a_1, a_2, \dots, a_n) = \begin{pmatrix} a_1 & 0 & \cdots & 0 \\ 0 & a_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & a_n \end{pmatrix}.$$

The *identity matrix* \mathbf{I} ,

$$\mathbf{I} = \begin{pmatrix} 1 & 0 & \cdots & 0 \\ 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 1 \end{pmatrix},$$

is a square, symmetric matrix with 1s running down the diagonal and all other entries equal to zero.

The identity matrix has the property that it has no effect when multiplied by another matrix:

$$\mathbf{IX} = \mathbf{X}$$

just as multiplying by 1 in scalar arithmetic.

The dimensions of the identity matrix \mathbf{I} are usually inferred from context. In this last equation, the dimensions of \mathbf{I} have to be the same as the first dimension of \mathbf{X} in order for this matrix multiplication to be defined. To make this point in a different way, if we assume that the $(n \times m)$ matrix \mathbf{X} is not square then we can also write somewhat ambiguously

$$\begin{matrix} \mathbf{I} \\ (n \times n) \end{matrix} \quad \begin{matrix} \mathbf{X} \\ (n \times m) \end{matrix} \quad = \quad \begin{matrix} \mathbf{X} \\ (n \times m) \end{matrix} \quad \begin{matrix} \mathbf{I} \\ (m \times m) \end{matrix} \quad = \quad \begin{matrix} \mathbf{X} \\ (n \times m) \end{matrix},$$

where the two appearances of \mathbf{I} represent different sized matrices within the same mathematical expression. For this reason, we will sometimes include the dimensions of matrices in equations when this removes the confusion.

4.4 Matrix Operations in R

The basic mathematical operations for vectors and matrices described in Sects. 4.2 and 4.3 can easily be implemented in R. The advanced matrix functions covered in Sect. 4.5 will be introduced using R to facilitate the discussion. The advanced operations involving determinants, inverses, and eigenvalues,

for examples, are best described in terms of their computational procedures. The use of these procedures will be more fully appreciated in subsequent chapters.

We add two vectors $\mathbf{x} + \mathbf{y}$ using the same notation in R: namely $\mathbf{x} + \mathbf{y}$. The inner product² of a vector with its self $\mathbf{x}'\mathbf{x}$ is computed by omitting the second argument: `crossprod(x)`. All of these operations are only defined when \mathbf{x} and \mathbf{y} have the same length. The following dialog illustrates these operations:

```
> x <- seq(2,8,2)
> x
```

```
[1] 2 4 6 8
```

```
> y <- 4:1
> y
```

```
[1] 4 3 2 1
```

```
> x+y
```

```
[1] 6 7 8 9
```

```
> crossprod(x,y)
```

```
[,1]
[1,] 40
```

```
> crossprod(x)
```

```
[,1]
[1,] 120
```

Notice that the `crossprod` function returns a 1×1 matrix, not a scalar. The `*` operation for vectors performs a component-wise product of vectors:

```
> x * y
[1] 8 12 12 8
```

and not the vector cross product.

²There should be no confusion here with a totally different operation familiar to physicists and engineers called the *vector cross product* that is only valid for vectors in three dimensions. Of two vectors $\mathbf{x}'\mathbf{y}$ is defined in (4.1) and computed using `crossprod(x,y)`.

The *outer product* $\mathbf{x}\mathbf{x}'$ is an $n \times n$ matrix. This is computed using the `%o%` operator as in `x %o% x`. The vector outer product operation is illustrated in the following dialog:

```
> x
[1] 2 4 6 8
> x %o% x
[,1] [,2] [,3] [,4]
[1,]    4     8    12    16
[2,]    8    16    24    32
[3,]   12    24    36    48
[4,]   16    32    48    64
```

Notice how R prints the matrix values, bordered by a useful index notation. The heading for each row and column reminds us of the subscripts we would use to address that row or column. So, for example, we have

```
> (x %o% x)[, 3]
[1] 12 24 36 48
> (x %o% x)[2,]
[1] 8 16 24 32
```

showing how we access the third column and second row of the matrix outer product, respectively. Both of these are treated as vectors.

We can easily build special types of matrices using `diag` to form a diagonal matrix and `matrix` to build a matrix with specified values.

So, for examples,

```
> diag(1, 4, 4)
[,1] [,2] [,3] [,4]
[1,]    1     0     0     0
[2,]    0     1     0     0
[3,]    0     0     1     0
[4,]    0     0     0     1
```

is a 4×4 identity matrix and

```
> matrix(1, 4, 4)
```

```
[,1] [,2] [,3] [,4]
[1,] 1 1 1 1
[2,] 1 1 1 1
[3,] 1 1 1 1
[4,] 1 1 1 1
```

is a 4×4 matrix of all 1s.

We can also construct a 4×4 matrix with the counts $1, \dots, 16$:

```
> matrix(1 : 16, 4, 4)

[,1] [,2] [,3] [,4]
[1,] 1 5 9 13
[2,] 2 6 10 14
[3,] 3 7 11 15
[4,] 4 8 12 16
```

running down columns.

If we wanted the counts to run across the rows, we can transpose this matrix with the `t` function

```
> t(matrix(1 : 16, 4, 4))

[,1] [,2] [,3] [,4]
[1,] 1 2 3 4
[2,] 5 6 7 8
[3,] 9 10 11 12
[4,] 13 14 15 16
```

The `diag` function can be used to both build diagonal matrices and extract the diagonal elements of an existing matrix:

```
> diag( t(matrix(1 : 16, 4, 4)))

[1] 1 6 11 16
```

We can add two matrices with `A + B` and multiply element-by-element `A * B`. These operations are valid only when `A` and `B` have the same dimensions:

```
> A

[,1] [,2] [,3] [,4]
[1,] 1 2 3 4
[2,] 2 4 6 8
[3,] 3 6 9 12

> B
```

```
[,1] [,2] [,3] [,4]
[1,] 2 4 6 8
[2,] 4 8 12 16
[3,] 6 12 18 24
```

> A + B

```
[,1] [,2] [,3] [,4]
[1,] 3 6 9 12
[2,] 6 12 18 24
[3,] 9 18 27 36
```

> A * B

```
[,1] [,2] [,3] [,4]
[1,] 2 8 18 32
[2,] 8 32 72 128
[3,] 18 72 162 288
```

The multiplication of two matrices is accomplished by writing A %*% B. This operation is illustrated as follows:

> A

```
[,1] [,2] [,3] [,4]
[1,] 1 2 3 4
[2,] 2 4 6 8
[3,] 3 6 9 12
```

> t(B)

```
[,1] [,2] [,3]
[1,] 2 4 6
[2,] 4 8 12
[3,] 6 12 18
[4,] 8 16 24
```

> A %*% t(B)

```
[,1] [,2] [,3]
[1,] 60 120 180
[2,] 120 240 360
[3,] 180 360 540
```

Recall that the product of a 3×4 matrix and a 4×3 matrix is a 3×3 matrix.

We can also solve linear equations in R. Consider the system of linear equations

$$a_{11}x_1 + a_{12}x_2 + \cdots + a_{1,n}x_n = b_1$$

$$a_{21}x_1 + a_{22}x_2 + \cdots + a_{2,n}x_n = b_2$$

$$\vdots \quad \vdots \quad \vdots \quad \vdots$$

$$a_{n1}x_1 + a_{n2}x_2 + \cdots + a_{n,n}x_n = b_n$$

These equations can be written in the more compact, matrix notation

$$\mathbf{Ax} = \mathbf{b}$$

for known matrix $\mathbf{A} = \{a_{ij}\}$ and vector $\mathbf{b} = \{b_i\}$. We want to solve these equations for vector $\mathbf{x} = \{x_i\}$ satisfying relationships. The solution in R is obtained by `solve(A, b)`.

As a numerical example, suppose $\mathbf{b} = \{9, 7, 5, 3\}$ and \mathbf{A} is a 4×4 matrix of random values that were generated uniformly between 0 and 1.

```
> (b <- c(9, 7 5, 3)
[1] 9 7 5 3
> (A <- matrix(runif(16),c(4,4)))
[,1]      [,2]      [,3]      [,4]
[1,] 0.6692485 0.5644291 0.4361838 0.7869338
[2,] 0.9458449 0.4710188 0.8120588 0.5741354
[3,] 0.3366968 0.1971159 0.3774943 0.3954844
[4,] 0.1841985 0.9128133 0.3773530 0.2363638
> solve(A,b)
[1] -1.9162283 -0.5453288  2.7192532 11.9503542
```

Algebraically, we can write $\mathbf{x} = \mathbf{A}^{-1}\mathbf{b}$ where \mathbf{A}^{-1} is the inverse of \mathbf{A} . The inverse \mathbf{A}^{-1} can be obtained in R using `solve(A)`:

```
> solve(A)
[,1]      [,2]      [,3]      [,4]
[1,] 1.4205610 2.15995584 -5.478218 -0.8099599
[2,] 0.5768595 0.04273936 -1.881024 1.1229594
[3,] -2.8628620 0.01850019 5.301603 0.6158308
[4,] 1.2357195 -1.87784541 3.069534 -0.4579570
```

The matrix inverse operation is explained in Sect. 4.5.2.

In the next section, we look at more advanced matrix operations. These are best introduced along with the corresponding R code.

4.5 Advanced Matrix Operations

The methods described in this section make the leap to beyond what a human could reasonably accomplish with pencil and paper alone. These concepts are important and are needed for subsequent chapters. To ease the discussion, we include the R code that accomplishes these tasks in order to show the reader that these methods can be implemented with a minimum amount of effort for any specific set of numerical values. The reader wishing to learn more about these advanced properties of matrices is referred to the classic textbook by Lang (2010).³ Golub and Van Loan (1983) is another excellent reference for learning more about the computational aspects of matrix operations

4.5.1 Determinants

The *trace* of a square matrix is the sum of its diagonal elements. The *determinant* is another numerical value associated with a square matrix.

As an example, consider the 2×2 matrix

$$\mathbf{A} = \begin{pmatrix} a & b \\ c & d \end{pmatrix}.$$

The trace of \mathbf{A} is $a + d$ and the determinant is

$$\text{Det}(\mathbf{A}) = ad - bc. \quad (4.5)$$

For another example, the trace of the 3×3 matrix

$$\mathbf{B} = \begin{pmatrix} a & b & c \\ d & e & f \\ g & h & i \end{pmatrix}$$

is $a + e + i$ and the determinant is

$$\text{Det}(\mathbf{B}) = a(ei - fh) + b(fg - id) + c(dh - eg). \quad (4.6)$$

As we can see from these two examples, the determinant is a polynomial in the matrix elements. These expressions quickly grow in complexity with the size of the matrix so, in general, it is best to find determinants numerically in R as in this example:

```
> (x <- matrix(rnorm(25), 5, 5))
```

³Serge Lang (1927–2005) French-born, American mathematician.

```

[,1]      [,2]      [,3]      [,4]      [,5]
[1,] 0.8773400 -0.5657782 1.7634118 1.8728550 0.9928573
[2,] 0.1017325 -0.3619644 0.8324341 1.4387591 0.2699057
[3,] 0.8026365 -0.6943805 -0.8926545 1.2955549 1.7452754
[4,] 0.9237657 1.2665737 -0.3078966 -0.2517838 1.0968427
[5,] 1.8795828 -0.5785956 -0.3837322 1.2007208 0.7950999

> det(x)

[1] -7.170792

```

In this example, we use R to generate a 5×5 matrix (denoted as \mathbf{x}) whose elements are sampled from a standard normal distribution. The `det(x)` function returns the determinant of this matrix.

Some special cases of determinants are worth mentioning. The determinant of a diagonal matrix is the product of its diagonal entries. So we have

$$\text{Det}(\text{Diag}(x_1, x_2, \dots, x_n)) = \text{Det} \begin{pmatrix} x_1 & 0 & \cdots & 0 \\ 0 & x_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & x_n \end{pmatrix} = x_1 x_2 \cdots x_n.$$

Similarly, the determinant of the identity matrix \mathbf{I} is equal to 1 regardless of its size.

The determinant of a matrix is equal to the determinant of its transpose so that

$$\text{Det}(\mathbf{A}) = \text{Det}(\mathbf{A}').$$

The determinant of a scalar c multiple of an $n \times n$ matrix \mathbf{A} satisfies

$$\text{Det}(c\mathbf{A}) = c^n \text{Det}(\mathbf{A}).$$

The determinant of a product of square matrices is the product of the individual determinants:

$$\text{Det}(\mathbf{AB}) = \text{Det}(\mathbf{A}) \text{Det}(\mathbf{B}).$$

The *rank* of a matrix is the maximum number of linearly independent rows and columns when these are considered as vectors. A square matrix whose rank is equal to the number of rows (or columns) is said to be of *full rank* or *nonsingular*. A square matrix that is less than full rank has a determinant of zero and is said to be *singular*.

4.5.2 Matrix Inversion

The *inverse* of a square matrix \mathbf{A} (when it exists) is denoted by \mathbf{A}^{-1} and has the property that the product

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

is equal to the identity matrix.

Let us draw comparisons between inverses of matrices and the parallel in scalar operations. The inverse of a matrix is analogous to what the reciprocal is to a scalar. The scalar 1 is its own reciprocal, just as the identity matrix \mathbf{I} is its own inverse. Corresponding to the scalar value zero, which does not have a reciprocal, a matrix with a zero determinant does not have an inverse. Conversely, any square matrix with a nonzero determinant will have an inverse.

In the 2×2 matrix

$$\mathbf{A} = \begin{pmatrix} a & b \\ c & d \end{pmatrix}$$

the inverse is given by

$$\mathbf{A}^{-1} = \frac{1}{ad - bc} \begin{pmatrix} d & -b \\ -c & a \end{pmatrix} \quad (4.7)$$

provided the determinant $ad - bc$ is nonzero.

The inverse of the 3×3 matrix

$$\mathbf{B} = \begin{pmatrix} a & b & c \\ d & e & f \\ g & h & i \end{pmatrix}$$

is given by

$$\mathbf{B}^{-1} = \frac{1}{\text{Det}(\mathbf{B})} \begin{pmatrix} A & B & C \\ D & E & F \\ G & H & I \end{pmatrix},$$

where $\text{Det}(\mathbf{B})$ is the determinant given in (4.6) and

$$\begin{aligned} A &= ei - fh & B &= ch - bi & C &= bf - ce \\ D &= fg - di & E &= ai - cg & F &= cd - af \\ G &= dh - eg & H &= bg - ah & I &= ae - bd \end{aligned}$$

This inverse exists only when the determinant is nonzero.

As with a matrix determinant, we see that the mathematical complexity of finding the inverse increases greatly with the size of the matrix. Fortunately for us, matrix inverses can be calculated numerically in R with little effort on our part. The following example illustrates this, continuing with the same matrix \mathbf{x} generated earlier in this section to illustrate the determinant.

Here is the \mathbf{x} matrix again:

```
> x
```

	[,1]	[,2]	[,3]	[,4]	[,5]
[1,]	0.8773400	-0.5657782	1.7634118	1.8728550	0.9928573
[2,]	0.1017325	-0.3619644	0.8324341	1.4387591	0.2699057
[3,]	0.8026365	-0.6943805	-0.8926545	1.2955549	1.7452754
[4,]	0.9237657	1.2665737	-0.3078966	-0.2517838	1.0968427
[5,]	1.8795828	-0.5785956	-0.3837322	1.2007208	0.7950999

We use the `solve()` function to find the inverse:

```
> solve(x)
```

	[,1]	[,2]	[,3]	[,4]	[,5]
[1,]	0.1588468	-0.3984637	-0.33113613	0.04831542	0.59711329
[2,]	-0.5552320	1.1185653	-0.28424175	0.69540112	-0.02176659
[3,]	0.6985182	-0.5875821	-0.19048830	-0.04702547	-0.18979125
[4,]	-0.6586654	1.4906931	-0.04002048	0.18067946	0.15505461
[5,]	0.5522533	-0.7788176	0.54445190	0.09628027	-0.49543987

Just to check, we can multiply the matrix \mathbf{x} by its inverse:

```
> x %*% solve(x)
```

	[,1]	[,2]	[,3]	[,4]	[,5]
[1,]	1.000000e+00	-6.661338e-16	1.110223e-16	4.163336e-17	-1.110223e-16
[2,]	1.665335e-16	1.000000e+00	5.551115e-17	2.775558e-17	0.000000e+00
[3,]	0.000000e+00	-2.220446e-16	1.000000e+00	1.387779e-16	-1.110223e-16
[4,]	1.110223e-16	-2.220446e-16	0.000000e+00	1.000000e+00	-1.110223e-16
[5,]	-5.551115e-17	1.110223e-16	1.110223e-16	-1.387779e-17	1.000000e+00

The resulting product is very nearly an identity matrix: There are 1s running down the diagonal and the off-diagonal entries are either zero or quantities within rounding error of zero (about $\pm 10^{-16}$). This is another reminder that performing numerical computations will usually result in very small numerical errors that (hopefully) do not greatly distort the final answers. The study of numerical algorithms and the corresponding rounding errors is examined in the mathematical field of *numerical analysis*.

A useful relationship between matrix determinants and inverses is

$$\text{Det}(\mathbf{A}^{-1}) = 1/\text{Det}(\mathbf{A}).$$

The inverse of a matrix is not always needed when it is part of a more complex mathematical expression. As an example of avoiding the use of the matrix inverse, suppose we want to compute the quadratic form $\mathbf{b}'\mathbf{A}^{-1}\mathbf{b}$ in R. (We will need to calculate similar expressions when we evaluate the multivariate normal density function, given in (7.2).) We can obtain this in R as

```
b %*% solve(A,b)
```

without having to separately find the inverse matrix \mathbf{A}^{-1} .

There are closely related matrix operations that include inverses when these exist, and other similar properties when they don't. These generalized inverses of matrices are described in Sect. 4.5.5.

4.5.3 Eigenvalues and Eigenvectors

Let us introduce another advanced topic in matrix algebra. Every square matrix has an associated set of *eigenvalues* and *eigenvectors*. If \mathbf{A} is a square matrix, then consider the linear equation

$$\mathbf{A}\mathbf{x} = \lambda\mathbf{x} \quad (4.8)$$

for some eigenvector \mathbf{x} and a scalar eigenvalue λ .

Intuitively, (4.8) says that the effect of multiplying the vector \mathbf{x} by \mathbf{A} is the same as multiplying it by a scalar. Multiplication of a vector by a scalar results in changing its length by either stretching ($\lambda > 1$), shrinking ($0 < \lambda < 1$), or reversing direction by changing its signs ($\lambda < 0$). A vector \mathbf{x} satisfying (4.8) is called an eigenvector of \mathbf{A} and the value λ corresponding to \mathbf{x} is called the eigenvalue. If one solution exists to (4.8) then there are an infinite number of these solutions. If (\mathbf{x}, λ) is a solution to (4.8), then, for example, $(2\mathbf{x}, \lambda/2)$ is also a solution. See Exercise 4.10 for more details. One useful way to avoid this ambiguity in R is to find a set of eigenvectors \mathbf{x} that are all of unit length and are mutually orthogonal. Vector length is defined in (4.4).

The identity matrix \mathbf{I} leaves vectors unchanged

$$\mathbf{I}\mathbf{x} = \mathbf{x}$$

so the eigenvalues λ s of the identity matrix are all equal to 1, and every vector \mathbf{x} is an eigenvector of the identity matrix.

Here are some useful properties of eigenvalues in relation to other topics already discussed. The eigenvalues $\lambda_1, \lambda_2, \dots, \lambda_n$ of an $n \times n$ matrix \mathbf{A} are related to the trace

$$\text{Trace}(\mathbf{A}) = \lambda_1 + \lambda_2 + \dots + \lambda_n \quad (4.9)$$

and the determinant

$$\text{Det}(\mathbf{A}) = \lambda_1 \lambda_2 \cdots \lambda_n . \quad (4.10)$$

The *characteristic polynomial*

$$p(\lambda) = \text{Det}(\mathbf{A} - \lambda \mathbf{I}) \quad (4.11)$$

is a polynomial in λ and the roots of the equation $p(\lambda) = 0$ determine the eigenvalues. In practice, R uses a different algorithm to find eigenvalues.

An $n \times n$ matrix will have n eigenvalues. Just as a polynomial may have multiple roots, some of the eigenvalues may be repeated, corresponding to multiple roots⁴ of $p(\lambda) = 0$. A polynomial may have complex roots, and the eigenvalues may be *complex numbers*. Complex numbers are expressible as $\alpha + \beta i$ where $i^2 = -1$. Complex roots will appear as *complex conjugates*. That is, if $\alpha + \beta i$ is a complex root of a polynomial with real-valued coefficients, then $\alpha - \beta i$ will also be a root of this polynomial.

Eigenvalues and eigenvectors can be obtained in R using

```
evs <- eigen (A)
```

for a symmetric matrix \mathbf{A} . Then `evs$val` is the vector of eigenvalues and `evs$vec` are the corresponding eigenvectors.

For very large matrices we might only require the eigenvalues. In which case, to save computing time, use

```
eigen(A, only.values =TRUE)$values
```

and only the eigenvalues are computed.

In R we can calculate the eigenvalues of the 5×5 matrix \mathbf{x} examined previously,

```
> eigen(x)$values
[1] 3.502643+0.0000i -1.124313+1.140676i -1.124313-1.140676i
[4] -1.589936+0.0000i  0.501957+0.0000i
```

In this numerical example we see that two of the five eigenvalues are complex conjugates. We also have

```
> prod(eigen(x)$values)
[1] -7.170792+0i
> det(x)
[1] -7.170792
```

⁴A quadratic equation, for example, always has two roots and we say that $x^2 = 0$ has a root at $x = 0$ of multiplicity two.

illustrating the equality of the determinant and the product of the eigenvalues as stated in (4.10).

A square matrix \mathbf{A} is said to be *positive definite* if for every nonzero vector \mathbf{x} we have

$$\mathbf{x}' \mathbf{A} \mathbf{x} > 0$$

and nonnegative definite if $\mathbf{x}' \mathbf{A} \mathbf{x} \geq 0$.

See Exercise 4.11 for some properties of positive definite matrices and how to identify these. A useful property of positive definite matrices is that all of their eigenvalues are real and nonnegative.

4.5.4 Diagonalizable Matrices

A square matrix \mathbf{A} is said to be *diagonalizable* if it is expressible as

$$\mathbf{A} = \mathbf{X} \mathbf{D} \mathbf{X}^{-1} \quad (4.12)$$

for a diagonal matrix \mathbf{D} .

The numerical identification of the components of a diagonalizable matrix is very simple in R using the `eigen` function. The diagonal matrix \mathbf{D} in (4.12) is the diagonal matrix of the eigenvalues of \mathbf{A} . The eigenvectors provided by `eigen` are expressed as a matrix whose columns are mutually orthogonal vectors. That is, the \mathbf{X} in (4.12) is the matrix of eigenvectors.

Let us verify all of these statements in R. We begin by constructing a positive definite matrix called `apa`:

```
> (a <- matrix(rnorm(15), 5, 3)) # 5x3 matrix with random entries
[1,] [2,] [3,]
[1,] 0.4968134 -0.97565489 -0.6246059
[2,] 1.4922367 -0.10939041 -1.3471900
[3,] 1.5666928  1.82600963 -0.5806661
[4,] 1.3176006 -0.22123894 -1.2764140
[5,] -0.6809085 -0.07426517 -1.8700602

> (apa <- t(a) %*% a) # pos definite a'a matrix
[1,] [2,] [3,]
[1,] 8.210201 -4.913078 -2.044630
[2,] -4.913078  3.886116  1.608089
[3,] -2.044630  1.608089  0.733343
```

We find the eigenvalues and eigenvectors:

```
> (ax <- eigen(apa)) # eigenvalues and eigenvector as a matrix
```

```
$values
[1] 12.01145060  0.76052212  0.05768692

$vectors
[,1]      [,2]      [,3]
[1,] 0.8137227 -0.5811763 -0.009462608
[2,] -0.5363584 -0.7444990 -0.397543559
[3,] -0.2239980 -0.3285656  0.917534510
```

We can check that the matrix of eigenvectors is orthogonal:

```
> ax$vectors %*% t(ax$vectors)

[,1]      [,2]      [,3]
[1,] 1.000000e+00 -1.439820e-16 -1.908196e-17
[2,] -1.439820e-16  1.000000e+00 -1.665335e-16
[3,] -1.908196e-17 -1.665335e-16  1.000000e+00
```

which is very close to being an identity matrix, except for rounding errors in entries off the main diagonal.

Finally, we can verify the diagonalization process of (4.12)

```
> ax$vectors %*% diag(ax$values) %*% t(ax$vectors)

[,1]      [,2]      [,3]
[1,] 8.210201 -4.913078 -2.044630
[2,] -4.913078  3.886116  1.608089
[3,] -2.044630  1.608089  0.733343
```

returning the original matrix `apa` given above.

Properties of diagonalizable matrices are examined in Exercise 4.13.

4.5.5 Generalized Inverses

We may want to talk about matrices that are not invertable. The *generalized inverse* (or sometimes referred to as the *Moore–Penrose inverse*) corresponds to the matrix inverse when it exists and has a similar property when it doesn't. The generalized inverse \mathbf{A}^- of \mathbf{A} has the property that

$$\mathbf{A}\mathbf{A}^-\mathbf{A} = \mathbf{A}. \quad (4.13)$$

The generalized inverse is not unique. We show how to construct one in Exercise 4.12.

In R we can obtain a generalized inverse using the function `ginv` in the `MASS` library. Here is an example of its use. We begin by including the `MASS` package:

```

> library(MASS)
Attaching package: 'MASS'
> (z <- matrix(rnorm(15), 3, 5))
      [,1]      [,2]      [,3]      [,4]      [,5]
[1,] -1.019293 -1.1105161 -0.8835698 -1.56692865 0.3841926
[2,] -1.706265  0.5660277 -1.8179978  0.29282216 0.6521679
[3,]  0.556425 -0.5469372 -0.9581269  0.02266884 0.7840144
> (q <- t(z) %*% z)
      [,1]      [,2]      [,3]      [,4]      [,5]
[1,]  4.2599060 -0.1381812  3.4694761  1.1101408 -1.0681307
[2,] -0.1381812  1.8527737  0.4762167  1.8934466 -0.4863137
[3,]  3.4694761  0.4762167  5.0038186  0.8304212 -2.2762859
[4,]  1.1101408  1.8934466  0.8304212  2.5415241 -0.3932605
[5,] -1.0681307 -0.4863137 -2.2762859 -0.3932605  1.1876054

```

The matrix \mathbf{Z} is a 3×5 matrix of standard normal variates and

$$\mathbf{Q} = \mathbf{Z}' \mathbf{Z} \quad (4.14)$$

is a 5×5 symmetric, positive nonnegative definite matrix.

The eigenvalues of \mathbf{Q} should all be real and positive:

```

> eigen(q)$values
[1]  9.269311e+00  3.794984e+00  1.781333e+00 -1.290715e-16 -3.613510e-16

```

These eigenvalues are all real but the two smallest are within rounding error of zero because the 5×5 matrix \mathbf{Q} is of rank 3. See Exercise 4.8 for more details.

The generalized inverse of \mathbf{Q} is

```

> ginv(q)
      [,1]      [,2]      [,3]      [,4]      [,5]
[1,]  1.7573935  0.58990933  0.35307232 -0.18596570 -1.3996771
[2,]  0.5899093  0.33810377  0.06772675 -0.16774283 -0.5864543
[3,]  0.3530723  0.06772675  0.30962523 -0.09430042 -0.1568524
[4,] -0.1859657 -0.16774283 -0.09430042  0.13993652  0.2003483
[5,] -1.3996771 -0.58645427 -0.15685241  0.20034835  1.2424363

```

and we can check that this solution satisfies (4.13) using

```

> q %*% ginv(q) %*% q  -q
      [,1]      [,2]      [,3]      [,4]      [,5]
[1,] -2.220446e-16 -2.220446e-16 -1.942890e-16  4.440892e-16  2.498002e-16
[2,]  2.220446e-16  2.220446e-16 -1.526557e-16  2.220446e-16 -1.665335e-16
[3,] -1.387779e-16 -5.551115e-17 -8.881784e-16  4.440892e-16 -1.110223e-16
[4,]  2.220446e-16 -6.661338e-16  2.220446e-16  4.440892e-16  4.024558e-16
[5,]  1.110223e-16 -5.551115e-17  2.220446e-16  8.326673e-17  0.000000e+00

```

because this difference between

$$\mathbf{Q}' \mathbf{Q} (\mathbf{Q}' \mathbf{Q})^{-} \mathbf{Q}' \mathbf{Q}$$

and \mathbf{Q} is within rounding error (about 10^{-16}) of zero in all 25 elements of this 5×5 matrix.

4.5.6 Matrix Square Root

To end this section on advanced matrix operations, we note that there is also a *matrix square root*. By analogy to the scalar operation with the same name, for a square matrix \mathbf{Z} , is there a square matrix \mathbf{X} with the property that $\mathbf{X}^2 = \mathbf{Z}$? The answer is not every matrix \mathbf{Z} will have a square root, and when there is a square root, it may not be unique. When the square root exists, we write $\mathbf{X} = \mathbf{Z}^{1/2}$ using a familiar notation. See Exercise 4.14 to show that the square root may not be unique.

The matrix square root of a diagonal matrix with nonnegative entries $\{d_1, d_2, \dots, d_n\}$ is just the diagonal matrix with the square roots of the entries. That is, if

$$\mathbf{D} = \text{Diag}(d_1, d_2, \dots, d_n)$$

then

$$\mathbf{D}^{1/2} = \text{Diag}(d_1^{1/2}, d_2^{1/2}, \dots, d_n^{1/2}). \quad (4.15)$$

Just as there is no (real-valued) square root of a negative number, the square root only exists for nonnegative definite matrices. A nonnegative definite matrix will have no negative eigenvalues, so this provides an easy check for us in R.

An easy way to find the square root of a matrix is to express it as in the diagonalizable form given in (4.12) and use Exercise 4.12. The following R program includes a check for a nonnegative definite matrix:

```
msqrt <- function(a)  # matrix square root of positive definite matrix
{
  a.eig <- eigen(a)
  if ( min(a.eig$values) < 0) # check for positive definite
    warning("Matrix not positive definite")

  a.eig$vectors %*% diag(sqrt(a.eig$values)) %*% t(a.eig$vectors)
}
```

Let us provide a numerical example of this program and its use.

```
> (x <- matrix(rnorm(35), 7, 5)) # 7x5 matrix of normals
[,1]      [,2]      [,3]      [,4]      [,5]
[1,] 0.3798194 0.2114649 1.2076177 1.0124777 -1.49971761
[2,] 1.5125906 -0.9378462 0.4264717 1.3007917 -0.20352177
[3,] -0.2841299 -1.1639801 -2.0819616 -1.8749218 -0.52516122
[4,] -1.2978443 -1.0741596 1.7710925 -1.8331337 -0.54667111
[5,] 0.3154816 -0.7757654 2.4617252 -1.5434827 -0.63295035
[6,] -1.0363971 1.0355279 0.9133007 -0.6332664 0.41377237
[7,] -0.1596910 -0.9360372 1.5617765 -0.8657940 0.08946316
```

is a 7×5 of standard normals.

From this, we create a 5×5 symmetric, positive definite matrix:

```
> (z <- t(x) %*% x)      # pos definite, symmetric 5x5 matrix
[1,]      [,2]      [,3]      [,4]      [,5]
[1,]  5.3964714 -0.7819263 -1.022616  5.5716021 -0.6615621
[2,] -0.7819263  5.9832371 -2.049524  4.4976418  1.9079767
[3,] -1.0226159 -2.0495241 18.444907 -3.2958671 -2.8132511
[4,]  5.5716021  4.4976418 -3.295867 13.1258459  0.8410505
[5,] -0.6615621  1.9079767 -2.813251  0.8410505  3.4450550
```

We can see the symmetry and check that the matrix is positive definite:

```
> eigen(z)$values      # check positive definite
[1] 22.2951500 14.0726580  7.0743534  2.2363879  0.7169668
```

because all of the eigenvalues are positive.

We can find the matrix square root $Z^{1/2}$ using the `msqrt` program given above:

```
> (sqrtz <- msqrt(z))      # find matrix square root
[1,]      [,2]      [,3]      [,4]      [,5]
[1,]  1.9849903 -0.4102019 -0.1244228  1.11419094 -0.17640021
[2,] -0.4102019  2.1943311 -0.2449349  0.87546138  0.41648139
[3,] -0.1244228 -0.2449349  4.2449391 -0.38357917 -0.45032400
[4,]  1.1141909  0.8754614 -0.3835792  3.31074757  0.09904232
[5,] -0.1764002  0.4164814 -0.4503240  0.09904232  1.74008050
```

Finally, we can check the difference between $(Z^{1/2})^2$ and Z :

```
> sqrtz %*% sqrtz - z  # check properties of matrix sqrt
[1,]      [,2]      [,3]      [,4]      [,5]
[1,] -2.664535e-15  1.443290e-15 -1.332268e-15 -1.154632e-14  2.109424e-15
[2,]  1.665335e-15 -8.881784e-15 -1.332268e-15 -1.776357e-15 -1.776357e-15
[3,] -1.110223e-15 -8.881784e-16 -3.552714e-14  5.329071e-15  7.549517e-15
[4,] -1.065814e-14 -1.776357e-15  3.552714e-15 -3.907985e-14  1.998401e-15
[5,]  1.998401e-15 -1.332268e-15  7.549517e-15  1.776357e-15 -4.884981e-15
```

This difference is within rounding error of a matrix of all zeroes, confirming the properties of the matrix square root in R.

4.6 Exercises

- 4.1 Let $\mathbf{x}' = (2, 1, -5)$ and $\mathbf{y}' = (2, 1, 1)$.
- Find $\mathbf{x} + \mathbf{y}$.
 - Show that \mathbf{x} and \mathbf{y} are orthogonal.
 - Find a nonzero vector \mathbf{z} that is orthogonal to both \mathbf{x} and \mathbf{y} .
 - Show that any vector that is orthogonal to both \mathbf{x} and \mathbf{y} must be a scalar multiple of \mathbf{z} .
- 4.2 For vectors \mathbf{x} , \mathbf{y} , and \mathbf{z} with the same dimensions and scalar c verify that
- $\mathbf{x}'\mathbf{y} = \mathbf{y}'\mathbf{x}$
 - $\|c\mathbf{x}\| = |c| \|\mathbf{x}\|$ where $|c|$ is the absolute value of c
 - $\|\mathbf{x}\| = 0$ if and only if \mathbf{x} is the zero vector
 - Verify (4.2)
- 4.3 Let \mathbf{X} denote an $n \times n$ square matrix and \mathbf{y} is an n -tuple vector of all 1s. Interpret $\mathbf{y}'\mathbf{X}$ and $\mathbf{X}\mathbf{y}$.
- 4.4 Suppose \mathbf{X} , \mathbf{Y} , and \mathbf{Z} are matrices with the appropriate dimensions so that multiplication is defined.
- Prove that $(\mathbf{XY})\mathbf{Z} = \mathbf{X}(\mathbf{YZ})$.
 - Prove that $(\mathbf{XY})' = \mathbf{Y}'\mathbf{X}'$. Also $(\mathbf{XYZ})' = \mathbf{Z}'\mathbf{Y}'\mathbf{X}'$.
 - Suppose that \mathbf{X} and \mathbf{Y} are square matrices with the same dimensions. Show that \mathbf{XY} is not necessarily equal to \mathbf{YX} .
- 4.5 (a) Find a pair of vectors that are linearly independent but not orthogonal.
- (b) Suppose the vectors $\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_k$ are mutually orthogonal. Show that they are also linearly independent. *Hint:* If they are linearly dependent and orthogonal then they must all have zero length.
- 4.6 Consider the matrix
- $$\mathbf{A} = \begin{pmatrix} 2 & 1 \\ 1 & 1 \end{pmatrix}.$$
- Find the trace, determinant, and inverse of this matrix.
 - Multiply this matrix by its inverse and verify that your solution is correct.
 - Use (4.9) and (4.10) to find the eigenvalues for this matrix.

4.7 Let $\mathbf{X} = \{x_{ij}\}$ denote a matrix with n rows and p columns.

- (a) Show that $\mathbf{X}'\mathbf{X}$ is a symmetric matrix.
- (b) Verify that the i th diagonal element of $\mathbf{X}'\mathbf{X}$ is

$$\sum_{k=1}^n x_{ki}^2$$

and the (i, j) off-diagonal elements of $\mathbf{X}'\mathbf{X}$ are

$$\sum_{k=1}^n x_{ki} x_{kj}$$

for $i \neq j = 1, 2, \dots, p$.

(c) Suppose $\mathbf{A} = \{a_{ij}\}$ is a $p \times p$ symmetric matrix. Then verify that $\mathbf{B} = \mathbf{X}\mathbf{A}\mathbf{X}'$ is symmetric with diagonal elements

$$b_{jj} = \sum_{k=1}^n a_{jj} x_{kj}^2$$

and off-diagonal elements

$$b_{ij} = b_{ji} = \sum_{k=1}^n a_{ij} x_{ki} x_{kj}.$$

4.8 Show that the rank of an $n \times m$ matrix cannot be larger than the smaller of n and m . As a consequence, show that the 5×5 matrix \mathbf{Q} constructed in (4.14) cannot have rank greater than 3.

4.9 A *linear space* \mathcal{S} is a set of vectors with the properties that

- (i) The zero vector $\mathbf{0}$ is an element of \mathcal{S}
- (ii) if \mathbf{x} and \mathbf{y} are in \mathcal{S} then $\mathbf{x} + \mathbf{y}$ is also in \mathcal{S} .
- (a) Show that for any vector \mathbf{x} , the set

$$\mathcal{S}(\mathbf{x}) = \{c\mathbf{x} \text{ for every scalar } c\}$$

of every scalar multiple of \mathbf{x} is a linear space. We say that $\mathcal{S}(\mathbf{x})$ is the space *spanned* by the vector \mathbf{x} .

(b) More generally, consider the set of every linear combination of the vectors $\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n$:

$$\mathcal{S}(\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n) = \{c_1\mathbf{x}_1 + c_2\mathbf{x}_2 + \dots + c_n\mathbf{x}_n \text{ for all scalars } c_i\}.$$

Show that this is a linear space. Such a set is called the *linear space spanned by the vectors $\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n$* or more simply, the *span* of $\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n$.

- 4.10 Show that the set of all solutions in \mathbf{x} of (4.8) form a linear space. Specifically show that

(a) The zero vector $\mathbf{x} = (0, 0, \dots, 0)$ satisfies (4.8).

(b) If the eigenvectors \mathbf{x}_1 and \mathbf{x}_2 are both solutions to (4.8) with respect to an eigenvalue λ then the sum $\mathbf{x}_1 + \mathbf{x}_2$ of these eigenvectors will also solve (4.8).

- 4.11 Let \mathbf{Z} denote an arbitrary $n \times m$ matrix.

(a) Show that $\mathbf{Z}'\mathbf{Z}$ is symmetric.

(b) Show that $\mathbf{Z}'\mathbf{Z}$ is nonnegative definite. Hint: If $\mathbf{y} = \mathbf{Z}\mathbf{x}$ then $\mathbf{y}'\mathbf{y} = \mathbf{x}'\mathbf{Z}'\mathbf{Z}\mathbf{x}$.

(c) Show that every eigenvalue of $\mathbf{Z}'\mathbf{Z}$ must be nonnegative. Hint: If λ is an eigenvalue with eigenvector \mathbf{x} then $\mathbf{Z}'\mathbf{Z}\mathbf{x} = \lambda\mathbf{x}$. If we multiply on the left by \mathbf{x}' then we also have

$$\mathbf{x}'\mathbf{Z}'\mathbf{Z}\mathbf{x} = \lambda\mathbf{x}'\mathbf{x}.$$

- 4.12 Let \mathbf{Z} denote an arbitrary $n \times m$ matrix. The previous exercise showed that eigenvalues of $\mathbf{Z}'\mathbf{Z}$ are all real and nonnegative. Let us denote these by

$$\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_r \geq \lambda_{r+1} = \lambda_{r+2} = \dots = \lambda_m = 0$$

with corresponding eigenvectors $\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_m$. Refer to (4.13) and show that the matrix

$$\sum_{i=1}^r (1/\lambda_i) \mathbf{x}_i \mathbf{x}_i'$$

is a generalized inverse of $\mathbf{Z}'\mathbf{Z}$.

- 4.13 Suppose the matrix \mathbf{A} is expressible as in (4.12). Find \mathbf{A}^{10} .

4.14 In this exercise we explore properties of the matrix square root.

(a) Verify (4.15).

(b) Consider the 2×2 identity matrix

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

Show that the matrix square root of \mathbf{I} is not unique.

Specifically, consider any numbers r and s , at least one of which is nonzero. Then define

$$t = \sqrt{r^2 + s^2}$$

and define

$$\mathbf{J} = 1/t \begin{pmatrix} \pm s & \pm r \\ \pm r & \mp s \end{pmatrix}.$$

Show that $\mathbf{J}^2 = \mathbf{I}$.

Chapter 5

The Univariate Normal Distribution

THE NORMAL DISTRIBUTION is central to much of statistics. In this chapter and the two following, we develop the normal model from the univariate, bivariate, and then, finally, the more general distribution with an arbitrary number of dimensions.

Historically, the normal distribution was developed as an approximation to the binomial distribution by de Moivre¹ in 1738 but the more common attribution is to Gauss² in 1809. As a result, the normal distribution is often referred to as the *Gaussian distribution* or frequently as the *bell curve* because of the familiar shape of its density function.

5.1 The Normal Density and Distribution Functions

The density function of the *standard normal distribution* is

$$\phi(x) = (2\pi)^{-1/2} \exp(-x^2/2). \quad (5.1)$$

The distribution is called the standard normal because a random variable X sampled from this distribution will have zero mean and unit variance. This function is available in R as `dnorm()`.

¹Abraham de Moivre (1667–1754). French mathematician and probabilist.

²Carl Friedrich Gauss (1777–1855). German mathematician and physicist.

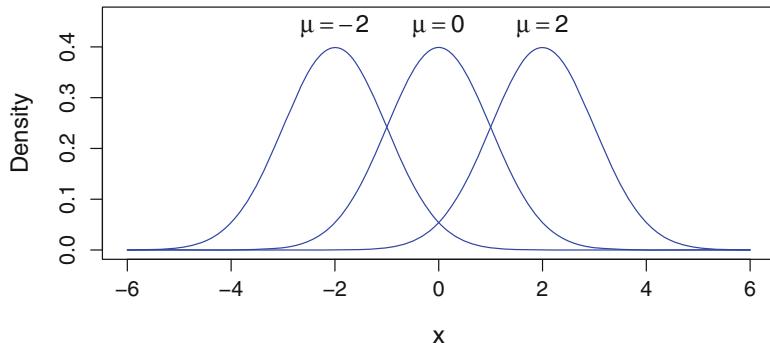


Figure 5.1: The normal distribution density function (5.2) for specified mean values, all with a standard deviation $\sigma = 1$

Of course we are not restricted to the use of standard normal variates. If X is a standard (zero mean, unit standard deviation) normal then the linear transformation

$$Z = \mu + \sigma X$$

is also normally distributed with mean μ and variance σ^2 .

This more general and useful form of the distribution of $Z = \mu + \sigma X$ defined for $\sigma > 0$ has density function

$$\phi(z | \mu, \sigma) = \sigma^{-1} (2\pi)^{-1/2} \exp\{-(z - \mu)^2/2\sigma^2\}. \quad (5.2)$$

In Fig. 5.1 we see that the familiar bell curve is shifted left and right by varying the value of the mean μ . When the value of the standard deviation σ is varied, Fig. 5.2 demonstrates that the curve can also have a sharp peak (when σ is small) or be broad and flat (when σ is large).

The cumulative distribution or area under the normal curve is much more important than the bell curve itself. That is, we usually want to describe the probability of an interval under the bell curve, but almost never need the value of the bell curve itself.

Specifically, let

$$\Phi(x) = \int_{-\infty}^x \phi(t) dt \quad (5.3)$$

denote the cumulative probability up to the value x .

The tail areas are symmetric so that

$$\Phi(-x) = 1 - \Phi(x)$$

for every value of x .

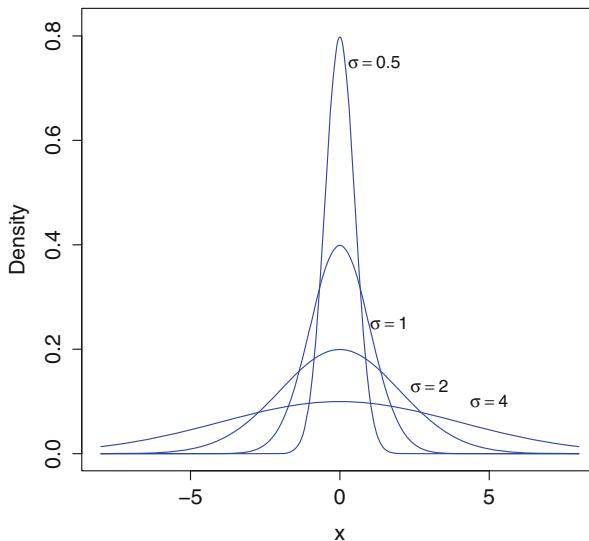


Figure 5.2: The normal distribution density function (5.2) with mean 0 and different values of the standard deviation as given

This integral, for the standard normal ($\mu = 0$ and $\sigma = 1$), is evaluated by `pnorm()` in R. The shape of Φ may be unfamiliar to many readers, so we present some examples in Fig. 5.3. In each of the curves of Φ in Fig. 5.3 we see all these begin close to zero on the left and increase monotonically up to one on the right. The curves shift left to right as the mean increases. Smaller standard deviations cause the curve to rise more quickly. The shape of the normal density in Figs. 5.1 and 5.2 should be familiar to the reader, but the shape in Fig. 5.3 is rarely displayed.

In R we can generate random samples from a standard normal distribution using the `rnorm()` function. This function was also illustrated in Sects. 2.5 and 4.5. The argument to `rnorm()` specifies how many random values are generated:

```
> rnorm(4)
[1] 1.1624076 -1.9219944 0.4634357 -2.5063903
> rnorm(5)
[1] -2.5397705 0.5856622 -1.3165089 3.3851341 1.5616724
```

Notice the random values generated are different with every invocation of `rnorm`. Your values will differ from these as well.

We calculate values of the standard normal density function ϕ given in (5.1) using `dnorm()` which may take a vector argument. Similarly, the cumulative normal Φ in (5.3) with $\mu = 0$ and $\sigma = 1$ is found using `pnorm()`.

We can illustrate these functions in R by plotting the values using

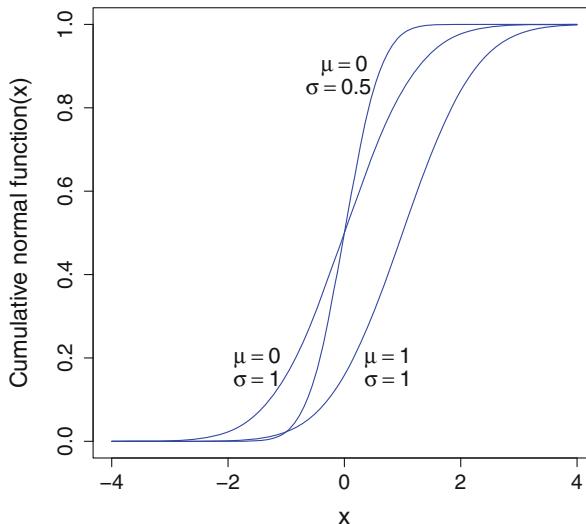


Figure 5.3: The cumulative normal distribution function (5.3) for means μ and standard deviations σ as given

```
> x <- (-50:50)/12
> plot(x, dnorm(x), type = "l")
```

to plot the standard normal density function in Fig. 5.1 and then

```
> plot(x, pnorm(x), type = "l")
```

to illustrate the cumulative distribution function with mean zero and standard deviation one, as in Fig. 5.3.

There is also the function `qnorm()` that calculates the *quantile function* from the normal distribution. The quantile is the inverse of Φ . That is, for any probability p ($0 < p < 1$), the normal quantile $x = x(p)$ is the value solving the equation

$$\Phi(x) = p. \quad (5.4)$$

You may be familiar with the use of this function for finding the critical value of a statistical test. Specifically, a standard normal distribution has 95 % of its area between the familiar values -1.96 and $+1.96$. We can obtain these values in R using the `qnorm` function:

```
> qnorm(.05/2)
[1] -1.959964
> qnorm(1 - .05/2)
[1] 1.959964
```

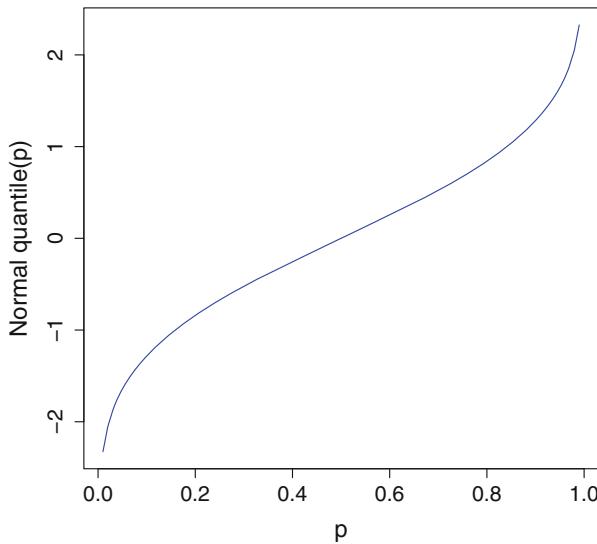


Figure 5.4: The quantile function $\Phi^{-1}(p)$ of the standard normal distribution

We use the argument of $0.05/2$ because we want half of the 0.05 probability in each of the two tails of the normal curve. A plot of the `qnorm()` function is given in Fig. 5.4. As p approaches either 0 or 1 , then this curve tends to $-\infty$ or $+\infty$, respectively.

To illustrate another use of this function in R, we generate a set of probabilities that are uniformly distributed between (but not including) 0 and 1 and then find the corresponding normal quantiles:

```
> x <- runif(6)
> x
[1] 0.6828715 0.4100933 0.5086939 0.7548347 0.8098490
[6] 0.7866481

> qnorm(x)
[1]  0.47574359 -0.22730502  0.02179419  0.68978305
[5]  0.87733996  0.79484489
```

In Exercise 5.2 you are asked to identify the distribution of the random values generated in this fashion.

5.2 Relationship to Other Distributions

Let us point out some simple relationships between the normal distribution and other important statistical distributions. The normal distribution is frequently used as an approximation to many other distributions and the behaviors of test statistics. A popular example is the normal approximation to the binomial distribution with a large sample size. Other examples appear in Exercises 2.4 and 5.4.

There is a close relationship between the normal and the chi-squared distribution. If x has a standard normal distribution then x^2 behaves as a chi-squared with 1 df. More generally, if x_1, x_2, \dots, x_k , each behave as independent, standard normals, then $x_1^2 + \dots + x_k^2$ behaves as chi-squared with k df. The ratio x_1/x_2 of two independent standard normals behaves as Student's t with 1 df, also known as the *Cauchy distribution*.³ See Sect. 5.5 for a discussion of Student's t -distribution.

Sums and differences of correlated, normally distributed variates also behave as normal. We will explore this property in the following two chapters when we talk about multivariate normal distributions.

5.3 Transformations to Normality

If you are reading this section, then it is likely that you are already suspicious that your data is not exactly normally distributed. In this section we will provide statistical tests to see if your data is “close enough” to being normal and some things you can do about it if it isn't. Of course, there are times when it is not worth testing for normality or even pretending the data is normally distributed because the non-normal shape is obvious. In this case, other techniques are available to us such as robust, nonparametric methods that do not rely on the assumption of normally distributed data. As an example, if the data values are binary valued, then the normal distribution is not appropriate and no amount of transformation will make this data look normal.

As a case study for this section, let us examine the median apartment rents for each of the 50 US states and DC given in Table 1.1.

The best way to start is to draw a histogram. In R we draw a histogram using the `hist(x)`. This command is discussed in Sect. 3.1. The histogram of the rent values appears in the upper left corner of Fig. 5.5. The data values have a longer right tail than the left (right skewed), and we are going to show how to repair that. There is also some evidence of a gap in the middle of the distribution, perhaps indicating that the data is sampled from two different

³Augustin-Louis Cauchy 1789–1857. French mathematician.

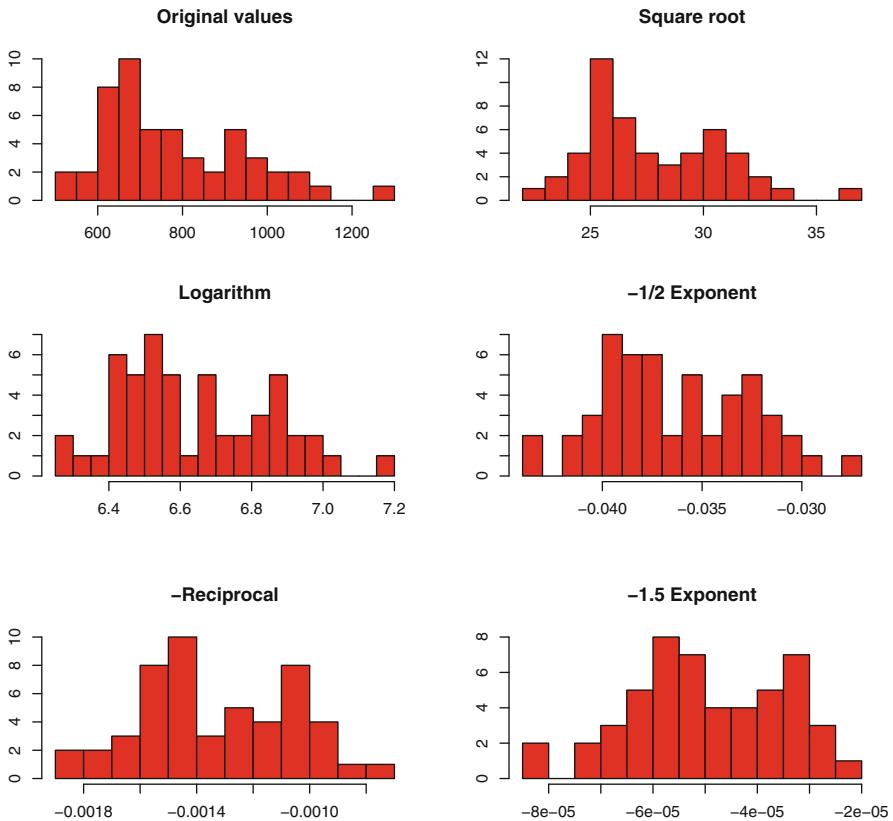


Figure 5.5: Histograms of the median apartment rents in Table 1.1. The data has been transformed using the power transformation (5.5)

populations. This bimodal feature is much harder to fix than the asymmetry, which we will discuss next.

It is possible and often useful to transform skewed data values in order to make them more symmetric. Clearly a linear transformation will not change the basic shape of the histogram. A nonlinear transformation is needed. The *power transformations* attributed to Box and Cox (1964) can be summarized as

$$\text{Power}(x) = \begin{cases} -x^\lambda & \text{for } \lambda < 0 \\ \log(x) & \text{for } \lambda = 0 \\ x^\lambda & \text{for } \lambda > 0 \end{cases} \quad (5.5)$$

for positive-valued data (x) and any specified value of λ . This function is called `bct` and is available in the `TeachingDemos` library.

The further λ is from 1, the greater the effect of the transformation.

Values of $\lambda < 1$ in this transformation will have the effect of pulling in a long right tail and spreading out values in a short left tail. This is what is needed for the rent data and we will explore these next. A negative sign is needed in the power transformation for values of $\lambda < 0$ because reciprocals of large numbers are small numbers and we need to preserve the order of the data, not reverse it. Values of $\lambda > 1$ in (5.5) will tend to push out the right tail of the distribution and this is the opposite of what is needed to make the distribution of the rent data more symmetric.

Histograms of transformed median rent values are given in Fig. 5.5. These include values of $\lambda = 1, 1/2, 0, -1/2, -1$, and -1.5 . Choosing the appropriate value of λ calls for more of a sense of aesthetics than mathematical rigor. In Fig. 5.5 we see that the square root ($\lambda = 1/2$) and log ($\lambda = 0$) transformations result in more symmetric improvements over the original data but are not strong enough. The reciprocal ($\lambda = -1$) and $\lambda = -1.5$ appear to overdo the transformation and begin to introduce a longer left tail. The reciprocal square root ($\lambda = -1/2$) seems to be a nice compromise, producing a more symmetric distribution, although there is not much we can do about the bimodal character of the data. Ideally, a separate statistical analysis could be applied to help identify characteristics and membership in two or more different populations. These methods are described in Chaps. 10 and 11.

Next we examine methods to check for normality. A simple graphical method for checking normality is the quantile–quantile plot or *QQ plot*. This plot compares the quantiles of the observed values with those of the theoretical distribution, hence the name *QQ*. The *QQ* plot displays the sorted, observed values against the values that we would expect to observe had they been sampled from a theoretical normal distribution. If the observed data was sampled from a normal distribution, then we would expect these values to form a nearly straight line.

What are the expected values from an ordered normal sample? To find these, begin by recalling the cumulative normal distribution function Φ given in (5.3). Consider then, a sorted sample $x_1 \leq x_2 \leq \dots \leq x_n$ from a standard normal distribution with mean $\mu = 0$ and standard deviation $\sigma = 1$.

We would expect that these ordered, standardized values to obey

$$\Phi(x_1) = 1/(n+1), \quad \Phi(x_2) = 2/(n+1), \quad \dots, \quad \Phi(x_n) = n/(n+1). \quad (5.6)$$

In other words, the theoretical, expected sample values should be spread out evenly with all n observations having equal cumulative probabilities between each. See Exercise 5.2 for more details.

We can take the set of equations in (5.6) and invert Φ using the normal quantile function to obtain the expected normal quantiles. These values are close approximations to where the ordered values should be expected to occur

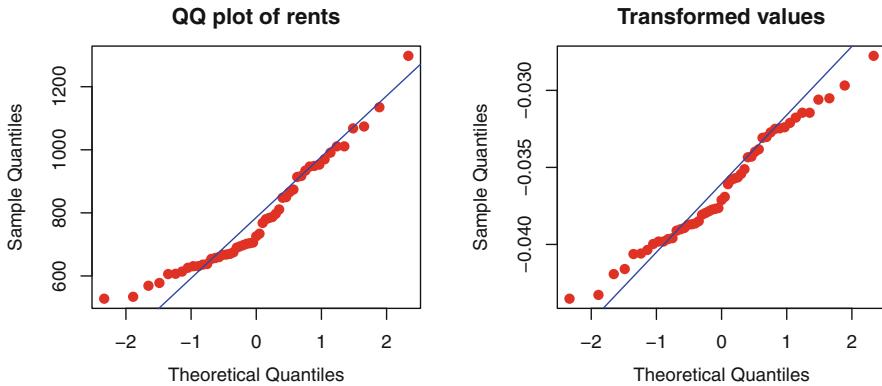


Figure 5.6: QQ plot of the original apartment rent values on *left* and power transformed with $\lambda = -1/2$ on the *right*

in the sample. Specifically, the expected quantiles for the QQ plot are

$$\hat{x}_1 = \Phi^{-1}(1/(n+1)), \quad \hat{x}_2 = \Phi^{-1}(2/(n+1)), \quad \dots \quad \hat{x}_n = \Phi^{-1}(n/(n+1)). \quad (5.7)$$

The quantile function $\Phi^{-1}()$ is plotted in Fig. 5.4 and can be calculated using the `qnorm()` function in R.

The QQ plot consists of a scatterplot of the paired values (\hat{x}_i, x_i) . Ideally, this should appear as a straight line if the x_i were a “perfect” sample with all observations appearing exactly where we would expect them to be. In the QQ plot we should expect to see the greatest deviations from the straight line at its ends, partly because the sampled values at the extremes will have greater variability than those observations nearer to the center of the distribution.

An example of a QQ plot for the rent data appears in Fig. 5.6. The plot on the left is for the raw data. The graph on the right is of the transformed data raised to the power $\lambda = -1/2$. This was the power we decided was best in the histogram plots of Fig. 5.5.

In R we draw a QQ plot for data in `y` with the code

```
qqplot(y)
qqline(y)
```

The `qqplot()` command produces the data plot, and the `qqline()` command adds the diagonal line as a useful visual reference. The line is drawn between the first and third quartiles of the observed data. The quartiles divide the observed data into four equal sized groups so that 1/4 of the data values are below the first quartile and 1/4 are above the third quartile. The `qqplot()` statement accepts the options `pch=`, `cex=`, and `col=` to control the plot character, its size, and its color.

The QQ plot of the original rent values on the left half of Fig. 5.6 shows that the lower (left) tail is short relative to where the normal distribution would expect it. The sample in the first quartile is higher than the line anticipates, and the lower tail is not as spread out as it should be if the data more closely followed a normal distribution. The upper (right) tail looks about correct for the original data values.

The QQ plot for the $\lambda = -1/2$ transformed data on the right half of Fig. 5.6 follows the line more closely but both the upper and lower tails of this transformed distribution are slightly shorter than what the normal distribution would anticipate. The center of this plot shows a small bump that is indicative of the bimodal gap in the middle of the distribution. The center of the transformed values appear to hug the diagonal line more closely, but the upper tail does not have as good a fit as does the original data. The extremes of the sample will generally be more variable, so we should not expect the tails to follow the normal model as closely as the observations in the center.

To conclude this section, the power transformation gives us a continuous range of tools to reshape our data. The choice of λ is more art than science. In the next section we will try to quantify the degree of non-normality by applying different statistical tests to the data.

5.4 Tests for Normality

There are many ways in which the data can appear non-normal. Similarly, there are a wide range of tests of normality that can be applied. Each of these looks for a different deviation from the normal model. Using the words of hypothesis testing, the null hypothesis is that the data has been sampled from a normal population, but there are many possible deviations from this model to consider as alternative hypotheses. Similarly, we need to know what attributes of the normal distribution are being examined in each test. The R libraries `fBasics` and `norTest` provide a number of useful tests of normality. In this section, we will review a few of these.

Begin with a random sample $\mathbf{x} = (x_1, \dots, x_n)$ with sample mean \bar{x} . The simplest and most intuitive test available examines the observed and expected histograms. Suppose we cut up the real line into a small number of nonoverlapping intervals. Then we count the number of observations that fall into each of these categories, just as we would when constructing a histogram. The theoretical normal distribution also provides the number of counts that should be expected in each of these intervals. Finally, the observed and expected counts can be combined in a Pearson⁴ chi-squared statistic.

⁴Karl Pearson (1857–1936). British historian, lawyer, and mathematician.

If obs_i and exp_i are the observed and expected counts in the i -th interval then

$$\sum_i (\text{obs}_i - \text{exp}_i)^2 / \text{exp}_i$$

is the Pearson chi-squared statistic.

The `pchiTest` test in the `fBasics` library does the calculations for this test, including the p-value obtained from the corresponding chi-squared reference distribution. (This test is also available as `pearson.test` in the `nortest` library.) The default number of categories chosen by this method is the largest integer in $2n^{4/5}$ so that the number of interval categories⁵ increases almost in proportion to the sample size. There are options in the test that allow you to vary the number of categories.

The cut points of the intervals are chosen so each interval has the same expected number of counts. See Exercise 5.8 for an example of how this is done.

Here is an example of the use of the Pearson test. Consider the original apartment rents that we examined in Sect. 5.3 as a candidate for transformation:

```
> library(fBasics)
> pchiTest(housing$Apartment,
+           description="Original apartment values")
Title:
Pearson Chi-Square Normality Test

Test Results:
PARAMETER:
Number of Classes: 10
STATISTIC:
P: 12.7255
P VALUE:
Adjusted: 0.07909
Not adjusted: 0.1754

Description:
Original apartment values
```

In this case, ten interval categories are examined and R uses different methods for calculating the reference p-values. The adjusted p-values (adjusted for small sample sizes) provides a small amount of evidence to reject

⁵There is mathematical theory to suggest that $n^{4/5}$ is about the correct number of categories needed when drawing a histogram. See Tapia and Thompson (1978; p. 53) for details on this.

the null hypothesis of an underlying normal population. Ideally, the next step would be to examine the frequencies in each of the ten categories to see where the lack of fit occurs. See Exercises 5.8 and 5.9 for more detail on this test of the normal distribution for the transformed apartment rent data.

Let us examine a different test of the normal distribution based on higher moments of the sampled data. The *Jarque–Bera test* examines the third and fourth moments of the sampled data. The *skewness* of the sample is defined by the third moment about the sample mean:

$$\hat{\gamma}_3 = \text{skewness} = n^{-1} \sum (x_i - \bar{x})^3 / \text{var}(\mathbf{x})^{3/2}.$$

Skewness measures asymmetry of the sampling distribution. The skewness should have a value near zero for normally distributed data. Values far from zero indicate that the data was sampled from an asymmetric distribution. Positive skewness means that the right, upper tail of the data is longer than the left tail.

The *kurtosis*

$$\hat{\gamma}_4 = \text{kurtosis} = n^{-1} \sum (x_i - \bar{x})^4 / \text{var}(\mathbf{x})^2 - 3$$

is the fourth moment of the data, centered about its mean.

There is a “3” in the definition of kurtosis because in the normal distribution, the fourth central moment is $3\sigma^4$. Positive or negative values of the kurtosis indicate the tails of the sampling distribution are longer (heavier) or shorter (lighter), respectively, than a normal distribution. A large positive kurtosis may also indicate the presence of outliers in the data. Similarly, a negative kurtosis may be the result of the truncation of extremes in the data. Skewness and kurtosis may be computed in R on data using functions of the same name in the **fBasics** library.

The Jarque–Bera statistic

$$JB = n/6 (\text{skewness}^2 - \text{kurtosis}^2/4)$$

provides a test of the normal distribution by combining both the skewness and kurtosis for a data sample (Jarque and Bera 1987).

This statistic behaves as chi-squared with 2 df under the null hypothesis of normally distributed data. Statistically large values of JB are indicative of a poor fit for the normal distribution. In R, the `jbTest()` function calculates the value of the JB statistic and provides the corresponding p-value of the reference chi-squared statistic. This function is part of the **fBasics** library.

As an example of the use of this test, let us look at the apartment rents. The following examines the original, untransformed values and gives the R output:

> `library(fBasics)`

```

> jbTest(housing$Apartment,
+         title="Original apartment rents")

Title:
Original apartment rents

Test Results:
PARAMETER:
  Sample Size: 51
STATISTIC:
  LM: 5.499
  ALM: 6.3
P VALUE:
  LM p-value: 0.043
  ALM p-value: 0.053
  Asymptotic: 0.064

```

The `jbTest()` calculates both a finite sample (LM) and asymptotic (ALM) version of the JB statistic as well as their corresponding p-values. In this example, the three p-values are close in value to indicate a consensus of methods and small enough for us to question the adequacy of the fit of the normal distribution.

Let us run this test again on the transformed apartment rents using the transformation we found in Sect. 5.3. The R code and output, in part are as follows:

```

> jbTest(-housing$Apartment^(-1/2),
+         title="Transformed apartment rents")

. . .

P VALUE:
  LM p-value: 0.29
  ALM p-value: 0.331
  Asymptotic: 0.429

```

The three p-values given here provide good evidence of data sampled from a normal population. This is quantitative evidence of the benefit of transforming these data values. See also Exercise 5.9.

The *Kolmogorov-Smirnov test*^{6,7} is a nonparametric examination of the cumulative distribution function. This test compares the maximum difference between the cumulative distribution function of the data with that of

⁶Andrey Nikolaevich Kolmogorov (1903–1987). Soviet mathematician and probabilist.

⁷Nikolai Vasil'evich Smirnov (1900–). Soviet probabilist.

the theoretical normal distribution. Intuitively, this statistic measures how far the cumulative, ordered data values are from where we would expect them to appear. This is similar to the visual inspection we apply when we perform the QQ plot as in Fig. 5.6 except that it only measures the largest vertical difference between the ordered data and the fitted straight line.

In R, this test expects the data values to be standardized with respect to the mean and standard deviation. Here is an example, again examining the apartment rents:

```
> z <- housing$Apartment
> z <- ( z -mean(z)) / sd(z)
> ksnormTest(z)

Title:
One-sample Kolmogorov-Smirnov test

Test Results:
STATISTIC:
D: 0.1597
P VALUE:
Alternative Two-Sided: 0.1484
Alternative Less: 0.5633
Alternative Greater: 0.07421
```

The test method provides three p-values for alternative hypotheses that the largest difference of the two distribution functions are either one or two sided. Unless we have strong *a priori* concerns, the two-sided alternative hypothesis is the preferred approach. In this example, none of these three p-values indicates a large deviation from the normal distribution.

The *Shapiro–Wilk* test statistic is

$$W = \left(\sum a_i x_{(i)} \right)^2 / \text{std dev}(\mathbf{x}),$$

where a_i are constants that depend only on the sample size (Shapiro and Wilk 1965).^{8,9}

The $x_{(i)}$ are the ordered data values $x_{(1)} \leq x_{(2)} \leq \dots \leq x_{(n)}$. As with the Kolmogorov–Smirnov test, this statistic also measures how far the ordered data values are from where we would expect them to appear. Informally, the *Shapiro–Wilk* test examines how far the observed data deviates from the QQ plot, and the Kolmogorov–Smirnov test examined the maximum difference in the QQ plot, measured on a vertical scale.

⁸Samuel Sanford Shapiro (1930–). American statistician and engineer.

⁹Martin Bradbury Wilk (1922–2013). Canadian statistician and former Chief Statistician of Canada.

The `shapiro.test()` in R provides a formal p-value for the W statistic. Here is an example of its use:

```
> shapiro.test(housing$Apartment)

  Shapiro-Wilk normality test

  data:  housing$Apartment
  W = 0.9346, p-value = 0.007472

> shapiro.test(-housing$Apartment^(-1/2))

  Shapiro-Wilk normality test

  data: -housing$Apartment^(-1/2)
  W = 0.9737, p-value = 0.3136
```

The first of these two tests shows a large discrepancy between the original apartment rent data and a normal distribution. The second use of the `shapiro.test` demonstrates how much better the transformed values follow the normal distribution.

As we have shown in the past two sections, there are tests for normality and transformations to make our data look more normal. We point out that this exercise in transforming and testing is not the final goal. Usually our interest is in inference made on the data using some statistical method that depends on a normal distribution for its validity. The motivation for testing normality, then, is that our inference requires it, not that normality is an end unto itself.

But if this is indeed the case, then we should not be asking if our data is normally distributed. The real question is whether our data is close enough to the normal distribution in order to obtain valid statistical inference. Instead, we need to question the sensitivity of the statistical method to the assumptions of normality. Simulation methods in R are ideal for addressing such issues. Simulation methods are discussed in Sects. 2.2 and 2.6.

5.5 Inference on Univariate Normal Means

In this section we want to describe statistical inference on the population parameter μ . Given a random sample x_1, x_2, \dots, x_n from a univariate normal distribution with mean μ and variance σ^2 , the sample average \bar{x} ,

$$\bar{x} = n^{-1} \sum_i x_i,$$

is used to estimate μ .

The standard error of \bar{x} is σ/\sqrt{n} . This standard error would be ideal, except σ is rarely known in practice and needs to be estimated. The usual point estimate for σ^2 is

$$s^2 = (n - 1)^{-1} \sum (x_i - \bar{x})^2. \quad (5.8)$$

In Sect. 5.6 we will describe inference on σ^2 .

For a long while, researchers would substitute the value s for the unknown σ and treat $\bar{x}/(s/\sqrt{n})$ as normally distributed. Gosset¹⁰ pointed out the appropriate distribution while working at the Guinness Brewery in Dublin. His work was considered a trade secret so he published it in 1908 under the pen name “Student,” leading to the present name of “Student’s t-distribution.”

The distribution of $\bar{x}/(s/\sqrt{n})$ is that of Student’s t with $n - 1$ df if the underlying observed values x_1, x_2, \dots, x_n are sampled from a standard normal distribution. Figure 5.7 plots Student’s t-distribution for 1, 2, 5, and 10 df and compares these to a standard normal distribution. The lower df distributions have much longer tails than the normal, and above 10 df, these distributions are indistinguishable from the normal. The normal distribution corresponds to the t-distribution with infinitely many df.

We can now discuss inference on the mean μ of a normal population. There are three important forms of statistical inference that we can draw: a confidence interval of μ , a hypothesis test whether μ is equal to a specified value, and equality of means sampled from two different populations. A good way to illustrate these is to have R generate a random sample of normally distributed data for us.

In R we can generate standard normal variates and find their sample average, estimated variance, and standard deviation as in the dialog:

```
> sample <- rnorm(6)
> sample
[1] -1.0763316  0.1058763 -2.3284413  1.1132752  0.4492566 -1.1717192

> mean(sample)
[1] -0.4846807

> var(sample)
[1] 1.599197

> sd(sample)
[1] 1.264594
```

¹⁰William Sealy Gosset (1876–1937). British mathematician

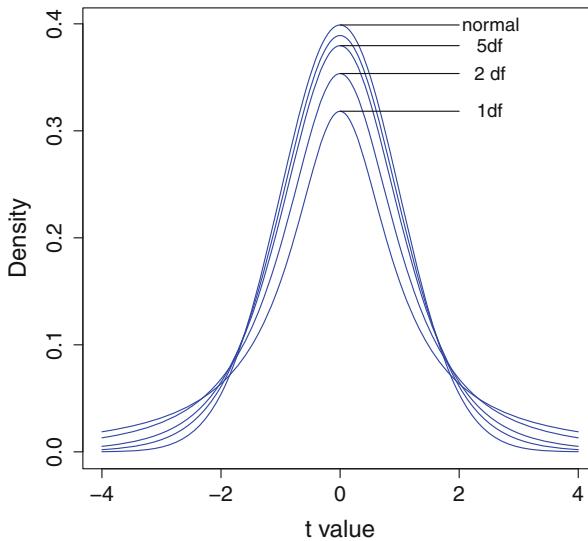


Figure 5.7: Density of normal and Student's t with 1, 2, 5, and 10 df

The one sample `t.test` program for this sampled data

```
> t.test(sample)

One Sample t-test

data: sample
t = -0.9388, df = 5, p-value = 0.3909
alternative hypothesis: true mean is not equal to 0
95 percent confidence interval:
-1.811790  0.842429
sample estimates:
mean of x
-0.4846807
```

calculates a 95 % confidence interval for the normal population mean μ and tests the hypothesis whether μ is equal to zero. In this present sample, there is no evidence against this hypothesis. Your values will be different every time you run this example.

To test other hypotheses about μ you can specify a known value for the null hypothesis, as in this example

```
> t.test(sample, mu=2)

One Sample t-test
```

```

data: sample
t = -4.8128, df = 5, p-value = 0.004829
alternative hypothesis: true mean is not equal to 2
95 percent confidence interval:
-1.811790 0.842429
sample estimates:
mean of x
-0.4846807

```

in which the small p-value 0.0048 shows that there is little evidence that μ is equal to 2.

The third important form of inference concerns the comparison of means from two different populations. So, for example,

```

> sample2 <- rnorm(5) + 1.5
[1] -0.5277086 2.5294779 3.0055344 2.9060771 3.2043778

```

generates a sample with a population mean of 1.5.

The corresponding two-sample t-test of equality of population means

```

> t.test(sample, sample2)

Welch Two Sample t-test

data: sample and sample2
t = -3.1238, df = 7.735, p-value = 0.01476
alternative hypothesis: true difference in means is not equal to 0
95 percent confidence interval:
-4.7194790 -0.6969859
sample estimates:
mean of x mean of y
-0.4846807 2.2235518

```

produces a relatively small p-value (0.014) providing evidence that the two population means are not equal. The 95 % confidence interval is that of the *difference* of the two population means. The Welch¹¹ t-test is a modification of the usual t-test that accommodates unequal population variances by introducing fractional df.

Let us use the `t.test` function to simulate the behavior of the univariate confidence interval. Specifically, Output 5.1 generates 50 different normal random samples of size 25 and finds a (univariate) 95 % confidence interval of the mean of each sample. In Fig. 5.8 we plot each of the confidence intervals and provide a histogram of their lengths.

In each of the 50 samples, the observed mean and standard deviations will vary, producing intervals of different lengths and centered at different places.

¹¹Bernard Lewis Welch (1911–1989). English statistician.

The location of the true population mean is indicated with a dotted line, but of course, this value would not be known to us in practice. The confidence intervals include the true value in 98 % of these fifty samples, which is close to the claimed coverage rate of 95 %. Figure 5.8 also includes a histogram of the lengths of these intervals.

The use of Fig. 5.8 helps us interpret confidence intervals, in general. This is an awkward concept to explain and can only be interpreted in the context of many repeated samples from the same population. The data is random, and so are the endpoints of the confidence interval. We will never know the true population mean, but with repeated sampling from the population, these random intervals are constructed in such a way that they should cover the true value 95 % of the time. Unfortunately, we usually observe only one sample from the population so the single observed confidence interval will either cover the true value or not. We cannot correctly talk about a probability associated with this single interval. The confidence interval is only associated with repeated sampling from the population.

Let us complete this section with a real-data example. Sullivan (2008) gives the data in Table 5.1 of the mathematics scores of a group of men and women. These were students in an elementary algebra course, enrolled at a community college over two semesters.

Let us begin by looking at the separate histograms, given in Fig. 5.9. Even though we see in this figure that the male students have a wider range, the women students have a larger standard deviation of values: 19.0 for women and 16.5 for men. One explanation for this discrepancy is that more women students had values at the extremes of their range but few males scored near their endpoints.

Another good first step is to check for normality using the QQ plot described in Sect. 5.4. The QQ plots in Fig. 5.10 confirm the deviations from normality that are apparent in Fig. 5.9. Specifically, the female observations have shorter tails than would be expected under a theoretical normal sample. This does not look too deviant to question the assumption of normally distributed data. The values of the male students look closer to that of a normal sample. No outliers are apparent in either male or female data.

These tests do not indicate problems with the normal distribution assumptions, so we can proceed and test the hypothesis of equality of population means:

```
> t.test(score[sex == female], score[sex == male])

Welch Two Sample t-test

data: score[sex == female] and score[sex == male]
t = 1.0226, df = 70.327, p-value = 0.31
alternative hypothesis: true difference in means is not equal to 0
95 percent confidence interval:
-3.845393 11.939686
sample estimates:
```

Output 5.1: Program to produce Fig. 5.8 of simulated univariate confidence intervals for a normal mean

```

reps <- 50                      # number of intervals to generate
sim.mean <- 2                    # true population mean
cover <- 0                      # count of coverage of true value
ints <- NULL                     # start a list of intervals
for (i in 1 : reps)              # generate the confidence intervals
{
  int <- t.test(rnorm(25, mean = sim.mean, sd = 5))$conf.int[1 : 2]
  ints <- rbind(ints, int)
  if(int[1] <= sim.mean &&
     int[2] >= sim.mean) cover <- cover + 1
}
ints                         # print these intervals
cover <- cover / reps
cover                         # percent coverage of true values

pdf(file = "simCI.pdf")    # capture graphics in file
op <- par(mfrow = c(1, 2))# side-by side plots

plot(0,0, xlim = c(min(ints[, 1]) - .5, max(ints[, 2]) + .5),
      ylim = c(0, reps), type = "n", ylab = "Simulation number",
      xlab = "Confidence interval") # create an empty frame
for (i in 1 : reps)           # plot the intervals
{
  lines(ints[i, ], c(i, i), col = rainbow(6)[4], lwd = 3.5)
  points(ints[i, ], c(i, i), col = "red", pch = 16, cex = .5)
}
lines(rep(sim.mean, 2), c( -5, reps + 5), lty = 3, col = "blue")

lengths <- ints[, 2] - ints[, 1]
hist(lengths, xlab = "Lengths of intervals",
      main = " ", breaks = 10, col = rainbow(7)[5])

dev.off()                      # return to R graphics window
par(op)                         # reset plotting option

```

```

mean of x mean of y
71.69231 67.64516

```

The female students have a larger average score than the males. The p-value of 0.31 gives us no evidence that the population means are different from each other.

We next examine statistical inference on the normal variance parameter.

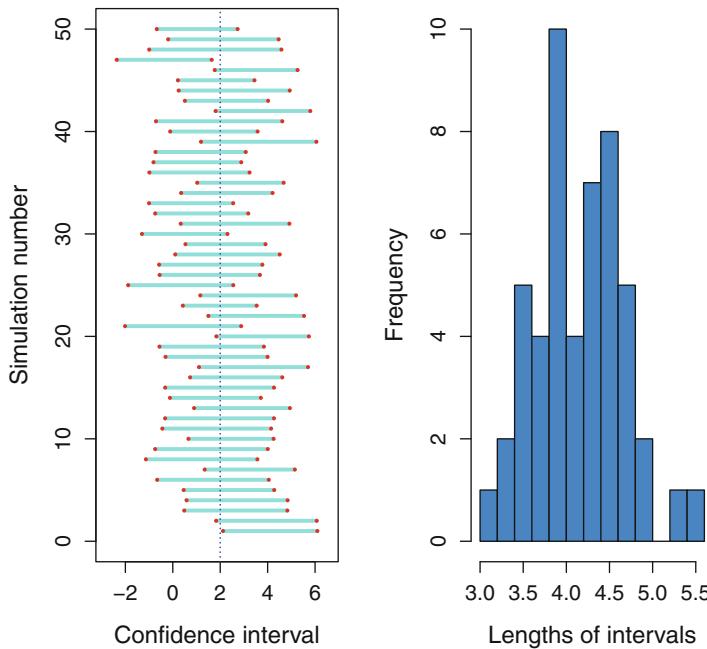


Figure 5.8: Simulated confidence intervals of a normal mean. The program in Output 5.1 produces this figure

5.6 Inference on Variances

As in Sect. 5.5, let us begin by assuming that we have a random sample x_1, x_2, \dots, x_n from a normal distribution with mean μ and variance σ^2 . The variance is estimated by s^2 given in (5.8) and this is calculated using the `var()` function in R.

Let us illustrate how we can construct a 95% confidence interval for the population variance σ^2 . In a random sample from a normal population, the sample variance s^2 behaves as $\sigma^2 \chi^2 / (n - 1)$ where χ^2 is a chi-squared random variable with $n - 1$ df.

Let us illustrate this with a sample of size $n = 10$ from a normal distribution with mean $\mu = 0$ and variance $\sigma^2 = 6$:

```
> (sample <- sqrt(6) * rnorm(10))
[1]  5.8661171  0.3683464  0.8060940  0.1836058 -1.6013981  2.2258245
[7]  0.6948691 -0.2916154 -4.9956032 -1.8808992
```

and find the sample variance:

```
> var(sample)
[1] 7.957982
```

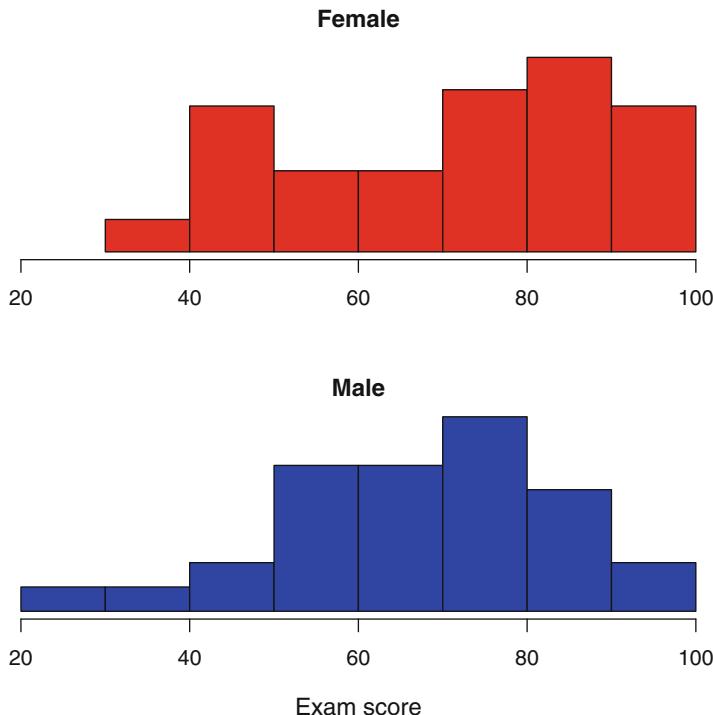


Figure 5.9: Histograms of math scores

Consider a 95 % confidence for a 9 df chi-squared random variable with equal probability 0.025 in each of the two tails of the distribution. In R we compute this as

```
> (chis95 <- c( qchisq(.975, 9), qchisq(.025, 9)))
[1] 19.022768 2.700389
```

so that the 95 % confidence interval for σ^2 from our sample is then

```
> 9 * var(sample) / chis95
[1] 3.765059 26.522781
```

We can also construct a *one-sided confidence interval* for σ^2 with all of the uncertainty at one end:

```
> (chis05 <- qchisq(.95, 9))
[1] 16.91898
```

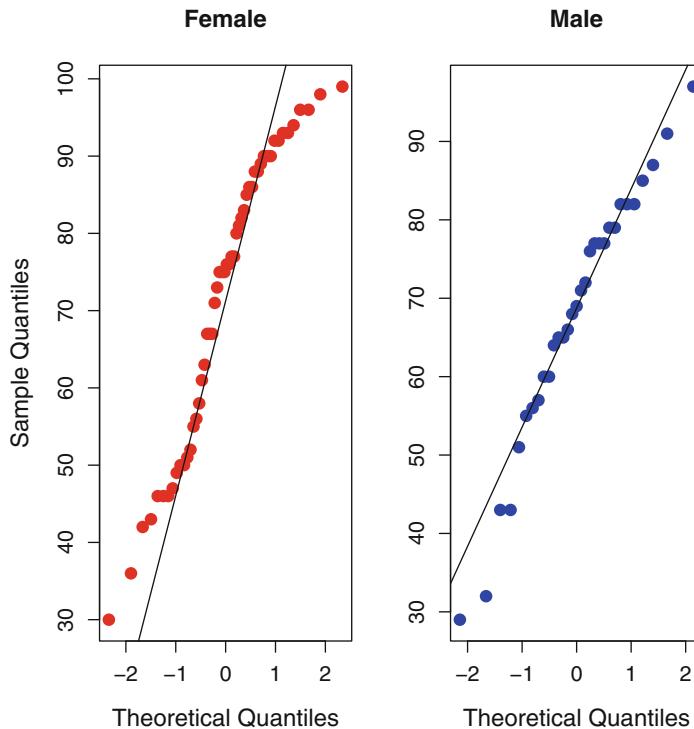


Figure 5.10: QQ plots of math scores

so that the one-sided 95 % confidence interval for σ^2 is all values greater than

```
> 9 * var(sample) / chis05
[1] 4.233225
```

so that all of the uncertainty is expressed at the lower estimate for σ^2 .

Exercise 2.5 describes several tests available in R for testing the equality of variances in different populations. These include the `bartlett.test()` test. Other tests of equality of variances available in R are `var.test()`, `fligner.test()`, `ansari.test()`, and `mood.test()`. Use the `help()` file to read about these tests.

5.7 Maximum Likelihood Estimation, Part I

In this section we want to introduce a very general process of parameter estimation and show how we can do this in R. We start with a simple example:

Table 5.1: Mathematics examination scores, by gender

Women	Men
94 90 96 73 71 75 52	77 57 79 65 68 65 55
86 93 86 50 30 46 36	72 66 29 69 85 82 43
82 55 75 47 80 92 56	60 64 82 91 51 60 76
43 77 63 76 67 99 93	43 82 87 32 71 77 77
75 90 92 88 76 61 77	79 97 56
49 67 81 89 88 42 51	
58 98 46 96 90 46 50	
67 83 85	

Source: Sullivan (2008)

estimating the mean and standard deviation from a normal sample. The reason for this apparent backward motion is to become familiar with a new method when the answer is already well known to us. Then we can use the new method and advance to more difficult problems where the solution is not obvious.

Let's begin by generating a random sample from the normal distribution with a specified mean and standard deviation:

```
> z <- rnorm(25, mean = 5, sd = 10)
> z[1 : 5]

[1] 3.861693 9.953657 14.686397 17.601439 -8.863527

> mean(z)

[1] 3.949079

> sd(z)

[1] 10.33858
```

This example generates 25 random values from a normal population with mean 5 and standard deviation 10 using the `rnorm` function. This function is previously described in Sect. 5.1, but notice how we are now using the `mean=` and `sd=` options. The `mean()` and `sd()` functions return the average and standard deviation of the sample. These are not the population values, of course, but are within sampling error of the true values. (It would take an extremely large sample to obtain the population parameters.)

Now suppose we didn't know how to estimate the mean and standard deviation and R did not include these functions to make it so easy for us. To estimate these parameters we will need to introduce two important principles:

(1) the likelihood of the data and (2) an estimate the parameters using those values that maximize this likelihood function.

The *likelihood* of a normal observation is the density function $\phi(z | \mu, \sigma)$ given in (5.2). The likelihood function is evaluated using the `dnorm()` function in R. Different likelihood functions will be used for different statistical distributions and models, but we will stay with this example for now.

The observations z_i are independent in this example so the *joint likelihood* is the product of the individual likelihood functions:

$$\phi(\mathbf{z} | \mu, \sigma) = \prod_i \phi(z_i | \mu, \sigma). \quad (5.9)$$

The principle of *maximum likelihood* directs us to find the values of μ and σ that maximize this quantity. On one level this may seem counterintuitive because Figs. 5.1 and 5.2 seem to suggest that the parameters μ and σ are fixed and only z varies in ϕ . We now need to think about the likelihood function differently and consider the observed data \mathbf{z} as fixed. That is, we are fixing the data values in ϕ and letting the parameters vary.

Intuitively, the likelihood tells us how likely the observed data was to be observed. Maximum likelihood estimates are those parameter values that make the observed data as likely to occur as possible. In words, the observations are all that we have in order to estimate parameters. Maximizing the likelihood is a method to make the observed data look as good as possible. Such parameter estimates are called *maximum likelihood estimates* and are frequently abbreviated *mle's*.

Next we need to find values of μ and σ that maximize $\phi(\mathbf{z} | \mu, \sigma)$. Notice that the data in \mathbf{z} remains the same, while the parameters μ and σ are meant to vary. We can evaluate the likelihood for \mathbf{z} at any given parameter values using the `dnorm()` function in R. This is best performed as a function. (We discuss writing functions in R in Sect. 2.5.)

The function

```
lik <- function(parm) prod( dnorm(z, mean = parm[1], sd = parm[2]))
```

of a single, vector-valued argument evaluates the normal likelihood given in (5.9). The data in \mathbf{z} is external and is understood by the function.

The vector argument to the `lik` function is a 2-tuple consisting of the mean and the standard deviation. We can evaluate it at the known, true parameter values

```
> lik(c(5,10))
```

```
[1] 2.468186e-41
```

and see that the value of the likelihood near its maximum is an extremely small number.

The reason that the likelihood is so small (about 2×10^{-41}) is that each term $\phi(z_i)$ in (5.9) is smaller than 1, and some of these terms can be quite small. Multiplying these together results in a very small number. A problem with working with the likelihood, then, is that in sufficiently large sample sizes, the likelihood can be an extremely small number and R might round this number down to zero.

A useful way to avoid such extreme numbers is to take the *logarithm* of the likelihood function. The resulting log-likelihood

$$\Lambda(\mu, \sigma) = \log\{\phi(z | \mu, \sigma)\} = \log \left\{ \prod_i \phi(z_i | \mu, \sigma) \right\} = \sum_i \log\{\phi(z_i | \mu, \sigma)\} \quad (5.10)$$

is much easier to work with because it consists of *sums* of terms, rather than a *product* of terms. (Throughout this book, we always take logarithms to the base $e = 2.718\dots$)

The corresponding log-likelihood in (5.10) is calculated by the R function

```
llik <- function(parm) sum( dnorm(z, mean = parm[1],
sd = parm[2], log = TRUE ))
```

using the `log = TRUE` option in `dnorm`.

We then evaluate this function

```
llik(c(5, 10))
[1] -93.5025
```

and obtain a more useful number. The log-likelihood is a negative number because it represents the log of a fraction.

Is it acceptable to use the log of a function that we are maximizing rather than the original function itself? Taking logs is a reasonable approach because the maximum of the function will also occur at the same place that its logarithm is maximized. There are several reasons for using the logarithm as we will see. In statistical practice, when we talk about the likelihood function, we almost always mean the *log* of the likelihood so that we often forget to use the word *log* in writing and speaking. See Exercise 5.3 for more on this example.

Next, let's have a look at this log-likelihood function. Figure 5.11 illustrates the log-likelihood function $\Lambda(\mu, \sigma)$ in (5.10). This figure is plotted using the code given in Output 5.2. This code uses the `persp()` function which plots three-dimensional objects with options for different perspectives and shading.

The perspective plot of the log-likelihood $\Lambda(\mu, \sigma)$ is given in Fig. 5.11. This figure shows us that the log-likelihood Λ is a function of the parameters

Output 5.2: Code to produce Fig. 5.11

```

trange <- seq(from = 0, to = 10, length = 25) # range of theta
srange <- seq(from = 6, to = 14, length = 25) # range of sigma
drawll <- function(th,sig) # the log-likelihood
{
  sum(dnorm(z, mean = th, sd = sig, log = TRUE))
}
# evaluate the log-likelihood at every pair of parameter values
zvals <- matrix(0, length(trange), length(srange))
for (i in 1 : length(trange))
  { for (j in 1 : length(srange))
    { zvals[i, j] <- drawll(trange[i], srange[j])}
  }
}

persp( x = trange, y = srange, z = zvals, cex.lab = 1.2,
       zlim=c(min(zvals), max(zvals) + .5),
       xlab = "mean", ylab = "std deviation",
       zlab = "Log likelihood", col = rainbow(6)[3],
       axes = TRUE, box = TRUE, theta = -30, shade = .3)

```

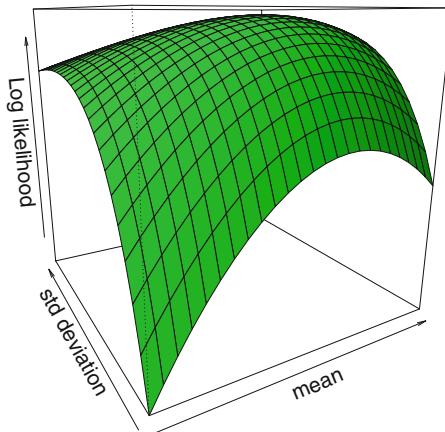


Figure 5.11: The log-likelihood function (5.10)

θ and σ . There is a clear single maximum in these two parameters, and then the log-likelihood falls off as we move away from its maximum. In Exercise 5.3 we find the exact mathematical expressions for the location of this maximum.

How do we use R to find the estimates of the mean and standard deviation parameters that maximize the log-likelihood? The `nlm` program is a very handy program and we will make repeated use of it. Given a function of several variables and a reasonable set of starting values for the parameters,

`nlm` will numerically locate the maximum as well as approximate the first and second derivatives at this minimum. (The `nlm` function was introduced in Sect. 2.7.)

The `nlm` program was written to find the *minimum*, but we are interested in finding a *maximum*. We work around this by defining the *negative log-likelihood*:

```
nl1 <- function(par)      # negative, normal log-likelihood
  -sum(dnorm(z, mean = par[1], sd = par[2], log = TRUE))
```

which will be minimized.

As with the `llik` function, this function calculates the negative log-likelihood function. It is defined by a vector of arguments representing the two parameters to be estimated. The first, `parm[1]` is the mean, and the standard deviation is `parm[2]`.

The `nlm` program is invoked with the name of the function followed by a set of reasonable starting values:

```
nlm(nl1, c(10, 15))  # call nlm with neg log-lik and initial values
```

The output from this program contains the minimum of the negative log-likelihood, estimates of where this occurs, estimated gradient, the number of iterations it took, and finally, an error message:

```
$minimum
[1] 90.06128

$estimate
[1] 7.127638 8.877439

$gradient
[1] 1.870154e-06 5.884479e-06

$code
[1] 1

$iterations
[1] 11

Warning messages:
1: In dnorm(x, mean, sd, log) : NaNs produced
```

Let's explain this output in reverse order, beginning with the error message. The `nlm` program looks for a function minimum and tries many different parameter values in order to get there. The program does not know that the standard deviation must be a positive number and may have tried something invalid in its search. This produced several error messages along the way.

The `$gradient` is a numerical estimate of the first derivatives in each of the two directions of μ and σ . These values are both very close to zero. This is a good indication that the extreme of the function has been achieved. Intuitively, we are at the top of the mountain when the landscape is flat in every direction.

The `$estimate` is the set of parameter values that maximize the log-likelihood (and minimize the negative log-likelihood). The first of this pair is exactly the same as the sample mean (7.127638) except possibly differing in the last digit.

The sample standard deviation (9.060493) and the maximum likelihood estimate of σ (8.877439) are noticeably different, however. The difference is explained in Exercise 5.3. Briefly, the usual estimate of the sample variance s^2 given in (5.8) divides the summation by $n-1$ but the maximum likelihood estimate of σ^2 divides by n . That is, the maximum likelihood estimator of σ^2 is

$$\text{maximum likelihood estimator}(\sigma^2) = n^{-1} \sum (z_i - \bar{z})^2 \quad (5.11)$$

and not the more familiar $n-1$ denominator given by s^2 in (5.8). In other words, these two estimates of σ should differ by a factor of $\{n/(n-1)\}^{1/2}$.

In Sect. 2.7, we showed how to capture the output from `nlm`. This ability allows us to use portions of the output in subsequent steps of R. For example, we may want to use the values of the parameter estimates in later steps.

In such simple examples as the estimation of the mean and standard deviation, the mathematics and computer output confirm each other. We will continue the discussion of maximum likelihood estimation in Sect. 6.5. Let's end this section with a numerical method that will bring us to more complicated examples where the mathematics can become burdensome and the answer may not be known in advance.

In this next example, suppose we have data from a normal distribution and want to estimate the *ratio* of the mean to the standard deviation. That is, the (positive-valued) normal mean is denoted by $\mu > 0$ and the standard deviation obeys the relationship

$$\sigma = \alpha\mu$$

for some parameter $\alpha > 0$ that we also need to estimate. This example might arise in a setting where larger values of the mean are associated with measurements that are less precise, such as where the *relative error* (α) remains the same.

In this example we need to estimate the parameters α and μ . It is not obvious what the analytic form of the maximum likelihood estimates are without resorting to calculus. The point of this exercise, then, is to tackle a problem that would otherwise be difficult for us to solve without the help of R.

The negative, log-likelihood function for this model

```
prop <- function(par)           # negative log-likelihood
  -sum(dnorm(z, mean = par[1],
  sd = par[1] * par[2], log = TRUE ))
```

is a function of two parameters: `par[1]` is the mean μ and `par[2]` is the parameter α .

We can then generate some random data values for this problem and use `nlm` to fit the model:

```
(z <- rnorm(50, mean = 10, sd = 20)) # generate some data
nlm( prop, c( 5,5))                 # maximize with starting values
```

In this example, we generate 50 normal variates with known mean ($\mu = 10$) and standard deviation ($\sigma = 20$) so the true ratio α is equal to 2. The `nlm` function minimizes the negative log-likelihood, based on initial starting values of 5 for μ and 5 for α . Usually, our starting values for `nlm` are just good guesses in the neighborhood of the answer. You might try other starting values to see how well `nlm` works, and perhaps, whether it works at all. See Exercise 5.6 for more details.

A portion of the output from `nlm` includes the following:

```
$minimum
[1] 218.96

$estimate
[1] 9.090690 2.123380

$gradient
[1] -1.067062e-05 -4.542913e-05
```

The estimates are then $\hat{\mu} = 9.09$ and $\hat{\alpha} = 2.12$. Both of these estimates are reasonably close to the population values of 10 and 2, respectively. The two gradient values are close to zero indicating good convergence to an extreme minimum of the negative log-likelihood.

There are also error messages, omitted here, indicating attempts by `nlm` to fit the log-likelihood function where it is not defined, specifically where a trial value of the standard deviation $\sigma = \alpha\mu$ might be a negative number. Sometimes `nlm` gets caught in these invalid regions and never seems to get out. One way to avoid this situation is for us to start with reasonable initial values in the search for maximum likelihood estimates. Again, see Exercise 5.6 for guidance.

In conclusion, in this section we showed how we can write programs in R that allow us to fit mathematical models that are unlike those we might see in a textbook. This is an important skill for the data analyst because it opens a much wider range of models to consider as we explore data. In Sect. 6.5

we examine other properties of maximum likelihood estimation in R including hypothesis testing of parameter values and approximating the standard errors of the estimated parameters. In Sect. 7.4, we use maximum likelihood to fit different models and compare these in terms of a formal test of hypothesis. This test of hypothesis allows us to compare different models of the covariance matrix in a multivariate normal distribution.

5.8 Exercises

- 5.1 Consider some data such as the apartment rent values or the CD4 counts. Transform these values to more normal-looking distributions using the Box–Cox transformation (5.5) for different values of λ . Find the value of λ that provides the best fit according to the Jarque–Bera test, the Kolmogorov–Smirnov test, or the Shapiro–Wilk test. Are these different λ s close in value? Explain why this may (or not) be the case.
- 5.2 (a) If u is distributed as uniform between 0 and 1, what is the distribution of the normal quantile x satisfying the equation $\Phi(x) = u$?
 (b) In an ordered sample $u_1 \leq u_2 \leq \dots \leq u_n$ of n observations sampled from a uniform distribution on $(0,1)$, intuitively, where would we expect these values to appear? Use this result to motivate the use of (5.6).
- 5.3 (a) Use the functional form of ϕ given in (5.2) and find a mathematical expression for the likelihood function (5.9).
 (b) Find a mathematical expression for the log of the likelihood.
 (c) Show that the maximum likelihood estimate of σ^2 of the normal log-likelihood is achieved in (5.11). Notice how this expression for the estimate of σ^2 differs from the usual estimate s^2 of the sample variance given in (5.8). The estimator s^2 has the property of being *unbiased*. Argue that with large samples, it should not matter which of these two estimators we use.
- 5.4 The Poisson¹² distribution is defined on nonnegative integers. In the Poisson distribution, the mean is equal to its variance. If X has a Poisson distribution with mean $\lambda > 0$ then

$$\Pr[X = j] = e^{-\lambda} \lambda^j / j! \quad (5.12)$$

for $j = 0, 1, \dots$

¹²Siméon Denis Poisson (1781–1840). French mathematician and physicist.

- (a) Use `rpois(25, lambda=10)` to generate a sample of 25 observations from a Poisson distribution with mean 10.

Examine the QQ plot and test this data for normality. Repeat this exercise using larger and/or smaller Poisson means. Comment on what you see. Confirm that when the mean λ is large, then the Poisson distribution is very similar to the normal.

- (b) Program the Poisson likelihood (5.12). Use `nlm` to obtain the maximum likelihood estimate of the single parameter λ for a sample of Poisson observations.

- (c) What is the functional form of the one-parameter normal distribution when the mean and the variance are equal?

- (d) Program the likelihood of the one parameter normal distribution that you found in part c. Use `nlm` to obtain the maximum likelihood estimate of the single parameter from the sample of Poisson observations you used in part b. How does this estimate compare with the estimate you obtained in part b?

- (e) Use calculus to show the sample mean is the maximum likelihood estimator of λ in a Poisson sample. Does this agree with the estimate you obtained in part b?

- (f) Use calculus to find a closed-form expression for the maximum likelihood estimator of the one parameter normal distribution in part c. Does this agree with the estimate obtained in part d?

- 5.5 (a) Show that the standard normal density function $\phi(x)$ is symmetric about $x = 0$. That is, show $\phi(x) = \phi(-x)$.

- (b) Show that $\phi(x | \mu, \sigma)$ is maximized in x at $x = \mu$. That is, the normal mean is also the mode.

- (c) What does the cumulative normal distribution function $\Phi(x | \mu, \sigma)$ look like when σ becomes very large? What does this say about the distribution of samples from this population?

- (d) What does Φ look like when σ is very small? Similarly, what does this suggest about samples from this distribution?

- 5.6 Try other starting values for the `nlm` program in Sect. 5.7 that fits a standard deviation proportional to the mean. What range of values provide reasonable answers with a relatively small number of iterations? Does your finding depend on the size of the normal sample z ? What happens if you start with invalid parameter values, such as negative estimates of the standard deviation?

- 5.7 Consider the housing data examined in Sect. 2.3. Suppose the average apartment cost is expressible as a linear function of housing costs. That is,

$$\text{Apartment rent} = \alpha + \beta \text{ Housing cost} + \text{error}$$

for parameters (α, β) where the errors are normally distributed with mean zero and variance σ^2 .

- (a) Does this seem to be a reasonable model for the data? Refer to Fig. 3.7, for example, to make your case. Interpret this model in terms of real estate values in different states.
- (b) Write a function in R to calculate the negative log-likelihood in terms of the three parameters (α, β, σ) for this model. Use `nlm` to obtain the maximum likelihood estimates of these parameters.

- 5.8 Find the cutoff points of the categories of the `phiTest` of normality. Specifically, begin with a data set and estimate the mean $\hat{\mu}$ and standard deviation $\hat{\sigma}$. The cut points defined in (5.7) for a standard normal distribution determine the limits of k categories with equal probabilities.
- 5.9 (a) Examine the transformed apartment rents with $\lambda = -0.5$ to see if this provides a better normal fit for this data.
- (b) Find the value of λ that provides the best transformation according to the Pearson test. Does this transformation yield a more normal looking QQ plot than the one in Fig. 5.6?
- (c) Similarly, find the power transformation value of λ that yields the best fit according to the Jarque–Bera test. Compare this value of λ to the value you obtained in part b.
- 5.10 Write a program in R that fits a model for normally distributed data in which the variance σ^2 is proportional to the squared mean μ^2 . That is, $\sigma^2 = \alpha\mu^2$ for some $\alpha > 0$ that needs to be estimated. To avoid any problems that `nlm()` might run into, put a check in your program so that α is a positive number. One way around this possible error is to express α as e^θ for an arbitrary value of θ .
- 5.11 The `hills` data set in the `MASS` library contains the record times of foot races held in the Scottish hills. Obtain the data in R as a `data.frame` using

```
> library(MASS)
> hills
```

	dist	climb	time
Greenmantle	2.5	650	16.083
Carnethy	6.0	2500	48.350
.	.	.	
Cockleroi	4.5	850	28.100
Moffat Chase	20.0	5000	159.833

For each of 35 hills, the data set provides the length of the race, the gain in altitude, and the time of the winning runner in 1984.

- (a) Use R to find means and standard deviations of the distances, altitudes, and times. Are these useful summaries of this data? Do these measurements capture the multivariate character of the observations?
- (b) Why might you expect the distribution of race times, altitudes, and distances to be skewed?
- (c) Plot the data in R and verify that this is indeed the case. See if transformations of the data provide more symmetric distributions. Use the `pairs()` display or other graphical methods described in Chap. 3 to help you make your point.
- (d) There was debate about whether the time value for Knock Hill should be 18.65 or 78.65. Which of these values do you think is the correct one? What statistical evidence can you provide?

Chapter 6

Bivariate Normal Distribution

THE BIVARIATE NORMAL DISTRIBUTION helps us make the important leap from the univariate normal to the more general multivariate normal distribution. To accomplish this, we need to make the transition from the scalar univariate notation of the previous chapter to the matrix notation of the following chapter.

Let us begin with an exploration of the `swiss` data given in the `datasets` library of R. This data is a collection of six demographic variables from 47 French-speaking cantons (provinces) of Switzerland in 1888. At that time, Switzerland was undergoing a *demographic transition* from a time of high fertility rates to the lower rates more commonly associated with developed nations. The `help(swiss)` for this data in R contains more details on the other variables in this data set as well as links for additional data for other parts of Switzerland. This data set will be examined again in Exercise 11.2.

Consider the paired observations made on young men drafted into the army. Figure 6.1 contains a scatterplot of the 47 provinces, plotting percentage of men who claimed agriculture as their principal occupation and the percentage of men with academic examination scores at the highest level. Every canton is represented by one observation in this figure. (The options for the graphical output in the bivariate boxplot routine `bvbox` are discussed in Exercise 3.6.)

One way to think about these observations is as a cloud scattered in the figure. At the center of the cloud observations are more densely gathered, resulting in a thicker fog. At the edges of the scatter plot, observations are more widely dispersed and less frequent. The concept of density of observations will be continued in this chapter and is more formally expressed in

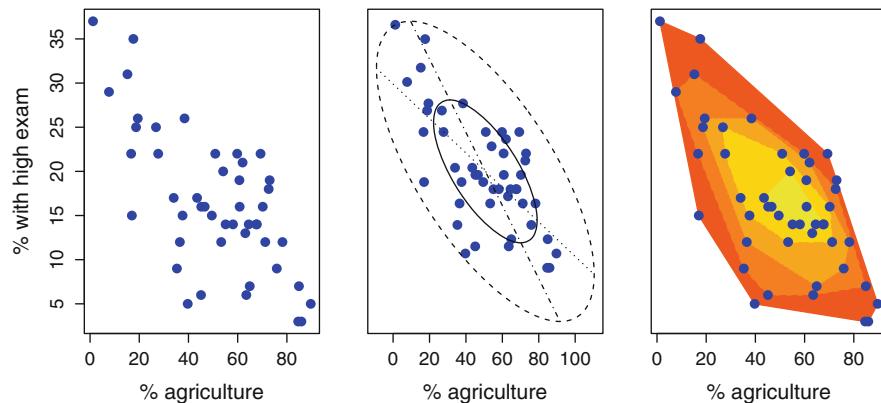


Figure 6.1: Scatterplot of percentage agriculture and high examination scores in 47 Swiss cantons. Data represented as raw scatterplot, bivariate boxplot, and as a five-layer peeling convex hull

the bivariate normal density function given in (6.1), below. Figures 3.10 and 3.22 also use graphical methods to estimate the density of similar sets of observations.

There are several features worth noting in Fig. 6.1. Chief among these is the high degree of association we see: Cantons with lower levels of agriculture are more likely to have higher examination scores. In regression methods (Chap. 9) we try to explain the means of one set of variables from the values of others. In this example we cannot say one of these measurements directly causes the other. The examination scores and agriculture work appear to be negatively associated with each other. Both are probably the result of additional factors.

While there are attributes we can say about either agriculture or examination scores individually, the chief objective of multivariate analysis is to describe the *association* between these two measurements. In this chapter we will use this data to motivate the bivariate normal distribution and show how we model the association between the paired observations of agriculture and examination scores.

6.1 The Bivariate Normal Density Function

Suppose X and Y have normal distributions with respective means (μ_X, μ_Y) and standard deviations (σ_X, σ_Y). Both of the standard deviations are positive valued. In addition to these four parameters there is a *correlation coefficient* ρ of X and Y defined for $-1 < \rho < 1$.

The joint density function is given for all (x, y) by

$$\begin{aligned}\phi(x, y) &= \frac{1}{2\pi\sigma_X\sigma_Y\sqrt{1-\rho^2}} \\ &\times \exp\left[-\frac{1}{2(1-\rho^2)}\left\{\frac{(x-\mu_X)^2}{\sigma_X^2} + \frac{(y-\mu_Y)^2}{\sigma_Y^2} - \frac{2\rho(x-\mu_X)(y-\mu_Y)}{\sigma_X\sigma_Y}\right\}\right]\end{aligned}\quad (6.1)$$

This expression may be intimidating at first glance but a considerable simplification is possible. Notice that every appearance of x is expressed as $(x - \mu_X)/\sigma_X$ which is the representation of a standard normal with mean zero and variance one. A similar expression holds for every appearance of y .

We can then write (6.1) in the much simpler form

$$K \exp\left\{-\left(x^2 + y^2 - 2\rho xy\right)/2(1-\rho^2)\right\}, \quad (6.2)$$

where x and y represent *marginal* standard normal random variates.

When $\rho = 0$, both (6.1) and (6.2) can be expressed as the product of two normal density functions. A product of densities signifies independence so $\rho = 0$ is a special case. See Exercise 6.8 for details. In Exercise 6.3 we see that uncorrelated normals are not necessarily independent. Uncorrelated bivariate normals must be independent.

A study of independence is antithetical to the purpose of multivariate data. We collect data on both x and y in which their relationship is one of the prime motivations of the study.

The value of $K = K(\rho, \sigma_X, \sigma_Y)$ is chosen in (6.2) so that the two-dimensional integral of this expression is equal to 1. In multivariate analysis, the word *marginal* refers to the variables taken individually. All values of ρ between -1 and $+1$ are possible. The limits are usually of little interest because $\rho = -1$ or $+1$ corresponds to settings where X and Y are exactly linear functions of each other.

Specifically, if $\rho = 1$ then Y is expressible as the linear combination

$$Y = \rho(X - \mu_X)\sigma_Y/\sigma_X + \mu_Y$$

with a positive slope σ_Y/σ_X . If $\rho = -1$, then this slope is negative.

If there is a perfect linear relationship between X and Y , then the bivariate data is expressible as a one-dimensional problem. As an example, knowing the temperature in Celsius does not tell us any more than knowing the value in Fahrenheit. The estimation of the slopes and intercepts of linear relationships and related linear regressions is discussed in Chap. 9.

In summary then, values of correlations near -1 , 0 , or $+1$ are all special cases to be treated differently. Most of our interest lies in situations where ρ is either between -1 and 0 or else between 0 and $+1$.

The marginal distribution is that obtained by integrating out the other variable(s). The marginal distributions of X and Y are also normal with the same respective means and variances as given in the bivariate distribution (6.1). A simple approach to analyzing and modeling bivariate normal data, then, would be to consider each variable separately. This defeats the purpose of multivariate analysis in which we want to describe the relationship between X and Y .

In discussion of the bivariate normal distribution, another parameter that is frequently discussed in describing the relationship between X and Y is the *covariance*. The covariance is defined as the expected value of

$$(X - \mu_x)(Y - \mu_y).$$

In terms of the parameters of the bivariate normal distribution, the covariance is equal to

$$\text{Cov}(X, Y) = \rho \sigma_X \sigma_Y. \quad (6.3)$$

The covariance is represented by the symbol σ_{XY}^2 . In Sect. 6.3 we discuss estimating the covariance.

It is often convenient to express the variances and covariance in a symmetric matrix, denoted by Σ . The variances appear on the diagonal and the off-diagonal is the covariance:

$$\Sigma = \begin{pmatrix} \sigma_X^2 & \sigma_{XY}^2 \\ \sigma_{XY}^2 & \sigma_Y^2 \end{pmatrix} = \begin{pmatrix} \sigma_X^2 & \rho \sigma_X \sigma_Y \\ \rho \sigma_X \sigma_Y & \sigma_Y^2 \end{pmatrix}. \quad (6.4)$$

There is also a matrix representation of (6.1). Let us define $\mu = (\mu_1, \mu_2)$ to be the vector of means and use (6.4) to denote the matrix of variances and covariance. We can verify

$$\text{Det}(\Sigma) = \sigma_X^2 \sigma_Y^2 (1 - \rho^2)$$

from (4.5) and find Σ^{-1} using (4.7).

The density function of the bivariate normal distribution (6.1) can be written as

$$\phi(\mathbf{x} | \mu, \Sigma) = (2\pi)^{-1/2} \text{Det}(\Sigma)^{-1/2} \exp \left\{ -1/2(\mathbf{x} - \mu)' \Sigma^{-1} (\mathbf{x} - \mu) \right\} \quad (6.5)$$

for $\mathbf{x} = \{x, y\}$, using matrix notation.

What does the bivariate normal density function look like? Figure 6.1 suggests ellipses stacked on top of each other. The appearance is similar to an oval wedding cake, as seen in Fig. 6.2. These images are all drawn with $\sigma_X = \sigma_Y$. If the marginal standard deviations were not equal, then

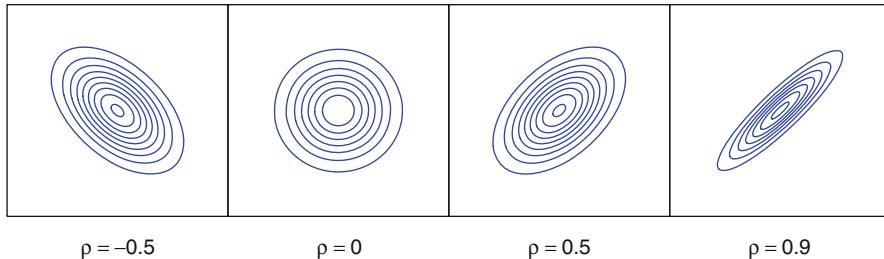


Figure 6.2: Contours of a bivariate normal density function with specified correlations

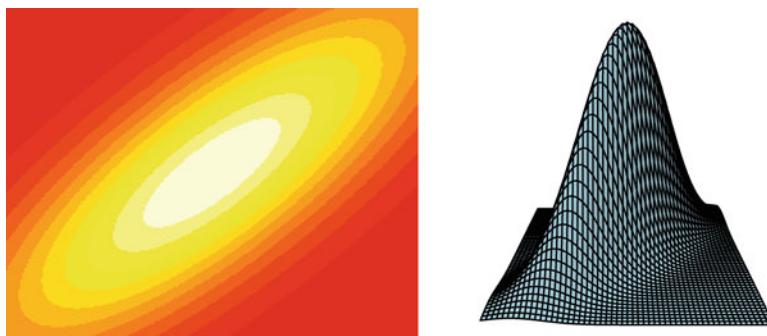


Figure 6.3: A bivariate normal density function with correlation 0.8, drawn using `image` and `persp`, both in the `graphics` package

these figures would be stretched vertically (for larger values σ_Y) or stretched horizontally (for larger σ_X).

The contours of constant density of $\phi(x, y)$ are ellipses. These are circular for a correlation of zero, indicating that the shape is the same any way we rotate the figure. The ellipses will tilt either towards the right or the left depending on whether the correlation is positive or negative. It is clear that the correlation in the Swiss data plotted in Fig. 6.1 corresponds to a negative correlation. Correlations close to either -1 or $+1$ result in thin ellipses corresponding to the almost perfect linear relationship between the two variables.

See Exercise 6.2 for details on how to draw the contour plots of Fig. 6.2. Two other graphical methods for depicting the bivariate normal density function are given in Fig. 6.3 using a heat image and a perspective plot.

In R there are a variety of computing options. The `fMultivar` library, for example, offers a variety of functions, specific to the bivariate normal distribution. In particular, the `dnorm2d` function in `fMultivar` calculates the bivariate normal density (6.1).

6.2 Properties of the Bivariate Normal Distribution

There are important features of the bivariate normal distribution that will be described here: marginal and conditional distributions of the bivariate normal are also normally distributed, as are linear combinations. These features also hold in the more general multivariate normal distribution studied in the following chapter. The marginal distributions refer to X or Y considered alone. Conditional distributions refer to X at a given value of Y or vice versa.

The marginal distributions of the bivariate normal distribution are also normally distributed. This is generally a useful property because it suggests that each variable in a multivariate data set can be examined individually. Of course, such an approach loses the multivariate character of the observations.

Another useful property of (6.1) is that the conditional distributions are also normally distributed. Specifically, for any given value or range of X , the corresponding values of Y are also normally distributed. In practical terms of data analysis, this suggests that we can examine the Y values as normals, separately for different ranges of X .

As an example, Fig. 6.4 divides the agriculture rates into quartiles. (Each quartile contains one quarter of the observations.) Within each quartile, we plot the corresponding set of examination scores giving a series of four boxplots. The model of the bivariate normal distribution suggests that each of these four separate boxplots should depict a different normal distribution. This is a popular approach for examining bivariate data.

We should expect, for example, some ordering among the means across the data slices. We can exploit this property and use all of the observations to measure this trend, rather than look at the data though a number of small slices. In Chap. 9 we discuss linear regression which estimates the slope and intercept of this trend.

When we sample from the bivariate normal density function (6.1), the conditional distribution of Y for any given value of $X = x$ is also normally distributed with mean

$$\mu_Y + \rho(x - \mu_X)\sigma_Y/\sigma_X \quad (6.6)$$

and variance

$$(1 - \rho^2)\sigma_Y^2. \quad (6.7)$$

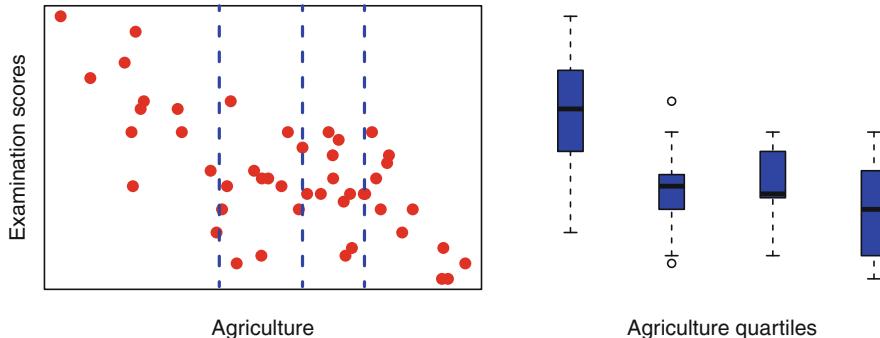


Figure 6.4: Scatterplot of Swiss agriculture and examination scores. Boxplots are given for each quartile of the agriculture values

We can make several points on the basis of these last two equations. In (6.6), we see that the conditional mean of Y is a linear function of a known value of X . This property is explored in Chap. 9 on linear regression. Notice the conditional variance of Y in (6.7) is always smaller than the marginal variance, σ_Y^2 . This reduction in the variance demonstrated the benefit achieved by knowing the value of X . Further, the conditional variance in (6.7) is the same for every value of X . One assumption of linear regression is the constant variance, conditional on X , yet independent of the value of X .

Another important feature of the bivariate normal distribution is every linear combination of X and Y is also normally distributed. For any values of α and β , the random variable $\alpha X + \beta Y$ also has a (univariate) normal distribution. This is a useful property and will be more fully exploited in Chap. 8 when we seek to reduce the dimensionality of a multivariate problem by combining several variables together in this linear fashion.

We can use this property to transform a correlated bivariate normal pair and into two independent normals. Specifically, suppose (X, Y) are a pair of random variables sampled from the density function (6.1) with some correlation ρ , not necessarily equal to zero.

Define

$$Z_1 = X / \sqrt{2\sigma_X} + Y / \sqrt{2\sigma_Y} \quad (6.8)$$

and

$$Z_2 = X / \sqrt{2\sigma_X} - Y / \sqrt{2\sigma_Y}. \quad (6.9)$$

Marginally, both Z_1 and Z_2 are distributed as standard normals. The joint distribution of (Z_1, Z_2) is also a bivariate normal with $\rho = 0$.

Uncorrelated bivariate normal random variates are also independent. This construction of Z_1 and Z_2 illustrates that we can begin with correlated normal variates and create a linear combination of these that is uncorrelated.

On the basis of a simple linear transformation of the data, we can create a pair of independent observations, remove the correlation, and eliminate the need to describe the multivariate character of the paired observations. The problem with this approach is that Z_1 and Z_2 may not have simple interpretations. They represent linear combinations of measurements that are conceptually different from each other. This lack of simple interpretation results from two different combinations of the original measurements. In the Swiss data example, Z_1 and Z_2 represent sums and differences of agriculture rates X and examination scores Y . It is not intuitive how to interpret sums and differences of these two measurements in the present example. However, in Chaps. 8 and 10, this feature will be exploited to identify groups of variables that can be combined in order to reduce the dimensionality of the data.

In summary, the marginal and conditional distributions of the bivariate normal are also normally distributed. Linear combinations of normals are also normally distributed. These properties are also true of the more general multivariate normal distribution described in Chap. 7.

6.3 Inference on Bivariate Normal Parameters

We estimate the mean and standard deviation parameters of the bivariate normal distribution in the familiar manner used in the univariate distribution. So we have

$$\hat{\mu}_X = \bar{x} = n^{-1} \sum_{i=1}^n x_i$$

and

$$\hat{\sigma}_X^2 = s_X^2 = (n-1)^{-1} \sum_{i=1}^n (x_i - \bar{x})^2$$

with similar expressions for $\hat{\mu}_Y$ and $\hat{\sigma}_Y^2$.

The sample covariance σ_{XY} is estimated by

$$\hat{\sigma}_{XY} = (n-1)^{-1} \sum_{i=1}^n (x_i - \bar{x})(y_i - \bar{y}).$$

The correlation ρ is estimated by the *Pearson correlation coefficient*

$$\hat{\rho} = \sum_{i=1}^n (x_i - \bar{x})(y_i - \bar{y}) \Big/ \sqrt{\sum(x_i - \bar{x})^2 \sum(y_i - \bar{y})^2}. \quad (6.10)$$

In R, we calculate these statistics using the functions `mean`, `var`, `cov`, and `cor`, respectively.

It is often convenient to express the collected estimators of variances and covariance in a symmetric matrix, denoted by \mathbf{S} . The variances appear on the diagonal, and the off-diagonal is the covariance:

$$\mathbf{S} = \begin{pmatrix} s_X^2 & \hat{\rho} s_X s_Y \\ \hat{\rho} s_X s_Y & s_Y^2 \end{pmatrix}.$$

This matrix is used to estimate the population variance matrix Σ that was introduced in (6.4).

Let's review with an example of the Swiss data. To find the means of the data in each column of this data.frame, we write

```
> colMeans(swiss[, 2 : 3])
Agriculture Examination
50.65957    16.48936
```

Note that the `data.frame` variable labels are attached to the estimates.

Standard deviations of `data.frame` data are obtained using `sapply(., sd)` as in this example:

```
> sapply(swiss[, 2 : 3], sd)
Agriculture Examination
22.711218    7.977883
```

to estimate these univariate values.

The estimator \mathbf{S} of variances and covariances

```
> var(swiss[, 2 : 3])
Agriculture Examination
Agriculture    515.7994  -124.39283
Examination   -124.3928    63.64662
```

is a symmetric matrix. The covariance, on the off-diagonal, is a negative number.

A separate estimate of the correlation coefficient ρ can be obtained using the `cor` function:

```
> cor(swiss[, 2 : 3])
          Agriculture Examination
Agriculture   1.0000000 -0.6865422
Examination  -0.6865422  1.0000000
```

which is also expressed as a symmetric 2×2 matrix.

The correlation of a variable with itself is always equal to 1, so the correlation matrix will always have 1s running down the diagonal. The off-diagonal value -0.687 confirms the negative correlation that is apparent in Fig. 6.1.

The `cor.test` function in R produces confidence intervals and tests the null hypothesis that the population correlation coefficient is zero:

```
> cor.test(swiss[, 2], swiss[, 3])

Pearson's product-moment correlation

data: swiss[, 2] and swiss[, 3]
t = -6.3341, df = 45, p-value = 9.952e-08
alternative hypothesis: true correlation is not equal to 0
95 percent confidence interval:
-0.8133545 -0.4974484
sample estimates:
cor
-0.6865422
```

The t-test in this output refers to the *Pearson product-moment correlation* transformation

$$t = \hat{\rho} \sqrt{(n - 2)/(1 - \hat{\rho}^2)}.$$

This statistic should behave approximately as a t-statistic with $(n - 2)$ df under the null hypothesis that X and Y are independent and uncorrelated.

The *Fisher Z-transformation* of the correlation is

$$Z = 1/2 \log\{(1 + \hat{\rho})/(1 - \hat{\rho})\}.$$

With large sample sizes, Z should behave approximately as normal with mean zero and standard error $1/\sqrt{n - 3}$ under the null hypothesis that X and Y are uncorrelated. The functions `CIR`, `CIz`, `r2z`, and `z2r` in the `psychometric` library perform these transformations and create confidence intervals of the correlation coefficient.

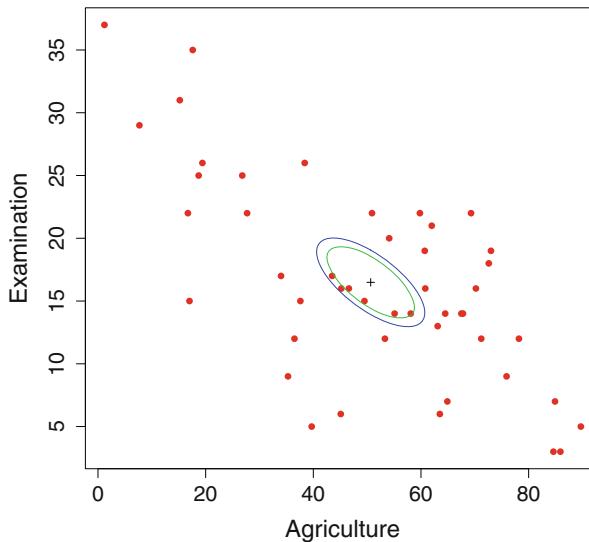


Figure 6.5: Joint 95 and 99 % confidence ellipsoids for bivariate means of Swiss agriculture rates and education scores

There are nonparametric estimators of ρ , as well. See Exercise 6.1 for two nonparametric estimators that are useful when the data contains suspected outliers or may not have been sampled from a bivariate normal parent population.

Marginal confidence intervals for the mean parameter were described in Sect. 5.5. The joint confidence interval of the bivariate normal mean vector $\mu = (\mu_X, \mu_Y)$ is expressed as an ellipse.

The joint confidence contours are values of μ such that

$$(\bar{x} - \mu)' S^{-1} (\bar{x} - \mu) = \chi^2_2/n \quad (6.11)$$

where χ^2 is the upper $1 - \alpha$ quantile of a chi-squared variate with 2 df.

An example of this appears in Fig. 6.5. This figure was drawn in R using the program code for the confidence ellipse of the bivariate means given in Output 6.1. The `bivCI` function returns m evenly spaced coordinates of the confidence ellipse of μ centered at the bivariate means. The ellipse is defined by (6.11) and much smaller than the range of the data. See Exercise 6.9 for more on this.

The `bivCI` function is defined and returns m points on a $1 - \alpha$ confidence ellipse. The code in this output plots the data. We next use `lines` to draw the 99 and 95 % confidence ellipses. The last `lines` statement puts the “+” sign in the center of the figure.

Output 6.1: R code to draw Fig. 6.5

```

bivCI <- function(s, xbar, n, alpha, m)
#  returns m (x,y) coordinates of 1-alpha joint confidence ellipse of mean
{
  x <- sin(2 * pi * (0 : (m - 1)) / (m - 1)) # m points on a unit circle
  y <- cos(2 * pi * (0 : (m - 1)) / (m - 1))
  cv <- qchisq(1 - alpha, 2)                  # chi-squared critical value
  cv <- cv / n                                 # value of quadratic form
  for (i in 1 : m)
  {
    pair <- c(x[i], y[i])          # ith (x,y) pair
    q <- pair %*% solve(s,pair) # quadratic form
    x[i] <- x[i] * sqrt(cv / q) + xbar[1]
    y[i] <- y[i] * sqrt(cv / q) + xbar[2]
  }
  cbind(x, y)
}

plot(biv, col = "red", pch = 16, cex.lab = 1.5)
lines(bivCI(s = var(biv), xbar = colMeans(biv), n = dim(biv)[1],
            alpha = .01, m = 1000),
      type = "l", col = "blue")
lines(bivCI(s = var(biv), xbar = colMeans(biv), n = dim(biv)[1],
            alpha = .05, m = 1000),
      type = "l", col = "green", lwd = 1)
# Add '+', sign
lines(colMeans(biv)[1], colMeans(biv)[2], pch = 3, cex = .8,
      type = "p", lwd = 1)

```

Table 6.1: US age-adjusted cancer rates for males in 50 states and DC for 2007 and 2008

State	2007	2008
	Rate	Rate
AL	584.5	591.0
AK	526.0	528.3
...		
WI	545.8	514.9
WY	508.9	520.0

Source: CDC

6.4 Tests for Bivariate Normality

The test of bivariate, and more generally multivariate normality, has received considerable attention. Because there are so many ways in which the multivariate normal can fail, we can find a variety of tests for each of these. We begin by pointing out that verifying marginal normality for each of the two variables does not assure that their joint distribution is bivariate normal. See Exercise 6.3 for an example of this behavior.

Rather than discussing tests specifically for the bivariate normal distribution, we will defer the discussion until Sect. 7.7 where we discuss tests for the more general, multivariate normal distribution. Among the most frequently used tests in R are `mvnormtest` in the `mvShapiroTest` library which performs a multivariate Shapiro–Wilk test and `mvnorm.etest` in the `energy` library which performs the energy test.

6.5 Maximum Likelihood Estimation, Part II

In this section, we will use likelihood function to both estimate parameter values and estimate standard errors of these estimates. We first introduced the concept of maximum likelihood estimation in Sect. 5.7 and demonstrated how it can be used to estimate parameters in models you develop. These models may constrain the parameters of the model, for example. The models can take a form that is unique to your application. This section shows how maximum likelihood estimation also provides estimates of the standard errors of the parameter estimates.

Refer back to Fig. 5.11. The peak of the likelihood function indicates the location of the maximum likelihood estimates. We are only interested

in the top so the derivative should be zero (or nearly so) in every direction. The `$gradient` estimate of `nlm` is very close to zero indicating how flat the log-likelihood is at its maximum.

The *second derivative* tells us how curved the log-likelihood is at its maximum. Informally, if the top of the peak is sharp, then there is little uncertainty about where the maximum is located. Conversely, if the top of the peak is broad and flat then the estimate is less reliable.

The `nlm` procedure gives us an estimate of this curvature in the direction of each parameter. The matrix of second derivatives is called the *Hessian*. The inverse of the Hessian matrix is a useful approximation to the variances and covariances of the estimated parameters. We will illustrate how to obtain these estimates in this section.

Another useful feature of maximum likelihood estimates is that these estimates are usually distributed as normal under a wide range of conditions. We can combine this feature with the approximate standard deviations and construct confidence intervals for parameters, as well as their point estimators. Again, this feature will be illustrated in R with an example in the present section.

Let us begin with a data example and then use `nlm` to fit a variety of different bivariate normal models to it. Table 6.1 lists the 2007 and 2008 US male all-cancer age-adjusted rates for each of the 50 states plus DC. Age-adjusted rates take into account the differing demographics of each state. A state with an older population, for example, should not be recording a higher rate of cancer than a younger state simply because of the age differences.

It is always a good idea to print a few of the data values and some summary statistics to verify that these are correct. Output 6.2 includes these for the cancer rate data.

Figure 6.6 plots the bivariate data. Three outliers are identified: Arizona (AZ) has very low rates in both years; DC and Nevada are extreme in this bivariate plot, but are not extreme in either of the 2 years. Multivariate outliers can appear but not be excessive in any of their marginal components. Other than these three points, there is nothing to indicate a lack of fit to the bivariate normal distribution. Figure 6.6 also contains a 45° line illustrating that most of the 2007 rates were higher than those in 2008. The correlation (0.889) of the data values is very high across the 2 years.

Let us fit a bivariate normal distribution to this data. We need an objective function for `nlm` that evaluates the function we need to maximize. There are five parameters to estimate: two means, two variances, and a correlation. A five-parameter objective function that finds the negative log-likelihood for the cancer data appears in Output 6.3. The five parameters in the code are the two means (`par[1]`, `par[2]`), the two variances (`par[3]`, `par[4]`), and the correlation (`par[5]`).

Just before the program ends and returns the value of the negative log-likelihood, the program prints out the value of the parameters, and the value

Output 6.2: Read cancer data and produce some summary statistics

```
> cancer <- read.table(file = "Cancer2007_8.dat",
+   header = TRUE, row.names = 1)
> cancer[1 : 3, ]      # look at the first few

  Rate2007 Rate2008
AL      584.5    591.0
AK      526.0    528.3
AZ      459.2    414.3

> cancer[49 : 51, ]      # look at the last few

  Rate2007 Rate2008
WV      602.1    566.5
WI      545.8    514.9
WY      508.9    520.0

> colMeans(cancer)      # some summary statistics

Rate2007 Rate2008
565.6039 548.7373

> sapply(cancer, sd)

Rate2007 Rate2008
42.95529 41.29989

> var(cancer)

  Rate2007 Rate2008
Rate2007 1845.157 1594.973
Rate2008 1594.973 1705.681

> cor(cancer)

  Rate2007 Rate2008
Rate2007 1.0000000 0.8990581
Rate2008 0.8990581 1.0000000
```

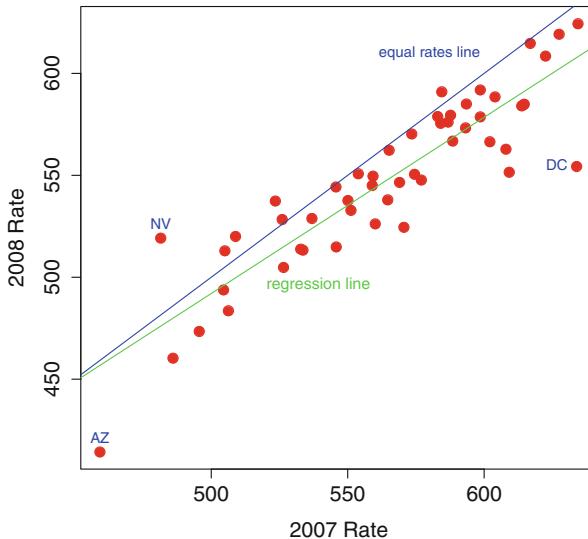


Figure 6.6: US male cancer rates in 2007 and 2008

the program is returning. This is a useful habit to get into. In its search for a minimum of the objective function, we will be able to watch the progress of `nlm`.

Some of the output from the model fitting appears in Output 6.4. The call to `nlm` includes the `hessian=TRUE` option producing an estimate of the Hessian matrix.

Most of the output consists of trial parameter values and the resulting negative log-likelihood. These preceded the output given here and most have been omitted except for the last two lines. The next items in the output, in order, are the value of the negative log-likelihood at its minimum, the parameter estimates, the estimated gradient, the estimated Hessian, some information about the computing effort listed under `$iterations`, and finally an indication of errors.

The estimated means (first two parameters) are the same as those in Output 6.2. The estimated variances are slightly smaller because these estimates have an n in the denominator, rather than the familiar $n - 1$ that we commonly use. The estimated correlation coefficient is about the same as in Output 6.2.

Much of this output (including the error message) was covered in Sect. 5.7. The gradients are all close to zero indicating an extreme of the function has been found. The warnings arise because `nlm` does not know about the ranges of parameter values, specifically that the variances must be positive and the correlation must be between -1 and 1 . (Similar warnings were described in Sect. 5.7.) Let us come back to this in a moment, but first, let's show how estimated standard errors can be obtained from the Hessian.

Output 6.3: Objective function for bivariate normal likelihood

```

library(mvtnorm)      # library with dmvnorm
biv5 <- function(par) # five parameter log-likelihood function
{
  cov <- par[5]* sqrt(par[3] * par[4])
  biv5 <- sum(
    -dmvnorm(cancer, mean=c(par[1], par[2]),
              sigma = matrix(c(par[3], cov, cov, par[4]), 2,2),
              log = TRUE) )
  print(c(par, biv5))
  biv5
}

```

Begin by capturing the output from `nlm`:

```
nlm.out <- nlm(biv5, c(45, 45, 1600, 1600, .8), hessian = TRUE)
```

Verify the output contains the estimated parameter values:

```
> nlm.out$estimate                      # parameter estimates
[1] 565.6097533 548.7412240 1702.6278244 1664.8481304 0.8955175
```

of μ_1 , μ_2 , σ_1^2 , σ_2^2 , and ρ , respectively.

This output also captures the Hessian matrix:

```
> nlm.out$hessian                      # estimated Hessian matrix
[,1]          [,2]          [,3]          [,4]          [,5]
[1,] 1.512443e-01 -1.369701e-01 -2.870247e-06 1.632584e-07 0.04117360
[2,] -1.369701e-01 1.546765e-01 2.345524e-07 -2.677687e-06 0.03584994
[3,] -2.870247e-06 2.345524e-07 3.015783e-05 -1.888685e-05 -0.08762491
[4,] 1.632584e-07 -2.677687e-06 -1.888685e-05 2.615282e-05 -0.04899606
[5,] 4.117360e-02 3.584994e-02 -8.762491e-02 -4.899606e-02 2361.51979607
```

Invert the Hessian matrix,

```
> solve(nlm.out$hessian)                # invert the Hessian matrix
[,1]          [,2]          [,3]          [,4]          [,5]
[1,] 33.3874221505 29.5656957245 1.793796e+00 2.400703e+00 -0.0009145817
[2,] 29.5656957245 32.6465638380 1.606956e+00 2.638535e+00 -0.0008967177
[3,] 1.7937963901 1.6069562639 1.015044e+05 8.360972e+04 5.5010045726
[4,] 2.4007031017 2.6385350535 8.360972e+04 1.086530e+05 5.3565794553
[5,] -0.0009145817 -0.0008967177 5.501005e+00 5.356579e+00 0.0007387387
```

to obtain an estimate of the variance matrix of the estimated parameters.

Output 6.4: A portion of the output from fitting a bivariate normal distribution

```
nlm(biv5, c(45, 45, 1600, 1600, .8), hessian = TRUE)

. . .

[1] 565.6097533 548.7412240 1702.6278244 1665.0146152 0.8956175 483.2521017
[1] 565.6097533 548.7412240 1702.6278244 1664.8481304 0.8957175 483.2518112
$minimum
[1] 483.2518

$estimate
[1] 565.6097533 548.7412240 1702.6278244 1664.8481304 0.8955175

$gradient
[1] 3.811412e-04 -1.424093e-04 -2.471923e-03 1.959478e-03 3.899459e-05

$hessian
[,1]      [,2]      [,3]      [,4]      [,5]
[1,] 1.512443e-01 -1.369701e-01 -2.870247e-06 1.632584e-07 0.04117360
[2,] -1.369701e-01  1.546765e-01  2.345524e-07 -2.677687e-06 0.03584994
[3,] -2.870247e-06  2.345524e-07  3.015783e-05 -1.888685e-05 -0.08762491
[4,]  1.632584e-07 -2.677687e-06 -1.888685e-05  2.615282e-05 -0.04899606
[5,]  4.117360e-02  3.584994e-02 -8.762491e-02 -4.899606e-02 2361.51979607

$code
[1] 2

$iterations
[1] 58

There were 38 warnings (use warnings() to see them)
```

The diagonal elements of the inverse

```
> diag(solve(nlm.out$hessian))          # diagonal elements
[1] 3.338742e+01 3.264656e+01 1.015044e+05 1.086530e+05 7.387387e-04
```

are of most interest to us because these are the estimated variances.

Finally, the square root of these entries

```
> sqrt( diag( solve( nlm.out$hessian ) ) ) # estimated se's
[1] 5.77818502 5.71371716 318.59759219 329.62551825 0.02717975
```

are the estimated standard errors for the five estimated parameters. The parameter estimates are approximately normally distributed with these standard errors so we can easily construct confidence intervals as we show in the following summary.

Let us conclude this section by constructing a summary `data.frame` of all the results obtained:

```
se <- sqrt(diag(solve(nlm.out$hessian)))
q <- qnorm(.975)          # normal 95% interval quantile
upper <- nlm.out$estimate + q * se  # upper 95% CI intervals
lower <- nlm.out$estimate - q * se  # lower 95% CI intervals
summary <- data.frame(
  cbind(nlm.out$estimate, se, lower, upper),
  row.names=c("mean1", "mean2", "var1", "var2", "rho"))
colnames(summary)[1] <- "estimate"
print(summary, digits = 3)
```

The resulting `summary` table is

	estimate	se	lower	upper
mean1	565.610	5.7782	554.285	576.935
mean2	548.741	5.7137	537.543	559.940
var1	1702.628	318.5976	1078.188	2327.068
var2	1664.848	329.6255	1018.794	2310.902
rho	0.896	0.0272	0.842	0.949

The data frame of these summary statistics is a good way to present results in an organized table. In Exercises 6.4 and 6.5, the reader is asked to fit other bivariate normal models to this data.

6.6 Exercises

6.1 See the help file on `cor.test` to learn about the Spearman's ρ and Kendall's τ . These are nonparametric estimators of the correlation coefficient. Nonparametric methods are used when there are outliers or the data may not follow the distribution assumed for the traditional method.

(a) Pick a data set and compute all three estimates of the correlation coefficient.

(b) Add some extreme outliers to the data set and compare the three estimates with those of the original data. Which methods appear to be most robust or insensitive to these introduced outliers?

6.2 Draw plots as given in Figs. 6.2 and 6.3.

(a) Contour plots can be produced by creating a square matrix of values of the bivariate normal density function. The bivariate normal is evaluated using `dmvnorm` in the `mvtnorm` library. More and more closely spaced points used in this matrix will result in smoother contours in your plot. Use this matrix in the `contour` program in the `graphics` library. See the `help` file for a list of the options available for contour plotting.

(b) Obtain images similar to those in Fig. 6.3 using `image` and `persp`.

6.3 There are bivariate distributions whose margins are normal but the joint distribution is not bivariate normal. Consider the function that generates n bivariate pairs

```
checker <- function(n)      # generates n pairs of marginal normals
                           # that are not bivariate normal
{
  checker <- NULL          # start a list
  for (i in 1:n)
  {
    x <- rnorm(2)          # pair of independent normals
    if(x[1]>0)  x[2] <- abs(x[2])
    else      x[2] <- -abs(x[2])
    checker <- rbind(checker, x)
  }
  checker
}
```

(a) Use the `checker` program to generate a large number of bivariate pairs. Plot the individual columns of this `data.frame` and test these using any of the methods described in Sect. 5.4 to see if the separate columns of data are marginally normally distributed.

(b) Plot the bivariate pairs to demonstrate the data does not follow a bivariate normal distribution.

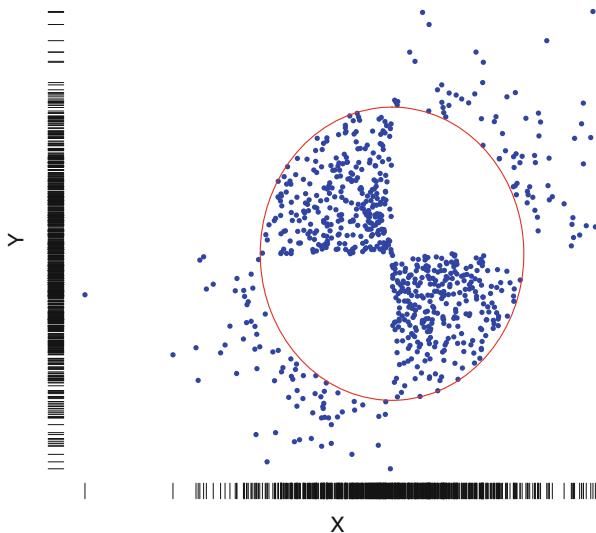


Figure 6.7: Uncorrelated marginal normals that are neither independent nor distributed as bivariate normal

- (c) The bivariate pairs generated in part (a) are positively correlated. Write a program in R that generates uncorrelated pairs that are marginally distributed as normal but do not follow a bivariate normal distribution. Here is one possible solution: Begin with uncorrelated pairs (X, Y) of bivariate normals and transform these to produce the scatterplot given in Fig. 6.7. The transformation is similar to the folding operation we used in the `checker` program. The red circle is added to help visualize that the transformation is different for observations close to and far from the origin.
- (d) Use simulation methods to estimate the diameter of the red circle that results in an uncorrelated bivariate distribution.
- 6.4 Fit an exchangeable bivariate normal model to the data in Table 6.1. A pair of random variables (X, Y) is said to be exchangeable if the ordered pair (X, Y) has the same distribution as does (Y, X) . This model has three parameters: the same mean for both year's cancer rates the same variance for both years and a correlation ρ . Use the Hessian to estimate the standard deviations of the parameter estimates.
- 6.5 Fit the bivariate normal distribution to the data of Table 6.1 in such a way to remove the chance of `nls` trying to use an invalid parameter value. Specifically, write an objective function in R with five arguments: two mean parameters, the two variances measured on a log scale, and

the correlation re-parameterized as

$$\rho = \theta / \sqrt{1 + \theta^2}$$

for all values of θ .

- 6.6 Verify the equivalence of the bivariate normal density function given in (6.1) and the matrix version in (6.5).
- 6.7 Redraw Fig. 6.4 using the coplot, illustrated in Fig. 3.18. Does this plot help show the conditional segments are also normally distributed? What can you say about the variances inside each slice relative to the variance of the whole sample?
- 6.8 When $\rho = 0$, show (6.1) and (6.2) can both be written as the product of two standard normal density functions ϕ given in (5.2).
- 6.9 Why are the ellipses so small in Fig. 6.5? Redraw this figure producing 95 and 99 % confidence ellipses for the population. *Hint:* These are obtained by omitting the “/n” in (6.11).

Chapter 7

Multivariate Normal Distribution

IN THIS CHAPTER, we generalize the bivariate normal distribution from the previous chapter to an arbitrary number of dimensions. We also make use of the matrix notation. The mathematics is generally more dense and relies on the linear algebra notation covered in Chap. 4. In Sect. 4.5 we pointed out there is a limit on what computations we can reasonably perform by hand. For this reason, we illustrate these various operations with the help of R.

The multivariate normal distribution is defined for a vector $\mathbf{x}' = (x_1, x_2, \dots, x_p)$ of p random variates. Recall from Sect. 4.1 that the prime ('') notation refers to the transpose of a vector or matrix. The number of dimensions p is a positive integer but otherwise is not restricted in this chapter. This results in a level of abstraction not found in the previous two chapters in which $p = 1$ and 2, respectively. The reader who has studied the material in those chapters and the linear algebra of Chap. 4 should be comfortable with the development here.

The mean of \mathbf{x} is a p -tuple vector of values denoted $\boldsymbol{\mu}' = (\mu_1, \dots, \mu_p)$ and the variance of \mathbf{x} is a $p \times p$ symmetric matrix $\boldsymbol{\Sigma}$. We will introduce the density function of \mathbf{x} . In this chapter we show how to draw statistical inference on $\boldsymbol{\mu}$ and $\boldsymbol{\Sigma}$ from a data sample.

7.1 Multivariate Normal Density and Its Properties

A useful concept when studying the multivariate normal distribution is the *quadratic form*:

$$\mathbf{x}' \mathbf{A} \mathbf{x} \quad (7.1)$$

for p -tuple vector \mathbf{x} and a square, $p \times p$ matrix

$$\mathbf{A} = \begin{pmatrix} a_{11} & a_{12} & \dots & a_{1p} \\ a_{21} & a_{22} & \dots & a_{2p} \\ \vdots & & \ddots & \\ a_{p1} & a_{p2} & \dots & a_{pp} \end{pmatrix}.$$

Notice although (7.1) involves vectors and a matrix, the result is a scalar. If $p = 1$ then (7.1) is

$$\mathbf{x}' \mathbf{A} \mathbf{x} = a_{11} x^2.$$

When $p = 2$ then the quadratic form (7.1) can be written as

$$\mathbf{x}' \mathbf{A} \mathbf{x} = x_1^2 a_{11} + (a_{12} + a_{21}) x_1 x_2 + a_{22} x_2^2.$$

More generally,

$$\mathbf{x}' \mathbf{A} \mathbf{x} = \sum_{i=1}^p a_{ii} x_i^2 + \sum_i \sum_j a_{ij} x_i x_j.$$

In this chapter we will also be interested in the special case where the matrix \mathbf{A} is symmetric. Recall from Sect. 4.3 that the matrix \mathbf{A} is symmetric if it is equal to its transpose: $\mathbf{A}' = \mathbf{A}$. Similarly, we can say that the matrix \mathbf{A} with entries $\{a_{ij}\}$ is symmetric if $a_{ij} = a_{ji}$ for all valid indices i and j .

In the case where \mathbf{A} is a square, symmetric matrix, then we have

$$\mathbf{x}' \mathbf{A} \mathbf{x} = \sum_{i=1}^p a_{ii} x_i^2 + 2 \sum_{i < j} a_{ij} x_i x_j.$$

The multivariate normal density function of \mathbf{x} can be expressed as a quadratic form $\mathbf{x}' \Sigma^{-1} \mathbf{x}$ for a square, symmetric, nonnegative definite matrix Σ of variances and covariances. Exercise 4.11 shows a square, symmetric

matrix is positive definite if and only if every eigenvalue is positive. Similarly, a square, symmetric matrix Σ is nonnegative definite if and only if every eigenvalue is nonnegative.

We can now introduce the multivariate normal distribution. The parameters of the *multivariate normal distribution* are the mean vector μ and the variance matrix Σ . The mean vector μ is a p -tuple and Σ is a $p \times p$, symmetric, non-negative definite matrix of variances and covariances.

The *multivariate normal density function* is

$$f(\mathbf{x} | \mu, \Sigma) = (2\pi)^{-1/2} \text{Det}(\Sigma)^{-1/2} \exp \left\{ -1/2(\mathbf{x} - \mu)' \Sigma^{-1} (\mathbf{x} - \mu) \right\}. \quad (7.2)$$

When \mathbf{x} is a scalar, this expression reduces to the usual univariate density function given in (5.2). Notice the quadratic form in the exponential function. The formula (7.2) may seem rather daunting at first glance. We will not have much need to refer to it because it is available as a programmed feature in R. This function is called `dvttnorm()` and is found in the `mvtnorm` library.

The vector $\mathbf{x} - \mu$ behaves as multivariate normal with mean vector $\mu = \mathbf{0}$ and variance Σ . A property of the multivariate normal variate \mathbf{x} is that every linear combination of \mathbf{x} also has a multivariate normal distribution. Specifically, if \mathbf{A} is an arbitrary $q \times p$ matrix, then $\mathbf{A}\mathbf{x}$ is a q -tuple that behaves as a multivariate normal with mean $\mathbf{A}\mu$ and $q \times q$ variance matrix $\mathbf{A}\Sigma\mathbf{A}'$.

The marginal and conditional distributions of the multivariate normal also behave as multivariate normal. Specifically, let us partition the multivariate normal vector \mathbf{x} into a pair of subvectors and write

$$\mathbf{x} = \begin{pmatrix} \mathbf{x}_1 \\ \mathbf{x}_2 \end{pmatrix}.$$

The corresponding vector of means has a similar representation:

$$\mu = \begin{pmatrix} \mu_1 \\ \mu_2 \end{pmatrix}$$

and the variance matrix can be partitioned as

$$\Sigma = \begin{pmatrix} \Sigma_{11} & \Sigma_{12} \\ \Sigma_{21} & \Sigma_{22} \end{pmatrix}.$$

The marginal distribution of \mathbf{x}_1 (ignoring \mathbf{x}_2) behaves as multivariate normal with mean μ_1 and variance matrix Σ_{11} . The conditional distribution of \mathbf{x}_1 given the value of \mathbf{x}_2 also behaves as multivariate normal with mean

$$\mu_1 - \Sigma_{12}\Sigma_{22}^{-1}(\mathbf{x}_2 - \mu_2) \quad (7.3)$$

and variance

$$\text{Var}(\mathbf{x}_1 \text{ given } \mathbf{x}_2) = \boldsymbol{\Sigma}_{11} - \boldsymbol{\Sigma}_{12}\boldsymbol{\Sigma}_{22}^{-1}\boldsymbol{\Sigma}_{21}. \quad (7.4)$$

These conditional means and variances generalize the bivariate values given in (6.6) and (6.6), respectively. As in (6.6), the conditional variance is independent of the value of \mathbf{x}_2 and is smaller than the unconditional variance, $\boldsymbol{\Sigma}_{11}$. The conditional mean given in (7.3) is linear in \mathbf{x}_2 . This linear relationship is the motivation for the multivariable linear regression models described in Chap. 9.

7.2 Inference on Multivariate Normal Means

Suppose we have multivariate normal observations $\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n$ where $\mathbf{x}'_i = (x_{i1}, \dots, x_{ip})$. We estimate the multivariate mean vector

$$\hat{\boldsymbol{\mu}} = \bar{\mathbf{x}} = n^{-1} \sum_{i=1}^n \mathbf{x}_i$$

as the component-wise sample averages.

The estimate of the variance matrix $\boldsymbol{\Sigma}$ is denoted by \mathbf{S} and the calculation is analogous to the method used in Sect. 6.3. Specifically, the diagonal elements of \mathbf{S} are marginal variances, and the off-diagonal elements are the corresponding covariances.

Usually \mathbf{S} will be positive definite. If some components of the data \mathbf{x}_i are linearly dependent or there are more observations n than components p , then the matrix \mathbf{S} will be singular and have a zero determinant. We calculate $\hat{\boldsymbol{\mu}}$ in R using `colMeans()`, and \mathbf{S} is found using the `var()` function.

Joint multivariate confidence intervals for the mean vectors $\boldsymbol{\mu}$ are constructed as ellipses, generalizing (6.11). Specifically, the $1 - \alpha$ confidence ellipse is the set of all values of $\boldsymbol{\mu}$ for which

$$(\hat{\boldsymbol{\mu}} - \boldsymbol{\mu})' \mathbf{S}^{-1} (\hat{\boldsymbol{\mu}} - \boldsymbol{\mu}) = \chi^2/n \quad (7.5)$$

where χ^2 is the upper $1 - \alpha$ percentile of the chi-squared distribution with p df.

There is a generalization of Student's t-test for multivariate data. The multivariate t-distribution is available as `pmvt()` function in R, but it is better to describe the test procedure. Specifically, suppose we have two p -dimensional multivariate normal samples denoted by $\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n$ and $\mathbf{y}_1, \mathbf{y}_2, \dots, \mathbf{y}_m$ with respective population means $\boldsymbol{\mu}_X$ and $\boldsymbol{\mu}_Y$. We estimate

the means as sample averages, so $\hat{\mu}_X = \bar{x}$ and $\hat{\mu}_Y = \bar{y}$. The sample covariance \mathbf{S} is estimated as the sample covariance from the pooled sample of $x - \hat{\mu}_X$ and $y - \hat{\mu}_Y$.

We want to test the null hypothesis that the population means μ_X and μ_Y are equal. One approach is to examine each individual component, marginally, and then perform a correction for the multiplicity of the tests. This approach has some loss of efficiency because of correlations between the individual variables (components of the \mathbf{x} 's and \mathbf{y} 's).

Intuitively, the solution is to examine a statistic based on the differences of means $\hat{\mu}_X - \hat{\mu}_Y$. Then use the analogy to (7.5) giving rise to the statistic

$$T^2 = (\hat{\mu}_X - \hat{\mu}_Y)' \mathbf{S}^{-1} (\hat{\mu}_X - \hat{\mu}_Y) \quad (7.6)$$

also known as the Hotelling¹ T^2 statistic. Under the null hypothesis of $\mu_X = \mu_Y$ the T^2 statistic behaves as a multiple of the F distribution.

Let us demonstrate the use of this generalization of the two sample t-test in an example from a physiology study. The `LASERI` data in the `ICSNP` library is a data frame with 32 measurements made on each of 223 healthy Finnish subjects. The subjects were monitored while in a supine position and then again with their heads elevated on a motorized table. We will concentrate on four measurements and their average differences: average heart rate (`HRT1T4`); average cardiac output (`COT1T4`); average systemic vascular resistance index (`SVRIT1T4`); and average pulse wave velocity (`PWVT1T4`). Each of these variables is expressed as a difference of the pre- and post-tilt values. Testing equality of means of pre- and post-values is the same as testing whether each of the variables in the data has a zero population mean. More detail on this study and the other variables in the data frame are available in `help(LASERI)`.

The four physiology measurements are plotted in Fig. 7.1 with the axes indicating the zero values. In each of the displays, the zero values seem to occur at or near the center of the data mass so it seems reasonable to test the hypothesis that the pre- and post-tilt means are equal. The one-sample Hotelling test for these differences is available in the `ICSNP` library and gives us

```
> HotellingsT2(LASERI[, 25:28])
Hotelling's one sample T2-test

data: LASERI[, 25:28]
T.2 = 101.6741, df1 = 4, df2 = 219, p-value < 2.2e-16
alternative hypothesis: true location is not equal to c(0,0,0,0)
```

¹Harold Hotelling (1885–1973). US mathematician, statistician, and economist.

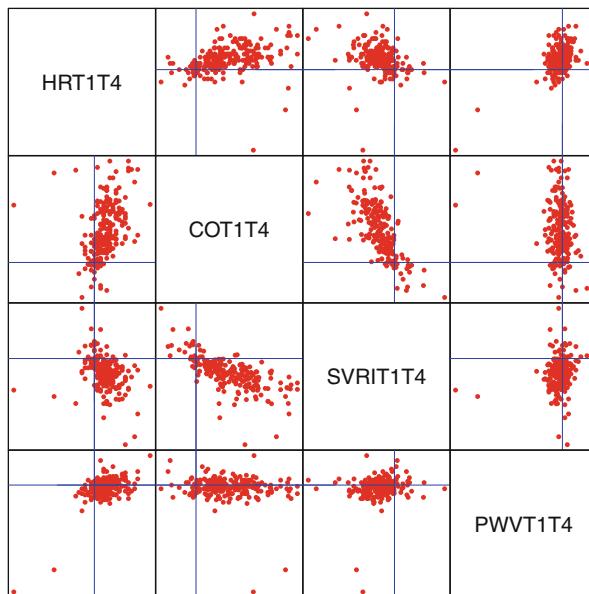


Figure 7.1: Differences in four physiological measures on 225 subjects in the LASERI study. The zero axes are indicated

providing considerable evidence that the mean measurements are very different in the supine and tilted positions. We conclude that tilting the subject results in very different measures.

Exercises 7.1 and 7.2 ask the reader to perform similar tests on multivariate normal means. In Chap. 9 on multivariable regression, we develop a wider set of models for mean parameters of multivariate normally distributed data. The remainder of this chapter discusses models of the multivariate normal variance parameters and tests of adequacy of the multivariate normal distribution as a model for sampled data.

We next introduce a larger example.

7.3 Example: Home Price Index

The Case–Schiller index is a measure of relative home prices in different US cities. This index does not simply look at average prices but, rather, compares the prices of the *same* homes when they were sold at an earlier date. The index for every city is standardized at the value of 1.00 in the year 2000. The index is updated monthly but only January values are examined here. Table 7.1 shows these values in several major US cities for recent years.

The values for the cities are not entirely independent and are subject to identical market forces such as changes in interest rates on mortgages. There

Table 7.1: The Case–Schiller home price index in January of recent years for several US cities

City	Year								
	2000	2001	2002	2003	...	2009	2010	2011	
Phoenix	1	1.0593	1.1161	1.1710	...	1.1713	1.1176	1.0154	
Los Angeles	1	1.1088	1.2145	1.4427	...	1.6655	1.7297	1.6988	
San Diego	1	1.1754	1.2879	1.5540	...	1.4826	1.5695	1.5703	
⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮
Portland	1	1.0392	1.0813	1.1369	...	1.5380	1.4729	1.3580	
Dallas	1	1.0649	1.1176	1.1389	...	1.1260	1.1730	1.1409	
Seattle	1	1.0670	1.1179	1.1580	...	1.5438	1.4509	1.3541	

Source: S&P Dow Jones Indices. Used with permission

was boom in housing prices in 2008 that affected all cities, but some were more affected than others. External forces in the global economy affect all cities, but in this examination we will treat the cities as independent and only model the correlation across years within each city.

The data is index values and compares relative change to the baseline value of 1.00 in the year 2000. Similarly, this does not allow a comparison of one city's prices with another but, rather, each city's change from the year 2000. Such changes are multiplicative: a value of 1.100 indicates a 10% increase in prices since 2000 for example, so we will take logarithms of this data in all subsequent examinations of this example. The spaghetti plot of the data appears in Fig. 7.2, with the annual means in red and the values for one extreme city identified.

The means and standard deviations for each year are plotted in Fig. 7.3. The year 2000 data is included with a mean and standard deviation of zero. The means (and to a smaller extent, the standard deviations) follow an inverted “U” shape: increasing between 2000 and 2008 and then decreasing in more recent years. In this section we want to develop models of the correlation structure between years. In the following sections we will model Σ and μ separately for the multivariate normal distribution.

The empirical correlation matrix of each year's data with all others is

```
> print(cor(CS), digits = 2)
   2001 2002 2003 2004 2005 2006 2007 2008 2009 2010 2011
2001 1.00 0.80 0.75 0.64 0.53 0.41 0.35 0.33 0.25 0.40 0.45
2002 0.80 1.00 0.96 0.88 0.76 0.65 0.58 0.56 0.53 0.60 0.64
2003 0.75 0.96 1.00 0.97 0.87 0.76 0.70 0.68 0.62 0.68 0.71
2004 0.64 0.88 0.97 1.00 0.96 0.87 0.82 0.78 0.66 0.68 0.71
```

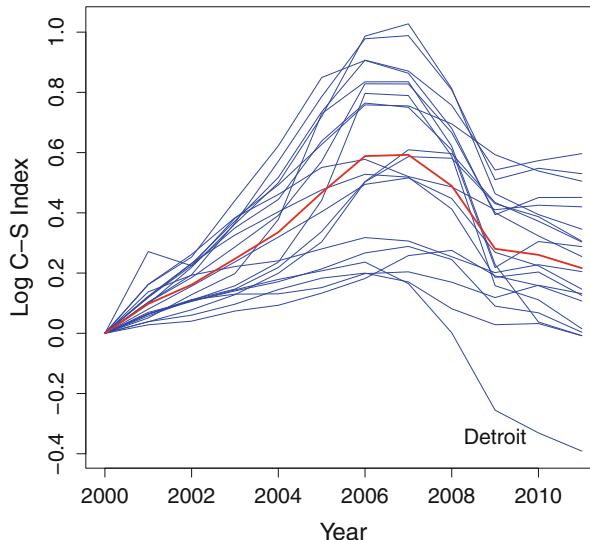


Figure 7.2: Spaghetti plot of home price data. Annual means are in red

```

2005 0.53 0.76 0.87 0.96 1.00 0.95 0.91 0.86 0.66 0.62 0.64
2006 0.41 0.65 0.76 0.87 0.95 1.00 0.99 0.93 0.69 0.63 0.62
2007 0.35 0.58 0.70 0.82 0.91 0.99 1.00 0.97 0.74 0.66 0.64
2008 0.33 0.56 0.68 0.78 0.86 0.93 0.97 1.00 0.87 0.79 0.77
2009 0.25 0.53 0.62 0.66 0.66 0.69 0.74 0.87 1.00 0.96 0.94
2010 0.40 0.60 0.68 0.68 0.62 0.63 0.66 0.79 0.96 1.00 0.99
2011 0.45 0.64 0.71 0.71 0.64 0.62 0.64 0.77 0.94 0.99 1.00

```

This mass of numbers is not particularly useful to us. One area of multivariate analysis is to model, fit, and interpret different patterns of the covariance matrix Σ . Models for this matrix are the subject of this section.

A more useful summary of this *time series* data is the autocorrelation. The autocorrelation is the average correlation between all pairs of years that differ by 1, 2 years, and so on. The differences are referred to as *lags*. More details for time series models are given in Chap. 12.

These autocorrelations are plotted in Fig. 7.4. Adjacent years, with a lag of one, have a very high correlation. Years with a lag of 2 years are also highly correlated, but a little lower than the 1 year lag. This monotone pattern continues, with lower correlations as the lag increases between years being compared.

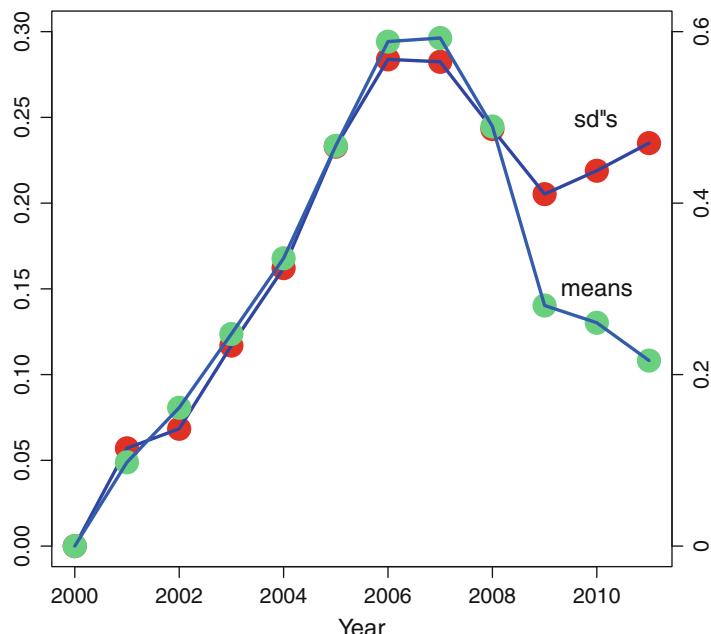


Figure 7.3: Means (*left scale*) and standard deviations (*right scale*) of home price data

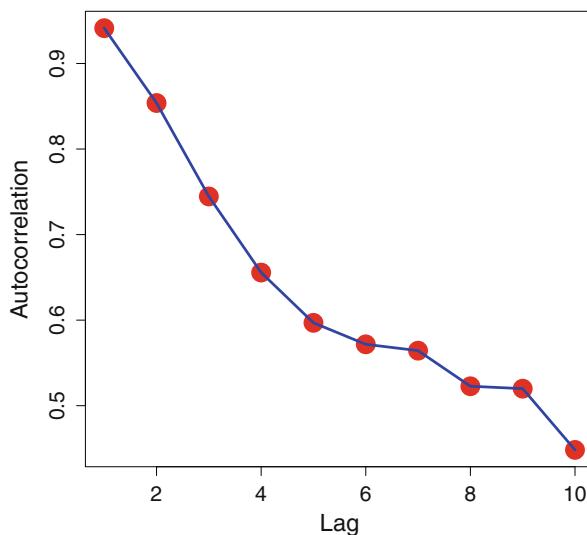


Figure 7.4: Autocorrelation of home price data

7.4 Maximum Likelihood, Part III: Models for Means

We introduced maximum likelihood estimation in Sects. 5.7 and 6.5. This technique allows us to fit a wider variety of models for which there may not exist software. Specifically, in Sect. 5.7, we show how to write programs in R to fit these, and in Sect. 6.5, we use the `nls` program to approximate variances of parameter estimates. In this section we will compare two different fitted models.

Suppose we have two or more competing models for our data and would like to choose the best of these. A simple procedure exists if the models follow a specific relationship with each other. Specifically, two models are said to be *nested* if one is a special case of the other.

As an example of nested models, let us consider the home price index given in Table 7.1. We will fit models for the mean parameters for the different years. The most general model is that of a different mean for each year. This model has 11 parameters: one for each year, excluding the reference year 2000.

A model with means that are linear in year has two parameters (the slope and intercept) and is included as a special case of a model with a different mean parameter for every year. These models are nested. As another example, the model with the same mean for every year is a special case of both the linear model and the model with 11 different mean parameters.

A useful result from mathematical statistics concerns the value of the log-likelihood for nested models and is attributed to Wilks.² The approximation is that twice the difference of two log-likelihoods for nested models, evaluated at their respective maximums, behaves as a chi-squared. The df is the difference in the number of parameters of the nested models.

This *likelihood ratio test* allows us to formally compare two hypothesized models and demonstrate whether the addition of more parameters is worthwhile. Of course, if neither model provides a good fit to the data, then a test of the parameters does not test the adequacy of the models.

Let us work with the home price data given in Table 7.1. The multivariate normal distribution modeling the vector of values for each city has both mean and variance parameters. These will be examined separately: In this section we will fit models to the mean parameters, and in Sect. 7.6 we will examine models for the variance parameters. A more thorough examination of models for means of multivariate normal data is discussed in Chap. 9 on linear regression models.

Begin with a general program that evaluates the negative log-likelihood of the home price data. It is best to write a separate function that evaluates the model of the means.

²Samuel Stanley Wilks (1906–1964). American mathematician, worked at Princeton University.

Output 7.1: A general program that evaluates the multivariate normal distribution

```

mvnMean <- function(parms)
# Log-likelihood function to fit means to a multivariate
# normal distribution to CS data
# meanModel is a function that determines the mean
# Requires the mvtnorm library.

{
  n <- dim(CS)[1]                      # sample size
  p <- dim(CS)[2]                      # number of variables

  mu <- meanModel(parms, p)            # mean vector of length p
  resid <-
    CS - t(matrix(rep(mu, n), p, n)) # subtract the mean
  vm <- var(resid)                   # the variance of the data
  mvnMean <- sum(dmvnorm(resid, log = TRUE,
    sigma = var(resid)))           # multivariate normal density
  print(c(parms, mvnMean))           # likelihood at this estimate
  -mvnMean                            # return negative to minimize
}

```

This program appears in Output 7.1 and will be called by `nlm` to maximize the log-likelihood. The variance matrix (`vm`) is just the empirical variance of the data and is not modeled. Notice that just as this program ends, it prints out the values of all parameters and the likelihood. This is a good method for judging the progress being made by `nlm`.

This program evaluates the negative log-likelihood of the home price data (`CS`) but does not specify a model for the means. The model for the means is determined by another function called `meanModel` that is specified separately. The function that determines the means can easily be changed to accommodate different models, as we will show next.

The `meanModel` program is a function of two arguments: the parameters (`parms`) passed to it from `nlm` and the number of multivariate means (`p`) that are required.

Here is a simple example of such a function:

```
meanModel <- function(parms, p)  rep(parms[1], p)
```

This function specifies a model with one mean for all years in the home-price data. Specifically, there is only one mean parameter. This function makes `p` copies of it and returns that vector of values.

Using this definition of the `meanModel` function, we fit a single-mean model with the R code

```
oneMout <- nlm(mvnMean, 0, hessian = TRUE) # capture output
oneMout                                     # print output
```

A portion of the output is as follows:

```
$minimum
[1] -273.1169

$estimate
[1] 0.05061963

$gradient
[1] 4.718004e-06

$hessian
[,1]
[1,] 32959.48

. . .
```

This output lists the minimum of the negative log-likelihood (-273.1), the estimated value of the single fitted mean (0.0506), the gradient (which is very close in value to zero), and the Hessian or curvature of the log-likelihood.

Finally, we compute the reciprocal, square root of the Hessian to obtain an estimate of the standard error of the estimated mean:

```
print(sqrt(1 / oneMout$hessian), 3)          # est'd std error
[,1]
[1,] 0.00551
```

We are not going to discuss the adequacy of this model except to fit other models for the mean vector and then show how much better these are, relative to increasing the log-likelihood. More detail on fitting regression models, including diagnostics, is discussed in Chap. 9 on multivariate linear regression.

As another example, we can use the function

```
meanModel <- function(parms, p) parms[1] + parms[2] * (1 : p)
```

to fit a model of the means that is linear in the year. The two parameters are, respectively, the intercept (`parms[1]`) and the slope (`parms[2]`) on year. In this model, the year is expressed less 2000. The effect of this recoding is to change the interpretation of the intercept but not the slope.

Output 7.2: R dialog fitting a linear model to the home price data

```

> linMout <- nlm(mvnMean, c(0, 0), hessian = TRUE)
> linMout

$minimum
[1] -286.9895

$estimate
[1] 0.06584120 -0.01725947

$gradient
[1] -2.160050e-06 -1.364242e-06

$hessian
      [,1]      [,2]
[1,] 32959.49 29067.81
[2,] 29067.81 118780.37

$code
[1] 1

$iterations
[1] 4

> invhess <- solve(linMout$hessian) # invert hessian matrix
> sqrt(invhess[1, 1]) # est'd std error of intercept

[1] 0.00622018

> sqrt(invhess[2, 2]) # est'd std error of slope

[1] 0.003276581

```

When we run this new definition of the `meanModel`, it replaces the previous definition of the function. The assignment (`<-`) operation is best thought of as *replacing* the definition rather than *assigning* a definition. Output 7.2 lists the R dialog fitting the linear model and providing parameter estimates.

The call to `nlm` uses the new definition of `meanModel` specifying the mean as a linear function of the year. The initial, starting values for the slope and intercept are both zero. The maximum of the log-likelihood function is 286.99.

Table 7.2: Log-likelihood tests of nested mean models for home price data

Model	Log-likelihood	Compared to one mean		Compared to previous model	
		Chi-squared	df	Chi-squared	df
One mean	273.12				
Linear	286.99	27.75	1	27.75	1
Quadratic	395.84	245.44	2	217.69	1
Separate	426.77	307.31	10	61.87	7

A three-parameter quadratic model of the mean can be fitted using

```
meanModel <- function(parms, p)
  parms[1] + parms[2] * (1 : p) / 10 + parms[3] * ((1 : p) ^ 2) / 100
```

In this function, we recode the year as

$$(year - 2000)/10.$$

The reason for dividing by 10 is to multiply the corresponding parameter values by this amount. Many algorithms will perform better when all parameter values are measured on the same scale, rather than a wide range of values. The interpretation of the parameters needs to be adjusted back when these are reported.

The function that fits a separate mean for every year returns a list of parameter values:

```
meanModel <- function(parms, p)  parms
```

where each of the parameters is the mean for one year.

Let us summarize the log-likelihood of these four nested mean models and the corresponding chi-squared tests in Table 7.2. In this series of models, we see strong evidence that each successive model provides a better fit leading up to the model with a separate mean for each year. Our goal is to provide a model with good explanatory value. The model with a different mean for every year fails to provide any simplification. The quadratic model has fewer parameters, and while statistically not as good as the 11 parameter model, it still provides a good intuitive summary of what we see in Fig. 7.3. That is, relative to the baseline year 2000, home prices increased to around 2008 levels and then declined.

7.5 Inference on Multivariate Normal Variances

The Wishart³ distribution is the generalization of the (univariate) chi-squared distribution to an estimated covariance matrix. In Sect. 5.6, we explained how the univariate sample variance is distributed as a multiple of the chi-squared distribution. The analogous multivariate sample variance matrix has a distribution known as the Wishart distribution. R has functions that can calculate the density of the Wishart distribution as well as generate random covariance matrices from a Wishart distribution. Unfortunately, finding cumulative distributions and tail areas from the distribution involves integrating the distribution over a subset of all symmetric, positive definite matrices. For one-dimensional data, the tail area is easily defined. In the case of random matrices, the range of the distribution of all covariance matrices is much more difficult to describe.

Rather than describing confidence intervals of the whole covariance matrix, we can model the matrix with a small number of parameters. In this section we will describe patterned covariance matrices that have useful interpretations. In Sect. 7.6, we will fit these in R and test hypotheses about them.

The *spherical covariance matrix* is so named because all contours of the density function are circular. In order for this to be the case, we must have all zero correlations. The spherical variance matrix is diagonal:

$$\text{Var}(\mathbf{X}) = \text{Diag}(\sigma_1^2, \sigma_2^2, \dots, \sigma_p^2) = \begin{pmatrix} \sigma_1^2 & 0 & \cdots & 0 \\ 0 & \sigma_2^2 & \cdots & 0 \\ \vdots & & \ddots & \\ 0 & 0 & \cdots & \sigma_p^2 \end{pmatrix}$$

and the corresponding correlation matrix is a $p \times p$ identity matrix.

Spherical covariance is the simplest pattern. It is the model for mutual independence of all p multivariate normal observations. Saying that all multivariate components of the distribution are mutually independent misses the point of modeling such data, however. The model of mutual independence tells us that nothing can be learned over p separate marginal analyses of each component of the data.

A special kind of multivariate dependence includes the *exchangeable* model. Exchangeable means that every multivariate component behaves the same as the others. An example of this appears in Fig. 1.2 where any one observation is representative of all others.

³John Wishart (1898–1956). Scottish mathematician and statistician.

The exchangeable dependence structure is also the same for every member of the multivariate observation. The result is that the exchangeable multivariate normal means and variances as well as every pairwise correlation are the same.

The exchangeable variance matrix is

$$\text{Var } \mathbf{X} = \begin{pmatrix} \sigma^2 & \rho\sigma^2 & \cdots & \rho\sigma^2 \\ \rho\sigma^2 & \sigma^2 & \cdots & \rho\sigma^2 \\ \vdots & \ddots & \ddots & \vdots \\ \rho\sigma^2 & \rho\sigma^2 & \cdots & \sigma^2 \end{pmatrix}. \quad (7.7)$$

The diagonal values are all equal to σ^2 and all of the off-diagonals are equal to $\rho\sigma^2$ for some $|\rho| < 1$.

The exchangeable correlation matrix is

$$\text{Corr } \mathbf{X} = \begin{pmatrix} 1 & \rho & \cdots & \rho \\ \rho & 1 & \cdots & \rho \\ \vdots & \ddots & \ddots & \vdots \\ \rho & \rho & \cdots & 1 \end{pmatrix}. \quad (7.8)$$

In the exchangeable covariance matrix in (7.7) there are two parameters: the variance σ^2 which is the same for all components of \mathbf{X} and the correlations between any pairs of components, ρ . In most cases we have $\rho > 0$ so there is a mutual positive correlation, and (7.7) will be positive definite. In very restrictive cases, we can also have ρ equal to a small negative value even though mathematically (7.7) may no longer be positive definite. What's more, it is difficult to describe a situation where every component is negatively correlated with every other. See Exercise 7.5 for an example of this behavior.

We can also have an exchangeable correlation matrix with different variances. In this case the covariance matrix is

$$\text{Var } \mathbf{X} = \begin{pmatrix} \sigma_1^2 & \rho\sigma_1\sigma_2 & \cdots & \rho\sigma_1\sigma_k \\ \rho\sigma_1\sigma_2 & \sigma_2^2 & \cdots & \rho\sigma_2\sigma_k \\ \vdots & \ddots & \ddots & \vdots \\ \rho\sigma_1\sigma_k & \rho\sigma_2\sigma_k & \cdots & \sigma_k^2 \end{pmatrix} \quad (7.9)$$

or equivalently,

$$\text{Var}(x_i) = \sigma_i^2$$

and

$$\text{Cov}(x_i, x_j) = \rho\sigma_i\sigma_j \text{ for } i \neq j.$$

The variances can all be different. The correlations are the same between all pairs and will also follow (7.8). We will fit the covariance matrix (7.9) to the home price data in Sect. 7.6.

Another commonly encountered patterned covariance matrix appears in observations that are measured in a temporal or serial manner such as the house-pricing data. We will discuss such time series data in more detail in Chap. 12, but for the present, we can intuitively understand observations that are closer to each other should be more highly correlated than observations that are farther apart. If the observations are measured in a uniform fashion (such as every day or every year), then we can expect these correlations to fall off in a prescribed fashion, as we see in Fig. 7.4.

The correlation matrix for autocorrelated observations is of the form

$$\text{Corr } \mathbf{X} = \begin{pmatrix} 1 & \rho & \rho^2 & \cdots & \rho^{k-1} \\ \rho & 1 & \rho & \cdots & \rho^{k-2} \\ \rho^2 & \rho & 1 & \cdots & \rho^{k-3} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \rho^{k-1} & \rho^{k-2} & \rho^{k-3} & \cdots & 1 \end{pmatrix}. \quad (7.10)$$

Specifically, adjacent years have correlation ρ . Years that are two apart have correlation ρ^2 and so on. This model is only useful when $0 < \rho < 1$. Notice that the exchangeable and autocorrelated correlation matrices have the same number of parameters but these have different interpretations and functional forms.

In the next section, we fit patterned variance matrices to the home price data in Table 7.1.

7.6 Fitting Patterned Covariance Matrices

As we see from the summary of fitted models in Table 7.2, the best fitting model for the mean has a separate parameter for every year. We concluded that although this model may be the best fitting one, it lacks a simple message to summarize the data in a succinct manner. By analogy, in Sect. 7.5 we saw that the full correlation matrix is more than we need and a simple patterned matrix can go a long way towards providing a succinct summary of the data.

Mathematically, we can separate the variances and correlations of the variance matrix Σ . Let σ denote the marginal standard deviations of the

multivariate normal \mathbf{x} and let \mathbf{R} denote the matrix of correlations. Then we can write

$$\Sigma = \text{Diag}(\boldsymbol{\sigma}) \mathbf{R} \text{Diag}(\boldsymbol{\sigma}). \quad (7.11)$$

Equivalently, it is more convenient in R to compute this as

$$\Sigma = \boldsymbol{\sigma} \boldsymbol{\sigma}' * \mathbf{R} \quad (7.12)$$

where $*$ represents element-by-element multiplication of two matrices.

Ideally, we can choose a functional form of \mathbf{R} with a useful interpretation such as any of the different matrices described in Sect. 7.5. Similarly, the vector of variances $\boldsymbol{\sigma}$ would be most useful if they followed a prescribed model rather than ranging freely.

We next fit some models using the home price data. Figure 7.5 plots the detrended home price data. That is, the mean value for each year has been removed leaving only the annual variability for us to model. Similarly, the mean of all data values is zero for each year so we do not need to consider the multivariate normal mean parameters. As we saw in Fig. 7.2, one unusual city (Detroit) stands out in this figure and is identified. We will model the variances of the data in Fig. 7.5 in this section. Figure 7.3 demonstrates variances increase up until about 2008 before they decline.

The observations within each city are positively correlated across the years. It is not clear what an appropriate model would be to model this correlation. We can solve this by fitting and then comparing a variety of models.

Next we need general code that allows us to fit a range of models. To do this, break the problem into several small modules that can be tested individually before going on to the next step.

Let us begin with code to build the correlation matrix \mathbf{R} in (7.11). The exchangeable correlation matrix (7.8) with specified size and ρ is created using

```
exchange.mat <- function(size = 1, rho = 0) # build exchangeable matrix
  matrix(rho, size, size) + (1 - rho) * diag(size)
```

Similarly, the autocorrelation matrix (7.10) can be built with

```
autocorr.mat <- function(size = 1, rho = 0) # autocorrelation matrix
  rho ^ abs(row(diag(size)) - col(diag(size)))
```

using code attributed to Peter Dalgaard.

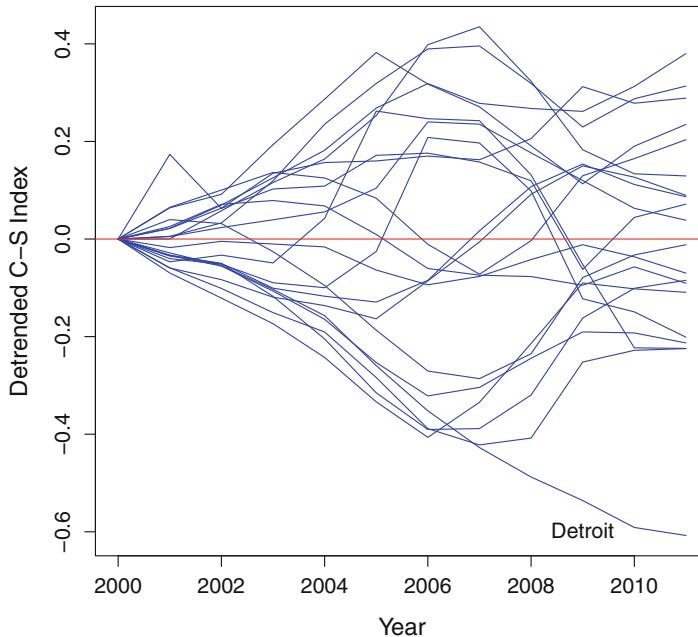


Figure 7.5: Detrended plot of home prices

Next, we write a shell that computes (7.12) from separate programs (`mv.vars` and `mv.cors`) that build the vector of variances σ and correlation matrix \mathbf{R} , respectively.

```

cov.model <- function(size, parms)
# shell to fit patterned covariance matrix
# mv.vars models variances, mv.cors models correlations
{
  rho <- parms[1] # rho is first parameter
  rho <- max(.0001, min(rho, .9999)) # must be between zero and one
  sigma <- sqrt(mv.vars(size, parms[-1])) # model for marginal st dev's
  sigma %*% t(sigma) * mv.cors(size, rho) # covariance matrix
}

```

We should consider the iterated, trial parameter values that will be passed to this program by `nlm` in its search for the maximum likelihood estimates of our model. Let us adopt the arbitrary convention that the first of these parameters will always denote the correlation ρ . The model for σ will depend on the other parameters sent by `nlm`.

In building Σ from trial parameters, `nlm` does not know that ρ must take values between zero and one, so this code enforces the restriction. A similar problem was encountered in Sect. 5.7 when we introduced `nlm` for obtaining maximum likelihood estimates. Similar adjustments will be made in subsequent code.

Output 7.3: Code to evaluate the multivariate normal likelihood for fitting the variance matrix. This program is called by `nlm`

```

fit.cov <- function(parms) # Shell called by nlm
  # Compute the log-likelihood of detrended home price data (detr)
  # Check for positive definite covariance matrix
{
  logl <- 0
  size <- dim(detr)[2]           # width of the detrended data
  cov <- cov.model(size, parms) # the trial built covariance matrix
  print(det(cov))              # check on trial covariance matrix
  if(det(cov) <= 1.0e-30)       # is the covariance positive definite?
  {
    cov <- cov + diag(size)    # adjust the covariance...
    logl <- -1000              # ... and penalize the likelihood
  }
  logl <- logl + dmvnorm(detr, mean = rep(0, size),
                         sigma = cov, log = TRUE)
  logl <- sum(logl)            # log likelihood of detrended data
  print(c(parms, logl))        # trace the progress of nlm
  -logl                         # return negative log likelihood
}

```

The last big step is to compute the log-likelihood of the detrended data (`detr`). The code in Output 7.3 is called by `nlm`, builds the covariance matrix `cov`, and evaluates the multivariate normal log-likelihood `logl` for the detrended home price data, `detr`.

The code for `fit.cov` given in Output 7.3 checks for a singular covariance matrix by flagging situations where the determinant is less than 10^{-30} . The choice of this threshold is arbitrary and was made after watching the printed values from this program. This assures that the matrix is positive definite. If the determinant falls below this value, the program adds a large value to the diagonal, making it more positive definite and also penalizing the log-likelihood. The routine ends by printing the parameter values and the log-likelihood so we can judge the progress made by `nlm`. This is a good practice when attempting to maximize the likelihood using iterative programs such as `nlm`.

The last step is to create a model for the vector of standard deviations, σ . Figure 7.3 provides strong evidence these are not all the same. We need to make sure that values of the parameters passed to us by `nlm` result in positive values of σ . We can avoid problems by modeling $\log \sigma$ as a function of parameters because all parameter values will be valid.

The model with a constant variance for all years

$$\log \sigma_i = \beta_0$$

is fitted using the code

```
mv.vars <- function(size, parms) rep(exp(parms[1]), size)
```

Similarly, we have the log-linear model

$$\log \sigma_i = \beta_0 + \beta_1(\text{year} - 2000)$$

and it is fitted by the R code

```
mv.vars <- function(size, parms)
  pmin( exp(parms[1] + parms[2] * (1 : size)), # log-linear vars
        rep(10, size)) # check for overflow
```

that checks that the σ_i are not too large. The `pmin()` function performs parallel minimums across each element of the vector arguments.

We also fit a quadratic term of the standard deviations on a log scale in order to capture the rising and falling values apparent in Fig. 7.3. This model is

$$\log \sigma_i = \beta_0 + \beta_1(\text{year} - 2000) + \beta_2(\text{year} - 2000)^2$$

and fitted in R using

```
mv.vars <- function(size, parms)
  pmin( exp(parms[1] + parms[2] * (1 : size)
            + parms[3] * (1 : size) ^ 2), # log-quadratic vars
        rep(10, size)) # check for overflow
```

We can fit different patterns of covariance matrices by assigning these functional values to `mv.vars` and `mv.cors`. There are two different correlation models (exchangeable and autocorrelation) and three different models for the marginal variances (constant, log-linear, and log-quadratic) for a total of six possibilities.

As an example of fitting one of these six models, we can write

```
mv.vars <- function(size, parms)
  pmin( exp(parms[1] + parms[2] * (1 : size)), # log-linear vars
        rep(10, size)) # check for overflow
mv.cors <- function(size, rho) exchange.mat(size, rho) # exchangeable
nlm(fit.cov, c(0.7, -5, 0.2), hessian = TRUE) # fit the model
```

to fit a log-linear model of standard deviations with an exchangeable correlation matrix.

Table 7.3: Fitted parameters, estimated standard errors, and log-likelihoods for variance models of the home price data

Model for σ	Likeli- hood	$\hat{\rho}$	SE $\hat{\rho}$	$\hat{\beta}_0$	SE $\hat{\beta}_0$	$\hat{\beta}_1$	SE $\hat{\beta}_1$	$\hat{\beta}_2$	SE $\hat{\beta}_2$
<i>Exchangeable correlation</i>									
One σ	125.8	0.650	0.079	-3.21	0.22				
<i>Autocorrelation matrix</i>									
One σ	256.2	0.927	0.017	-3.39	0.23				
Log- linear	149.8	0.673	0.076	-4.74	0.31	0.229	0.034		
Log- Quadratic	180.2	0.707	0.071	-6.65	0.33	0.977	0.089	-0.060	0.007
Log- Quadratic	292.1	0.939	0.016	-6.12	0.34	0.807	0.085	-0.050	0.007

The fitted values of all six models are summarized in Table 7.3. This table includes the maximized log-likelihood, estimated parameter values, and the corresponding estimated standard errors.

The exchangeable and autocorrelated correlation matrices are not nested so the differences in their log-likelihood values cannot be used as a hypothesis test using the likelihood ratio test. Even so, the likelihood values for the autocorrelated models are much larger, giving good evidence these are better summaries of the data. More formal tests of goodness-of-fit are described in the following section.

Within each of the two types of correlations, the log-linear model has a much larger log-likelihood than the model with a constant standard deviation, and the quadratic model exhibits an even higher log-likelihood. All of these comparisons can be made by differencing the log-likelihoods and treating these as one-half of a chi-squared with 1 df.

7.7 Tests for Multivariate Normality

Section 5.4 presents many different tests for univariate normality. The variety of these is motivated by all the different ways the sample can appear to deviate from the normal distribution. Most of the tests for multivariate normal described in this section are direct generalizations of those univariate methods. Tests will provide a p -value, quantifying the statistical significance of one deviation from the underlying assumption of normality. The test does not end there, however. After rejecting such a hypothesis, we should also explain how and where the normal model failed.

Visual examinations are among the best tools available. One familiar method is to plot the data in a pairwise scatterplot using `pairs()`. Every pairwise plot should appear to be sampled from a bivariate normal distribution. This is not a universal test of multivariate normality, but it can detect many serious deficiencies in the assumed model. Then again, there is no universal test for all of the possible deviations from this model.

Let us next examine a generalization of the QQ plot. We first need to summarize each multivariate observation as a univariate scalar. This is done by describing each observation in terms of its distance from the multivariate mean.

Define the measure

$$D_i^2 = (\mathbf{Y}_i - \bar{\mathbf{Y}})' \mathbf{S}^{-1} (\mathbf{Y}_i - \bar{\mathbf{Y}}). \quad (7.13)$$

The D^2 statistic is a popular metric called the *Mahalanobis distance*.⁴ This is a convenient way to express the *distance* between an observation \mathbf{Y}_i and the multivariate mean $\bar{\mathbf{Y}}$. A useful strategy is to plot the scalar D_i^2 values against chi-squared quantiles. Each D_i^2 is a scalar-valued measure of how far the observed value \mathbf{Y}_i is from the center of the fitted multivariate normal distribution.

The components of \mathbf{Y}_i are correlated and have different variances. For this reason, a simple Euclidean distance would not be appropriate. The \mathbf{S}^{-1} sandwiched between the $(\mathbf{Y}_i - \bar{\mathbf{Y}})$ standardizes the different components. See Exercise 7.6 for details. The formula for D_i^2 appears as the exponent of the normal density function given in (7.2) except the mean and variance have been replaced by their estimates. In other words, the likelihood (or value of the density function) of an observation \mathbf{Y}_i is approximately proportional to $\exp(-D_i^2/2)$.

The individual D_i^2 are not independent because all of the observations are used to estimate $\bar{\mathbf{Y}}$ and \mathbf{S} . However, as an approximation when there are many more observations than variable columns, the D_i^2 should behave as independent chi-squares with df equal to the number of data columns.

Let us illustrate the Mahalanobis distances for the candy nutrition values listed in Table 7.4. After reading the data into a `data.frame` called `candy`, the Mahalanobis distances are calculated in R using

```
mah <- mahalanobis(candy, colMeans(candy), var(candy))
```

where the second and third arguments are the estimated means and variances, respectively.

There are $p = 6$ data columns (calories, fat, saturated fat, carbohydrates, sugar, and sodium), so the ordered Mahalanobis distances from the overall

⁴Prasanta Chandra Mahalanobis (1893–1972). Indian scientist and statistician.

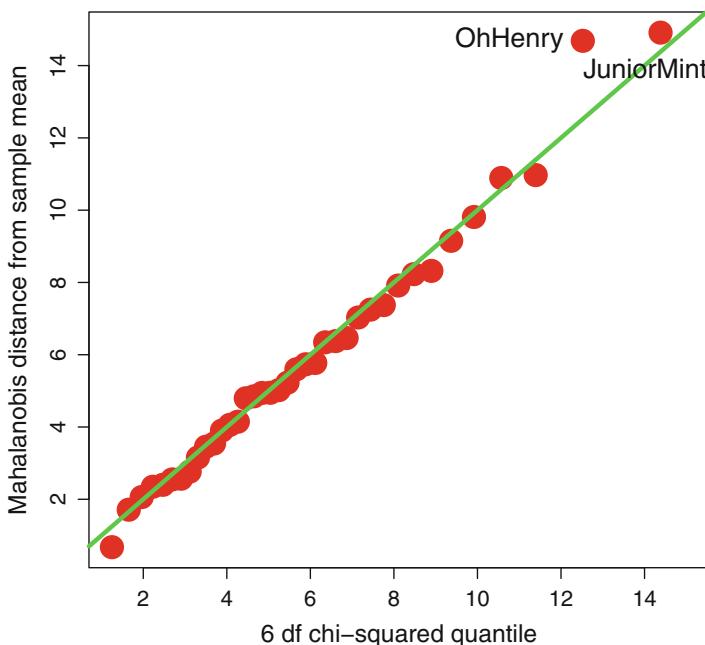


Figure 7.6: QQ plot of Mahalanobis distances of candy nutrition values

six-dimensional mean are compared to a chi-squared with 6 df. This is only an approximation because we are using estimates of the means and variances as their true values. Nevertheless, even a cursory examination of Fig. 7.6 shows this distribution is reasonable. The two most extreme candy brands are identified by name. In the present example, the identification of extreme brands refers to those that are most different from the overall average of all others.

All values in Fig. 7.6 appear to fall on the QQ line connecting the upper and lower quartiles of the chi-squared distribution and those of the data. From this plot, we see there is no evidence of a lack of fit, and the data values appear to follow a multivariate normal distribution.

We can create a test of the adequacy of the fit in this figure by converting the Mahalanobis distances from chi-squared values into normal quantiles. In this case we have:

```
> shapiro.test( qnorm( pchisq( mah, 6 )))
```

```
Shapiro-Wilk normality test
```

```
data: qnorm(pchisq(mah, 6))
W = 0.9893, p-value = 0.9711
```

Table 7.4: Nutritional values of popular candy brands

Name	Calories	Fat	Satfat	Carbs	Sugar	Sodium
100 Grand	190	8	5	30	22	90
3 Musketeers	240	7	5	42	36	90
5th Avenue	260	12	5	38	29	120
Almond Joy	220	13	8	26	20	50
Andes Mints	200	13	11	22	20	20
Baby Ruth	275	13	7	39	32	138
Butterfinger	270	11	6	43	29	135
Cadbury Dairy Milk	260	15	9	28	28	0
Charleston Chew	230	6	5	43	30	30
Dove Smooth Milk Choc.	220	13	8	24	22	25
Goobers	200	13	5	20	17	15
Heath Toffee	210	13	7	24	23	135
Hershey's bar	210	13	8	26	24	35
Hershey's Skor	200	12	7	25	24	130
Junior Mints	220	4	3	45	42	35
Kit Kat	207	10	7	26	20	22
M&M's, peanut	250	13	5	30	25	25
M&M's, plain	230	9	6	34	31	35
Milk Duds	230	8	5	38	27	135
Milky Way	240	9	7	37	31	75
Mounds	240	13	10	29	21	55
Mr Goodbar	250	16	7	25	22	50
Nestle Crunch	220	11	7	30	24	60
Oh Henry!	280	17	7	36	32	65
Payday	240	13	3	27	21	120
Raisinets	190	8	5	32	28	15
Reese's Fast Break	260	12	5	35	30	190
Reese's Nutrageous	260	16	5	28	22	100
Reese's Peanut Butter cups	210	13	5	24	21	150
Reese's Pieces	200	9	8	25	21	55
Reese's Sticks	220	13	5	23	17	130
Rolo	220	10	7	33	29	80
Snickers	230	11	4	32	27	115
Symphony	223	13	8	24	23	42
Twix	250	12	7	33	24	100
Whatchamacalit	237	11	8	30	23	144
Whoppers	190	7	7	31	24	100
Zero Candy Bar	200	7	5	34	29	105

Values collected from www.fatsecret.com. Used with permission

The `pchisq` program converts the Mahalanobis distances (`mah`) into p-values from the reference chi-squared distribution and then `qnorm` turns this into normal quantiles that are needed for the Shapiro–Wilk test. The p-value of the test confirms the good fit seen in Fig. 7.6.

In Fig. 7.7, we present the candy values in a parallel coordinate plot, identifying the two brands that were extreme in the Mahalanobis QQ plot

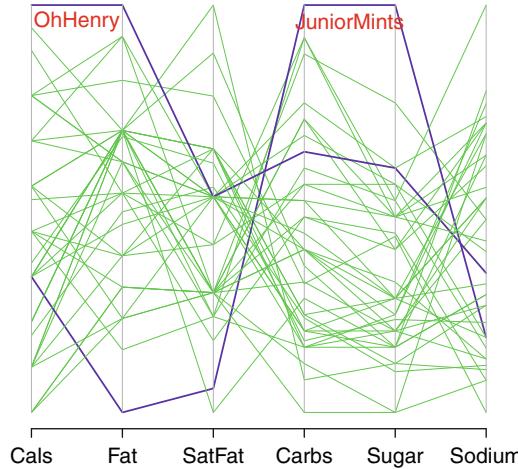


Figure 7.7: Parallel coordinates plot of candy nutrition values identifying the two extremes from Fig. 7.6

of Fig. 7.6. (Parallel coordinate plots were previously described in Sect. 3.5.) Oh Henry! has the largest calories and fat content of all brands. Junior Mints are highest in carbohydrates and sugar but also lowest in fat and very low in saturated fat.

Other tests for the multivariate normal are based on multivariate generalizations of skewness and kurtosis first described by Mardia (1970). By analogy to (7.13), define

$$D_{ij} = (\mathbf{Y}_i - \bar{\mathbf{Y}})' \mathbf{S}^{-1} (\mathbf{Y}_j - \bar{\mathbf{Y}}).$$

We can think of D_{ij} as a Mahalanobis distance between observations \mathbf{Y}_i and \mathbf{Y}_j .

The *multivariate skewness* is defined as

$$\hat{\gamma}_3 = N^{-2} \sum_{i \neq j} D_{ij}^3.$$

The statistic $N\hat{\gamma}_3/6$ will behave approximately as chi-squared with $p(p+1)(p+2)/6$ df when sampled from a multivariate normal distribution.

The *multivariate kurtosis* is defined as

$$\hat{\gamma}_4 = N^{-1} \sum_i D_{ii}^2.$$

The statistic $\hat{\gamma}_4$ will behave approximately as normal with mean $p(p+2)$ and variance $8p(p+2)/N$. The `mardia` test includes additional small sample corrections to approximate the behavior of $\hat{\gamma}_3$ and $\hat{\gamma}_4$.

von Eye and Bogat (2004) recommend multivariate skewness $\hat{\gamma}_3$ as a useful measure of goodness of fit for the multivariate normal. Schwager and Margolin (1982) show that the multivariate kurtosis $\hat{\gamma}_4$ is a good way to test whether multivariate outliers are present in the data. Both of these statistics are programmed in R and are available using the `mardia` function in the `psych` library. There are also versions in the `semTools` library.

If we return to the `candy` data, the R commands

```
> require(psych)
> mardia(candy)
```

return, in part,

```
n.obs = 38  num.vars =  6
b1p =  8.59  skew =  54.4  with probability =  0.54
  small sample skew =  60.02  with probability =  0.33
b2p =  44.86  kurtosis = -0.99  with probability =  0.32
```

and also produce the QQ plot that appears in Fig. 7.6.

From the statistical significance levels given here, we see that there is no evidence of extreme multivariate skewness or kurtosis in this data. Tests of skewness and kurtosis generalize the Jarque–Bera test to multivariate data. Another multivariate Jarque–Bera test is examined in Sect. 12.2 as a test of normality of residuals in a multivariate regression model.

Another test of the multivariate normal distribution is a generalization of the Shapiro–Wilk test for the QQ plot. The packages `mvnormtest` and `mvShapiroTest` both include a multivariate Shapiro–Wilk test.

The code and output for the `candy` data of Table 7.4

```
> library(mvnormtest)
> mshapiro.test( t(candy) )

  Shapiro-Wilk normality test

data:  Z
W = 0.8755, p-value = 0.0005544
```

indicates a poor fit to the multivariate normal distribution. The `mshapiro` program expects the data to be organized as variables in rows and cases in columns, so we must transpose the data matrix using the `t` function.

Let us see if we can identify the source of this problem by examining the individual QQ plots for each of the variables in this data. Figure 7.8 lists these and includes the individual p-values of the Shapiro–Wilk tests. Sugar

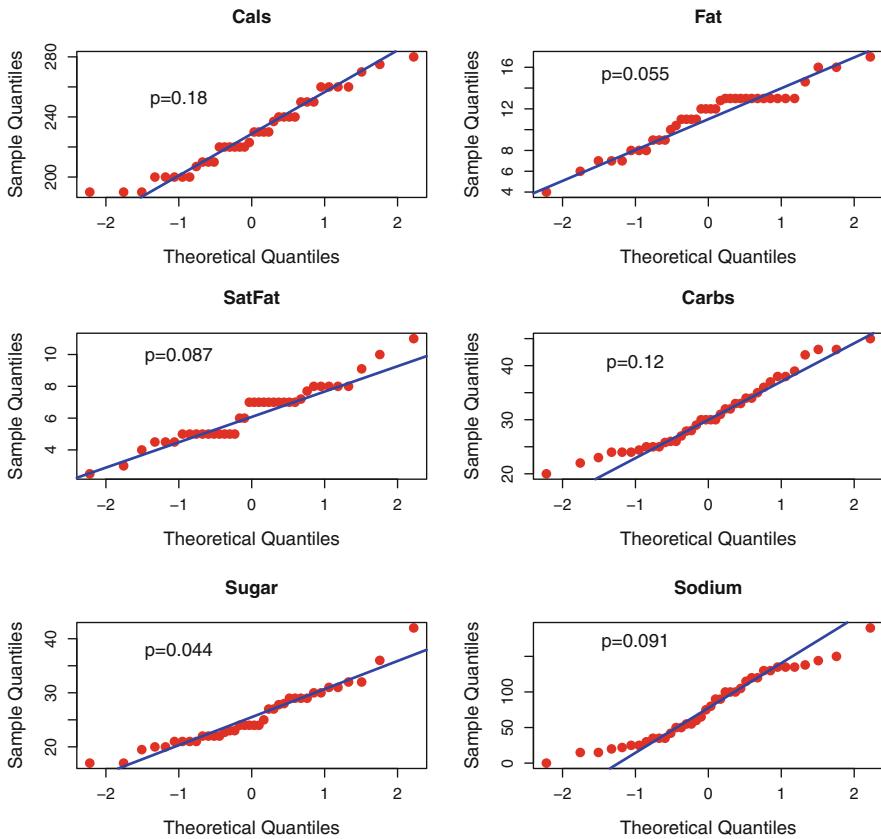


Figure 7.8: Univariate QQ plots for the candy data

and fat values approach statistical significance but their joint effect should be diminished when we take into account the multiplicity of these six hypothesis tests. That is, there is no one standout variable demonstrating a lack of fit. However, when taken collectively, the multivariate Shapiro–Wilk test indicates an overall deficiency. This is often the case with multivariate analyses of data: Overall outliers or lack of fit may not be apparent in marginal analyses of the same data.

As a final method of testing for multivariate normality, let us describe the *energy test*. The energy test is programmed in the library of the same name. Additional mathematical details are described in Székely and Rizzo (2005).

The energy test begins by standardizing the multivariate observations \mathbf{Y}_i by their sample means and variance \mathbf{S} . Specifically,

$$\mathbf{Z}_i = \mathbf{S}^{-1/2} (\mathbf{Y}_i - \bar{\mathbf{Y}}) \quad (7.14)$$

transforms a multivariate normal sample \mathbf{Y}_i into a multivariate sample with zero means and zero covariances.

Recall (see Exercise 4.14) that the matrix square root is not unique, so there is no unique way to perform this transformation. Briefly, the \mathbf{Z}_i are linear combinations of the multivariate data values for each observation and can be interpreted as the square root of the Mahalanobis distances.

The energy test compares the Euclidean distances between the transformed \mathbf{Z}_i and randomly sampled, uncorrelated multivariate normal random variables. The energy test can be written as

$$\text{Energy statistic} = 2A - B - C.$$

Here, B is the average Euclidean distance between the transformed \mathbf{Z}_i and C is the average distance between observations made on a simulated multivariate random sample \mathbf{X}_i with zero means and identity covariance matrix. The A term is the average distance between the \mathbf{X} 's and the \mathbf{Z} 's. Intuitively, this statistic has a large value if the distance between the observed and simulated values is greater than the distances within either the data values or the simulated values.

The energy test, performed on the candy data:

```
> library( energy )
> mvnorm.etest( candy )
```

```
Energy test of multivariate normality: estimated parameters
```

```
data: x, sample size 38, dimension 6, replicates 999
E-statistic = 1.1793, p-value = 0.7638
```

In this case there were 999 replicated random samples \mathbf{X}_i . The energy test does not indicate a lack of fit to the multivariate normal distribution. In Exercise 7.7, we show how to create and interpret *energy residuals* that are related to this statistic. We also point out the *MissMech* package which contains tests of the multivariate normal when there are missing values in the data.

Let us end this section with the same message we gave in Sect. 5.4 on testing for adequacy of the univariate normal distribution. There are many ways in which data can fail to follow a normal distribution. Similarly, there are many good tests available which may return contradictory results: some indicate a good fit while others demonstrate a poor fit.

The real question in this scenario is why are we interested in testing for the fit to the normal model? Most likely it is because we are performing some other statistical procedure that requires normally distributed data. If this is the case, we should be asking how robust the statistical procedure is and how sensitive it is to deviations from the normal model.

7.8 Exercises

- 7.1 The data frame `pulmonary` in the `ICSNP` measures the difference in pulmonary function in 12 workers after being exposed to cotton dust for 6 h. There are three measurements: forced vital capacity, forced expiratory volume, and closing capacity. Plot this data and test for fit to the multivariate normal distribution. Use the Hotelling T^2 statistic to test the hypothesis that the means are the same before and after exposure to the dust.
- 7.2 The data frame `bottle.df` in the `Hotelling` library summarizes a study of the chemical composition of six different Heineken beer bottles. Each bottle was examined ten times, and the glass was assayed for the composition of the elements manganese, barium, strontium, zirconium, and titanium.
- (a) Examine the data using plots to identify outliers. Identify any remarkable outliers or abnormalities. Test the data for multivariate normal distribution, both marginally and within each of the six bottles.
 - (b) Apply the Hotelling test to examine whether the multivariate normal means are the same across the six bottles. Is there evidence that the variance matrices are all the same?
- 7.3 Find the correlation matrix of the OECD PISA academic score data in Table 1.2. Is this suggestive of an exchangeable correlation? Fit this model for the correlation matrix. What is the estimated value of the off-diagonal elements? What does this value tell you? Other examinations of this data appear in Exercises 2.5 and 8.7.
- 7.4 Consider the home price data given in Table 7.1.
- (a) All index values are relative to the value 1 for every city in the year 2000. Does this motivate examining the logarithms of this data?
 - (b) Find the mean index value for each year, over all cities, to see the national trend. Plot these values. Is there evidence of a real estate “boom” or “bust?”
 - (c) Subtract this national, annual trend from each city’s values to identify outliers. Test the adequacy of the multivariate normal model.
- 7.5 Describe a situation where multivariate data is collected and every component is *negatively* correlated with every other. Can this happen in practice?
- 7.6 Show how the \mathbf{S}^{-1} in the sandwich of (7.13) corrects for the different variances. Specifically, write a program in R that computes the \mathbf{Z}_i defined at (7.14). Use R to show the variance of these transformed

Table 7.5: Percentages of obese students in upstate regions of New York State, 2010–2012

Region	Elementary schools		Middle and high schools	
	Overweight	Obese	Overweight	Obese
Central NY	16.8	18.6	17.5	20.7
Finger Lakes	16.0	17.0	16.7	19.5
Hudson Valley	15.2	16.1	16.9	16.6
Nassau-Suffolk	15.8	17.3	16.4	16.1
New York-Penn	16.3	17.5	16.4	20.8
NorthEastern NY	16.0	16.9	16.6	19.2
Western NY	15.2	17.1	17.1	19.8

Source: <https://health.data.ny.gov/>

values is an identity matrix. *Hint:* Use the program for calculating the matrix square root given in Sect. 4.5.6.

- 7.7 Let us look into the details of the energy test and develop a set of residuals for it. Let \mathbf{Z}_i be the normalized data values defined in (7.14) and let \mathbf{Y}_j ($j = 1, \dots, n$) be a set of random multivariate normal values with zero means and identity covariance matrix. Then define

$$\begin{aligned} A_i &= \text{Average } \|\mathbf{Z}_i - \mathbf{Y}_j\| \text{ over all } j \\ B_i &= \text{Average } \|\mathbf{Z}_i - \mathbf{Z}_j\| \text{ over all } j \neq i \\ C &= \text{Average } \|\mathbf{Y}_i - \mathbf{Y}_j\| \text{ over all } i \text{ and } j (i \neq j) \end{aligned}$$

where $\|\cdot\|$ is the Euclidean length defined in (4.4), and $\|\mathbf{Z} - \mathbf{Y}\|$ is the Euclidean distance between the vectors \mathbf{Y} and \mathbf{Z} .

- (a) Interpret the statistics A , B , and C in simple terms.
- (b) Define the *energy statistic residuals* as

$$\text{Energy residual}_i = 2A_i - B_i - C.$$

Write a program in R to calculate the energy residuals for a given set of data.

- (c) The energy residuals defined in this manner are functions of random values \mathbf{Y} and will not be the same every time you generate them. Show for large sample sizes n , the energy statistics have high correlation with the Mahalanobis distances on the data.

- 7.8 The data in Table 7.5 lists rates of student obesity in different regions of New York State for 2010–2012, excluding New York City.
- Display this data in a manner that identifies trends and/or outliers. Are the rates different in the two different grades?
 - Test for multivariate normality. Does the Mahalanobis distance identify the same outliers that you found in part (a)?
 - Fit a multivariate normal distribution to this data with different means and variances but an exchangeable correlation matrix. What is your estimate of the mutual correlation between the four different rates? Interpret this finding.
- 7.9 Write a program in R to calculate the autocorrelation function of the home price data plotted in Fig. 7.4.
- 7.10 There are *robust* estimators of the parameters of the multivariate normal distribution. Robust estimators are described in terms of their *breakdown*. Breakdown is the percentage of observations that can wander off to infinity without greatly affecting the estimator.
- Describe the breakdown properties of a sample mean versus the sample median for a univariate sample.
 - The `cov.rob` program in the `MASS` library performs robust estimation of the multivariate normal mean and variance parameters by identifying and using only those observations closest to the center of the data as measured by their Mahalanobis distance. Use `cov.rob` to estimate parameters of the numeric, demographic parameters in the `LASERI` data. How different are the estimates we obtain from `var`?
 - Try perturbing a fraction of the observations in `LASERI` by a huge amount and see how this affects the estimates. What percent of the observations can be changed before the estimates from `cov.rob` break down? How well do conventional estimators work under these circumstances? Also consider using the `cov.trob` program that estimates parameters of a long-tailed multivariate t-distribution.
- 7.11 Table 7.6 lists the percentage of Americans with disabilities, by age, according to the US Census. Fit a multivariate normal distribution to this data with separate models for the means and variances. As with rates in general, it may be useful to do all of the model fitting after taking logs of the data.
- Some rates are much higher than others and some disabilities increase faster with age. Fit separate models for the means of each disability, assuming all rates are independent. Use nested models to see if different slopes for each disability are better than one slope for all.

Table 7.6: Percentage of Americans with disabilities, by age

Disability	Age		
	65–74	75–84	85+
Vision	16.5	18.2	24.9
Hearing	34.9	40.6	48.1
Cognitive	22.6	28.0	39.1
Ambulatory	63.6	65.2	72.8
Self-care	20.2	26.9	42.4
Independent living	34.0	47.2	68.7

Source: Wan and Larsen (2014)

- (b) Describe a correlation structure for this data over age. Do the rates across ages appear dependent? Does this dependence appear exchangeable or autocorrelated?
- 7.12 In this exercise we consider two types of *banded* correlation matrices in which correlations are all zero if they are beyond a certain distance from the diagonal. Let us define elements $\{\sigma_{ij}\}$ of the matrix Σ with subscripts i and j equal to $1, 2, \dots, p$. The *banded exchangeable correlation matrix* is of the form

$$\sigma_{ij} = \begin{cases} 1 & \text{for } i = j \\ \rho & \text{for } |i - j| \leq k \leq p \\ 0 & \text{for } |i - j| > k \end{cases}$$

where correlations are zero between sequential observations if they are separated by more than k observations.

Similarly, the *banded autocorrelation matrix* is of the form

$$\sigma_{ij} = \begin{cases} 1 & \text{for } i = j \\ \rho^{|i-j|} & \text{for } |i - j| \leq k \leq p \\ 0 & \text{for } |i - j| > k \end{cases}$$

(a) Write programs in R that build these two matrices for specified parameters ρ and k . Your code will be similar to that used for `exchange.mat` and `autocorr.mat` in Sect. 7.6.

(b) Fit these correlation matrices to the home price data and build a table similar to that of Table 7.3. Is there evidence that these banded correlations fit better or worse than the correlations used in that table?

(c) Examine the home price data and test the adequacy of the multivariate normal distribution. Can you find other remarkable cities in addition to Detroit?

Chapter 8

Factor Methods

THE PREVIOUS CHAPTER described inference on the multivariate normal distribution. Sometimes this is more than we actually need. The multivariate distribution is used as a basis of modeling means and covariances. The covariances describe the multivariate relationship between pairs of individual attributes. In this chapter we go further and describe methods for identifying relationships between several variables concurrently. In the following chapter we will use regression methods to model the means.

In this chapter we want to express a multivariate setting in a smaller number of dimensions. Some measured variables will appear to act together in near unison behavior, while others will seem to act independently. The aim of this chapter is to develop methods to identify and characterize these relationships.

As with other statistical methods, it remains our responsibility to interpret the results the computer provides. It is not good enough for us to say that the software identified several variables that appear to act in parallel. We also need to explain this conclusion in terms of our knowledge of the original data. This final step is often overlooked and is needed to complete the data analysis.

Looking ahead to the following chapter, we will describe methods for modeling the mean vector in a multivariate normal distribution. The differences between the observed values and what these models expect are called *residuals*. The residuals of those models will be examined using the methods described in the present chapter.

Consider the data in Table 1.5 of investment recommendations. Every row sums to 100%, so we immediately see some reduction in dimension. In the following section we will demonstrate a much greater reduction in dimensionality with little loss of the variability of the original data.

8.1 Principal Components Analysis

It is reasonable to think of the multivariate normal as a football-shaped ellipse containing most of the population. It would be useful to describe the orientation of the football with its long axis. This long axis directs us to look at the largest orientation, or, in statistical terms, the axis with the largest variability. There are other directions for describing the orientation of our football, as well, and these are at right angles to the longest axis.

Principal components analysis is the identification of linear combination of variables that provides the maximum variability. The first principal component has the greatest variability. The second component has the maximum variability among all linear combinations that are orthogonal to the first. The third principal component is orthogonal to both the first and second, and so on for further components. In other words, principal components analysis reduces a large number of multivariate variables into a relatively small number of linear combinations of these that can be used to account for much of the variability in the data. Variables with the greatest variance will typically dominate the analysis. So in practice, the principal components analysis is often performed on the correlation matrix. (There are exceptions to this general rule, as we will point out.) The correlation provides the appropriate scaling so all variables can be compared on an equal footing. Similarly, in much of the following description of principal components analysis, we can interchangeably make use of the correlation and covariance matrices.

To perform a principal components analysis, we begin with a multivariate random vector $\mathbf{x} = (x_1, x_2, \dots, x_p)$ with mean $\boldsymbol{\mu}$ and covariance $\boldsymbol{\Sigma}$. For the moment, it is not necessary to assume that \mathbf{x} has a multivariate normal distribution.

Consider p different linear combinations of \mathbf{x} which we write out as

$$\begin{aligned} y_1 &= \mathbf{w}'_1 \mathbf{x} = w_{11}x_1 + w_{12}x_2 + \dots + w_{1p}x_p \\ y_2 &= \mathbf{w}'_2 \mathbf{x} = w_{21}x_1 + w_{22}x_2 + \dots + w_{2p}x_p \\ &\vdots && \vdots \\ y_p &= \mathbf{w}'_p \mathbf{x} = w_{p1}x_1 + w_{p2}x_2 + \dots + w_{pp}x_p \end{aligned} \tag{8.1}$$

for suitable multipliers w_{ij} resulting in p new random variables denoted by y_1, y_2, \dots, y_p , referred to as the *principal components* of \mathbf{x} .

The weights w_{ij} are also called *loadings* because they explain how much each of the original observations x_i contributes to each of the principal components. The loadings \mathbf{w}_i in (8.1) are chosen so that the y_i have the largest possible variances and are mutually uncorrelated.

For each $i = 1, \dots, p$ the variances of y_i can be expressed as

$$\text{Var } y_i = \mathbf{w}'_i \boldsymbol{\Sigma} \mathbf{w}_i . \quad (8.2)$$

Note that these variances can be made arbitrarily large by multiplying \mathbf{w}_i by a large scalar. To avoid this ambiguity, we restrict the loadings \mathbf{w}_i to have unit length so that $\mathbf{w}'_i \mathbf{w}_i = 1$.

The second criterion is to make the y_i mutually uncorrelated, so we set

$$\text{Cov } (y_i, y_j) = \mathbf{w}'_i \boldsymbol{\Sigma} \mathbf{w}_j = 0 \quad (8.3)$$

for all $i \neq j$ both between 1 and p .

The goal, then, is to make the variances in (8.2) as large as possible and have all of covariances in (8.3) equal to zero.

In order to achieve this end, we first notice that the objective functions in (8.2) and (8.3) are concerned with the $\boldsymbol{\Sigma}$ matrix and not the means $\boldsymbol{\mu}$ of \mathbf{x} . The means of \mathbf{x} can then be assumed to be zero. In Chap. 9, we will model the means $\boldsymbol{\mu}$ and then use factor methods on the residuals of a multivariate linear regression. These residuals all have zero means.

We usually don't know $\boldsymbol{\Sigma}$ and will need to estimate it using the sample variance matrix \mathbf{S} . Nothing in this formulation requires us to assume that \mathbf{x} has a multivariate normal distribution.

The solution is to examine the pairs of eigenvalues (λ_i) and eigenvectors (\mathbf{e}_i)

$$(\lambda_1, \mathbf{e}_1), (\lambda_2, \mathbf{e}_2), \dots, (\lambda_p, \mathbf{e}_p)$$

where $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_p \geq 0$ are the ordered eigenvalues of \mathbf{S} . In Sect. 4.5.3, we explain that the `eigen()` function in R calculates eigenvectors \mathbf{e}_i that all have unit length and are mutually orthogonal.

If the weights \mathbf{w}_i in (8.1) are replaced by the respective eigenvectors \mathbf{e}_i then the estimated variances of the principal components y_i are maximized with respect to the estimated covariance matrix \mathbf{S} , and these y_i are uncorrelated. The details of this assertion are verified in Exercise 8.1 but will not be proved here.

The estimated variances satisfy

$$\widehat{\text{Var}} y_i = \mathbf{e}'_i \mathbf{S} \mathbf{e}_i = \lambda_i . \quad (8.4)$$

To show that the estimated (y_i, y_j) are uncorrelated, we begin by recalling the eigenvector equation (4.8) so that

$$\mathbf{S} \mathbf{e}_j = \lambda_j \mathbf{e}_j$$

for every $j = 1, 2, \dots, p$.

If we multiply this equation on the left by \mathbf{e}_i and use (8.3) then we have

$$\widehat{\text{Cov}}(y_i, y_j) = \mathbf{e}'_i \mathbf{S} \mathbf{e}_j = \lambda_j \mathbf{e}'_i \mathbf{e}_j = 0$$

because the eigenvectors \mathbf{e}_i and \mathbf{e}_j are mutually orthogonal for $i \neq j$.

What does all of this say? We began with p dimensional multivariate observations \mathbf{x} . At (8.1) we re-expressed these as a different set of p dimensional observations \mathbf{y} that are linear combinations of the original \mathbf{x} s. In a way, nothing has been lost or gained. These principal components $\mathbf{y} = \{y_i\}$ are mutually uncorrelated so this makes them easier to manage, but more difficult to interpret.

The first of these, y_1 , has the largest variance, λ_1 . Second and subsequent components have smaller variances, so the first principal component captures the largest amount of variability in the data. The second component y_2 describes the largest amount of variability left over from y_1 because y_1 and y_2 are uncorrelated.

We can use (8.4) to say that the i -th principal component y_i captures

$$t_i = \lambda_i \left/ \sum_{j=1}^p \lambda_j \right. \quad (8.5)$$

fraction of the total variability.

If t_1 in (8.5) is a substantially large fraction, then we have reduced a p -dimensional problem down to one dimension with little loss of information or variability. Similarly, if t_1 and t_2 were both large fractions, then we would have a two-dimensional summary of the data with little variability omitted. A *scree plot* examines the ordered values of λ_i . This figure allows us to visualize how many principal components are needed to reasonably summarize the data. This plot will be illustrated in the following example.

8.2 Example 1: Investment Allocations

Now we can work out an example in R. Consider the investment recommendation data appearing in Table 1.5. Every financial management firm has a set of recommended percentages in each of eight different investment types. These sum to 100 %, so there is a lower dimensional data summary than what is presented.

The program `princomp` computes eigenvalues and eigenvectors and presents these in a suitable format. See Exercise 8.1 to verify these numerical values are indeed the same. The command line and the output appear in

Output 8.1: Command and output for principal components analysis of the financial recommendation data

```
> pc <- princomp(invest)
> summary(pc)

Importance of components:
                    Comp.1    Comp.2    Comp.3    Comp.4    Comp.5
Standard deviation     14.976263 7.4764087 6.3540720 3.44766464 2.64881614
Proportion of Variance 0.646986 0.1612404 0.1164641 0.03428767 0.02023912
Cumulative Proportion  0.646986 0.8082264 0.9246905 0.95897819 0.97921731
                                         Comp.6    Comp.7    Comp.8
Standard deviation      2.2348600 1.464974785 0.2528154516
Proportion of Variance 0.0144075 0.006190821 0.0001843721
Cumulative Proportion   0.9936248 0.999815628 1.0000000000

> pc$loadings

Loadings:
          Comp.1 Comp.2 Comp.3 Comp.4 Comp.5 Comp.6 Comp.7 Comp.8
USst    0.706  0.521 -0.182 -0.154      0.188      -0.356
Fst     0.734  -0.249  0.476  0.196      -0.348
Dst    -0.188 -0.135  0.840  0.286      0.163      -0.359
USb    0.114 -0.716 -0.413 -0.398      0.123      -0.352
Fb     -0.109  0.315  0.136 -0.800      0.221      0.224 -0.364
Db      0.161 -0.257 -0.887 -0.340
Alt   -0.686  0.410 -0.372 -0.166      0.149      0.208      -0.353
Cash      0.852  0.376 -0.356
```

Output 8.1. The **summary** statement describes the eigenvalues and the estimated cumulative proportion of the total variance explained for each principal component.

The R command

```
pc <- princomp(invest)
```

captures all the output from the principal components program.

The **summary(pc)** in the top half of Output 8.1 provides a simple explanation of the contributions of each principal component. The standard deviations are given by $\sqrt{\lambda_1} \geq \sqrt{\lambda_2} \geq \dots \geq \sqrt{\lambda_8}$ where the λ 's are the eigenvalues of the covariance matrix. From this output we also see the first two principal components account for over 80 % of the variability in the data. These contributions are calculated in (8.5). Subsequent principal components contribute much lower amounts. In other words, much of the variability within the original data can be explained by only two derived values. It remains for us to identify these and explain them in simple terms. To do this, we look at the factor loadings.

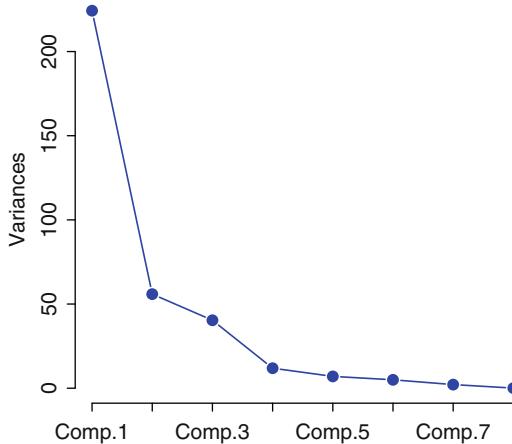


Figure 8.1: Screeplot for the investment recommendations

The `pc$loadings` shows the estimated eigenvector loadings w_{ij} in (8.1). Notice that several of these are printed as blanks. Omitted values are not zero but are close to zero in value and should be ignored. Similarly, only the largest (absolute) loadings are important to us. The eigenvectors of the covariance matrix provide additional details but these are often unnecessary.

In the case of the first principal component, the two largest loadings are 0.706 for US stocks (`USst`) and -0.686 for alternative investments (`Alt`). We can ignore the other much smaller loadings for this component. These two important loadings of the first principal component are then about equal for US stocks and alternatives but opposite in magnitude. In other words, the first principal component is roughly the difference between the recommended allocations to these two investment choices. This principal component makes up almost 65 % of the variability in the original data.

If we again look at Output 8.1, we see that the loadings for the second estimated principal component are almost entirely made up of the recommendations for US bonds (`USB`). This component is orthogonal to the first because it is made up of different information.

The screeplot for these data appears in Fig. 8.1. Specifically, this figure plots the ordered eigenvalues $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_8$ of the sample covariance matrix \mathbf{S} . This figure was obtained using the command

```
screeplot(pc, col = "red", pch = 16,
          type = "lines", cex = 2, lwd = 2, main = "")
```

It is clear from this figure that most of the variability is contained in the first principal component. Together, the first two principal components explain almost 81 % of the variability in the original data and have a simple interpretation. The remaining components represent smaller contributions and can be ignored as background noise.

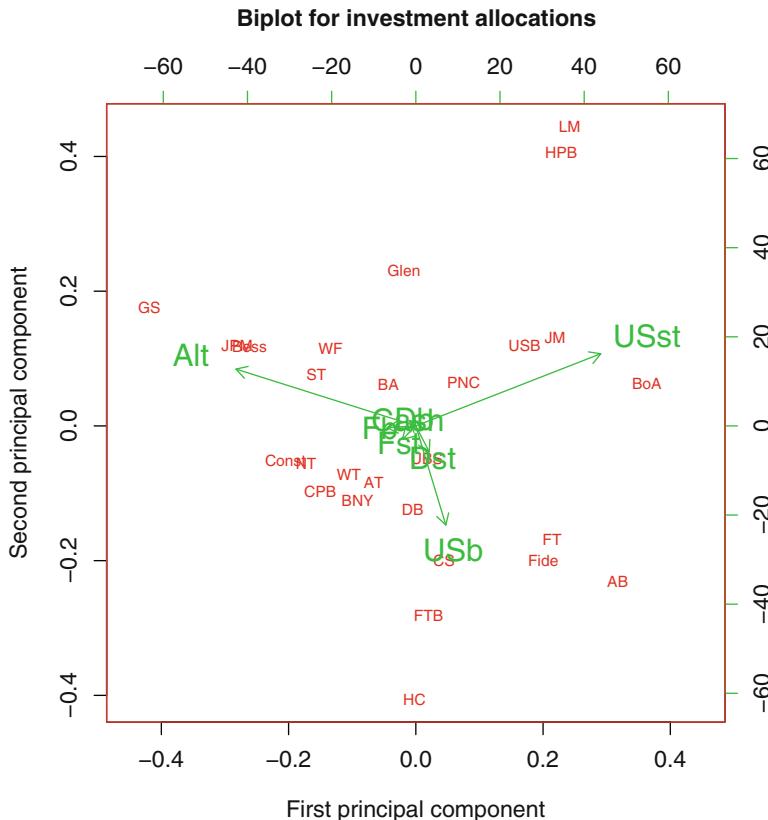


Figure 8.2: Biplot of the first two principal components of the investment recommendations, data appearing in Table 1.5

Another useful graphical method to help interpret the first two principal components is called the *biplot*. Figure 8.2 plots the estimated loadings of the first two principal components using arrows to indicate their direction. We can create this figure using `biplot(pc)` in R. The actual details for producing this figure are

```
pc <- princomp(invest)
biplot(pc, col = c(2, 3), cex = c(.75, 1.5),
       xlim = c( - .45, .45),
       xlab = "First principal component",
       ylab = "Second principal component",
       main = "Biplot for investment allocations")
```

where `col=` sets all colors and `cex` changes the fonts: smaller fonts for observations and larger for the principal components. The `xlim` option is used here because some of the text labels run outside the plot limits.

The US stocks `USst` and alternative investments `Alt` in Fig. 8.2 point in almost opposite directions along the x-axis. The allocation to US bonds `USb` is nearly at right angles to both of these and parallel to the y-axis. These three arrows illustrate our interpretation. The first component is the difference between US stocks and alternatives, in nearly a straight, horizontal line along the first component x-axis with very little change along the vertical, second component y-axis. The second component is made up almost entirely of US bonds and appears as an almost vertical line in this figure. The loadings for the other types of investments (cash or foreign stocks and bonds) play almost no role in the principal components analysis and their presence is lost in a jumble in the figure's center.

Finally, the biplot includes the names of the individual financial firms, located at their positions along these two principal components. A few notable standouts are worth mentioning. On the far left is GenSpring (`GS`) whose recommendations were very high in alternatives (45 %), few US stocks (13 %), and an average number of US bonds (23 %). On the far right is Bank of America (`BoA`) whose recommendations were largely US stocks (53 %), an average number of bonds (28 %), and no alternative investments. See Exercise 8.1 for more information about this example.

8.3 Example 2: Kuiper Belt Objects

Let us now examine a second example of principal components analysis for the Kuiper Belt objects given in Table 1.3. A brief summary of the computing in R is as follows:

```
> KuiPC <- princomp(Kuiper)
> summary(KuiPC)

Importance of components:
                                         Comp.1        Comp.2        Comp.3
Standard deviation      467.8570721 20.198455940 7.1584977540
Proportion of Variance  0.9978853   0.001859904 0.0002336135
Cumulative Proportion   0.9978853   0.999745186 0.9999788000
                                         Comp.4        Comp.5
Standard deviation      2.139420e+00 2.705506e-01
Proportion of Variance 2.086634e-05 3.336962e-07
Cumulative Proportion   9.999997e-01 1.000000e+00
```

From this we see 99.8 % of the variability is explained in the first principal component. On the surface, this appears to be a remarkable reduction in the dimensionality of the problem. The loadings

```
> KuiPC$loadings
```

Loadings:

	Comp.1	Comp.2	Comp.3	Comp.4	Comp.5
mag					0.999
albedo		0.876	0.480		
diameter	-0.999				
axis				-0.995	
Year		0.479	-0.872		

indicate that this first principal component is simply the diameter of the Kuiper object.

This finding can be explained by noting that the standard deviations of the individual measurements

```
> sapply(Kuiper, sd)
```

	mag	albedo	diameter	axis	Year
	1.720651	27.379290	486.254960	2.595953	20.746331

are all very different. By far, the largest of these is the diameter.

A better approach, then, is to record all of these values on the same scale. The principal components should be obtained from the correlation matrix in most cases. The instruction in R is to use the `cor=TRUE` option as in this dialog:

```
> KuiPCc <- princomp(Kuiper, cor = TRUE)
> summary(KuiPCc)
```

Importance of components:

	Comp.1	Comp.2	Comp.3
Standard deviation	1.7868751	1.1360500	0.6719163
Proportion of Variance	0.6385845	0.2581219	0.0902943
Cumulative Proportion	0.6385845	0.8967065	0.9870008
	Comp.4	Comp.5	
Standard deviation	0.219666359	0.129394388	
Proportion of Variance	0.009650662	0.003348582	
Cumulative Proportion	0.996651418	1.000000000	

The first two principal components account for almost 90 % of the variability. The biplot for this appears in Fig. 8.3 and the corresponding loadings are

```
> KuiPCc$loadings
```

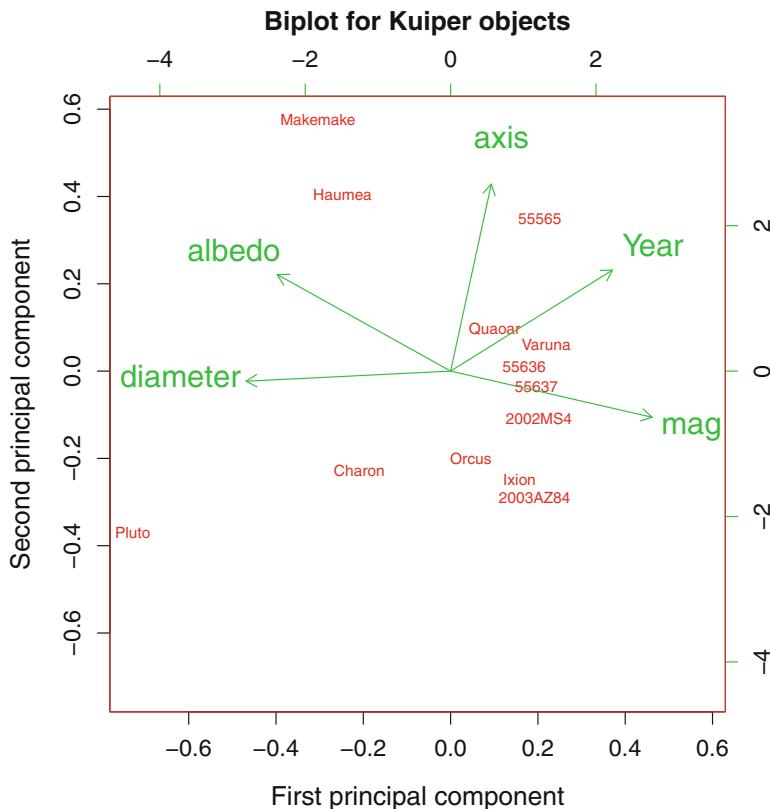


Figure 8.3: Biplot of the first two principal components of the Kuiper objects, data appearing in Table 1.3

Loadings:

	Comp.1	Comp.2	Comp.3	Comp.4	Comp.5
mag	0.538	-0.194	-0.188	-0.161	0.782
albedo	-0.463	0.405	0.446	-0.493	0.425
diameter	-0.546		-0.216	0.671	0.451
axis	0.109	0.785	-0.608		
Year	0.432	0.424	0.591	0.529	

	Comp.1	Comp.2	Comp.3	Comp.4	Comp.5
SS loadings	1.0	1.0	1.0	1.0	1.0
Proportion Var	0.2	0.2	0.2	0.2	0.2
Cumulative Var	0.2	0.4	0.6	0.8	1.0

The first principal component of the Kuiper objects is approximately

$$\text{Magnitude} + \text{Year of discovery} - \text{Albedo} - \text{Diameter}$$

and the second component is almost entirely the axis.

We are working with the correlation matrix, not the covariance, so all these measures have been divided by their standard deviations. The objects on the right side of the biplot are brighter, more recently discovered, less reflective, and smaller. Objects on top have tilted orbits. The opposite is true for objects appearing on the right or bottom of Fig. 8.3.

Why did we need to scale the Kuiper objects and use the correlation in order to obtain a reasonable principal components analysis while the investment recommendations provided an acceptable summary using the original data? The answer is that the investment recommendations were already measured on the same scale as percentages of the total. The multivariate data for the Kuiper objects were all different, and these were measured on different scales. The general rule is to perform principal components analysis on the scaled (correlation) matrix.

8.4 Example 3: Health Outcomes in US Hospitals

As a final example of a principal components analysis, Table 8.1 lists outcome data on US hospitals, as reported by Medicare. There are 16 variables measured and after deleting those cases with missing data, there are 1906 hospitals. This huge dataset is also available online.¹

There are too many variables and too many observations for the `pairs()` plot to be useful. There are simply too many plotted data points, and the computing is somewhat slow. This is a common difficulty in the analysis of such large datasets.

Principal components analysis proves to be a useful approach for starting the statistical examination of such data. The main benefit comes from reducing the large dataset to a 16×16 covariance matrix. Of course, much can be lost in this reduction, but the benefit is that we can easily identify some overall patterns without lengthy computing times.

The screeplot for these data appears in Fig. 8.4. This figure gives strong evidence that there is one component that can be used to summarize this large dataset. We examine the loadings of this first principal component (rounded to two digits):

```
> round(phosp$loadings[, 1], digits = 2)
```

¹See: <https://data.medicare.gov/>.

Table 8.1: Variables in Medicare data on US hospitals

Variable name	Measurement
SDeathN	Number of surgical deaths
SDeathR	Rate of surgical deaths
LungN	Number of collapsed lungs
LungR	Rate of collapsed lungs
ClotN	Number of clots
ClotR	Rate of clots
SplitN	Number of split incisions
SplitR	Rate of split incisions
CutsN	Number of cuts
CutsR	Rate of cuts
HADeathR	Rate of heart attack deaths
HADeathN	Number of heart attack deaths
HFDeathR	Rate of heart failure deaths
HFDeathN	number of heart failure deaths
PDeathR	Rate of pneumonia deaths
PDeathN	Number of pneumonia deaths

SDeathN	SDeathR	LungN	LungR	ClotN	ClotR	SplitN	SplitR
0.34	0.00	0.38	0.02	0.36	0.07	0.35	-0.03
CutsN	CutsR	HADeathR	HADeathN	HFDeathR	HFDeathN	PDeathR	PDeathN
0.38	0.00	-0.11	0.33	-0.07	0.34	-0.07	0.30

These loadings are chiefly composed of equal weighting of eight measures, each with weights in the range of 0.3–0.38. These measures are: `SDeathN`, `LungN`, `ClotN`, `SplitN`, `CutsN`, `HADeathN`, `HFDeathN`, and `PDeathN`. In every case, these variables represent the *number* of adverse events recorded and none of the measures of *rates*. This suggests that the rate values are generally not useful in discriminating between the different hospitals. Instead, the numbers of events are more representative of the size of the hospital than anything else. The principal components analysis, then, suggests we also need a variable indicating the size of the hospital, and this single measure might be the best summary of the variability of the hospitals in this data.

8.5 Factor Analysis

Factor analysis is a method for identifying groups of variables (or *factors*) whose actions appear to work in parallel. Within a single factor, several measured variables within every individual are highly correlated, whether positively or negatively. Other variables may seem to act independently of

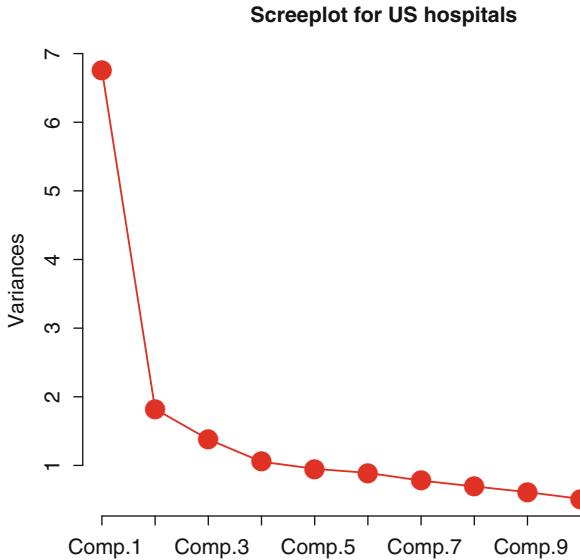


Figure 8.4: Screeplot for the US hospital data

all others. The aim of factor analysis is to identify and interpret these groups of factors. We will also need to estimate the appropriate number of factors needed to model the data.

Let us begin with an example from medicine. Hemangioma is the most common of all childhood cancer diagnoses. It appears as a lump of blood vessels on the skin. If left untreated it usually resolves within a few years. Some parents opt for surgical removal. The data in Table 8.2 is from a registry of surgically treated infants along with measurements on several genetic markers thought to be related to the disease. The age, measured in days, is the infant's age at the time of the surgery. The age, then, represents how long the infant was exposed to the tumor. It was hypothesized that exposure to the tumor might influence the magnitude of the expression of some of these genes over time. A cursory examination of this data reveals several extreme outliers.

The model for factor analysis is as follows. Suppose \mathbf{y} is a p -dimensional normal random vector with mean $\boldsymbol{\mu}$ and covariance matrix $\boldsymbol{\Sigma}$. The means $\boldsymbol{\mu}$ are removed from \mathbf{y} so we only model the random components of the observations. The idea is to see how well we can express the p -dimensional random vector $\mathbf{y} - \boldsymbol{\mu}$ as linear combinations of a relatively smaller number of m *factors* \mathbf{f} and their respective *loadings* $\boldsymbol{\Lambda}$ plus a randomly distributed error $\boldsymbol{\epsilon}$.

Mathematically we write

$$\mathbf{y} - \boldsymbol{\mu} = \boldsymbol{\Lambda} \mathbf{f} + \boldsymbol{\epsilon} \quad (8.6)$$

Table 8.2: Age, in days, and expression of genetic markers for infants who were surgically treated for hemangioma

Age	RB	p16	DLK	Nanog	C-Myc	EZH2	IGF-2
81	2.0	3.07	308975	94	6.49	2.76	11176
95	6.5	1.90	70988	382	1.00	7.09	5340
95	3.6	3.82	153061	237	0.00	5.57	6310
165	1.9	3.74	596992	88	0.00	2.47	7009
286	2.6	5.17	369601	282	12.23	1.63	7104
299	2.9	5.76	1119258	177	8.76	3.51	9342
380	1.9	2.40	214071	45	5.76	1.41	3726
418	7.1	3.38	69511	265	1.17	3.07	8039
420	6.4	3.37	81457	659	1.88	3.87	12583
547	6.4	4.05	64348	336	0.78	4.76	6505
590	1.8	5.15	164881	2012	35.65	9.45	32722
635	6.7	2.67	126016	3072	0.00	4.35	11763
752	1.8	3.28	567858	127	4.13	1.00	10283
760	7.3	0.92	43438	698	1.77	3.32	11518
1171	1.8	6.56	716260	392	12.92	2.90	13264
1277	1.3	0.05	94	15	0.36	3.83	30
1520	4.0	2.79	31125	454	0.62	2.33	1163
2138	0.5	0.00	2331	33	0.03	0.17	66
3626	4.2	4.24	560208	340	5.43	1.36	21174

Data courtesy of Dr. Deepak Nayar

In linear regression (covered in Chap. 9) we know the values of the m explanatory variables. In (8.6) the choice of explanatory variables is not known to us and must be determined. The value of m is specified by us in the program that fits this model.

Estimating the loadings $\mathbf{\Lambda}$ and factors \mathbf{f} is not possible without some additional assumptions. These assumptions are that both the unobservable factors and errors have zero means. Further, these are all assumed to be mutually and jointly uncorrelated.

Notice that neither (8.6) nor the subsequent derivation given below needs to specify a multivariate normal distribution. Briefly, (8.6) suggests the centered data $\mathbf{y} - \boldsymbol{\mu}$ can be expressed as a product of lower dimensional factors and loadings plus a small amount of random error $\boldsymbol{\epsilon}$.

Specifically we need to assume

$$\mathbf{E}\mathbf{f} = \mathbf{0} \quad \text{and} \quad \text{Cov}(\mathbf{f}) = \mathbf{E}\mathbf{f}\mathbf{f}' = \mathbf{I}, \quad (8.7)$$

$$E\epsilon = \mathbf{0} \quad \text{and} \quad \text{Cov}(\epsilon) = E(\epsilon\epsilon') = \Psi = \text{Diag}(\Psi_1, \Psi_2, \dots, \Psi_p). \quad (8.8)$$

In addition, the factors \mathbf{f} are uncorrelated with the errors ϵ :

$$\text{Cov}(\mathbf{f}, \epsilon) = \mathbf{0}. \quad (8.9)$$

Together, these assumptions are sufficient for us to fit the model (8.6).

These assumptions can also be used to describe an alternative form for the factor analysis model. If we begin in (8.6), then we can write

$$\begin{aligned} (\mathbf{y} - \boldsymbol{\mu})(\mathbf{y} - \boldsymbol{\mu})' &= (\mathbf{A}\mathbf{f} + \boldsymbol{\epsilon})(\mathbf{A}\mathbf{f} + \boldsymbol{\epsilon})' \\ &= \mathbf{A}\mathbf{f}(\mathbf{A}\mathbf{f})' + \boldsymbol{\epsilon}(\mathbf{A}\mathbf{f})' + \mathbf{A}\mathbf{f}\boldsymbol{\epsilon}' + \boldsymbol{\epsilon}\boldsymbol{\epsilon}' . \end{aligned}$$

Using the three assumptions (8.7)–(8.9) we can then express the covariance matrix Σ of \mathbf{y} as

$$\begin{aligned} \text{Cov}(\mathbf{y}) &= E(\mathbf{y} - \boldsymbol{\mu})(\mathbf{y} - \boldsymbol{\mu})' \\ &= \mathbf{A}E(\mathbf{f}\mathbf{f}')\mathbf{A}' + E(\boldsymbol{\epsilon}\mathbf{f}')\mathbf{A}' + \mathbf{A}E(\mathbf{f}\boldsymbol{\epsilon}') + E(\boldsymbol{\epsilon}\boldsymbol{\epsilon}') \\ &= \mathbf{A}\mathbf{A}' + \Psi \end{aligned} \quad (8.10)$$

demonstrating the equivalence of two formulations of the factor analysis models in (8.6) and (8.10).

In R we perform a factor analysis using `factanal(x, factors=m)` where \mathbf{x} is the data arranged in the usual fashion as columns of variables and rows for observations. The \mathbf{m} parameter specifies how many factors we want R to fit. Usually we try to fit a relatively small number of factors (three or four) because of the difficulty of interpretation. There is also a formal statistical hypothesis test performed in `factanal()` testing whether \mathbf{m} factors are adequate or not.

A factor analysis of the hemangioma data appears in Output 8.2 using three factors. The hypothesis test at the bottom of this table indicates that the eight measures (age and seven genetic markers) can be summarized as a three-dimensional measurement, plus a small amount of random error. We examine the three-factor loadings to see that `C.Myc`, `EZH2`, `IGF-2` collectively appear to work together in the first factor. The second factor is almost entirely the `DLK` marker. The third factor is almost represented by the `RB` marker. Age plays almost no part, contrary to our original hypothesis about the length of time the tumor burden is carried by the patient. Output 8.2 ends with a hypothesis test ($p = 0.33$) indicating that three factors are adequate to explain this data.

Output 8.2: Factor analysis for the hemangioma data

```
> factanal(hemangioma, factors = 3)
```

Call:

```
factanal(x = hemangioma, factors = 3)
```

Uniquenesses:

	Age	RB	p16	DLK	Nanog	C.Myc	EZH2	IGF.2
	0.962	0.035	0.292	0.005	0.616	0.005	0.491	0.254

Loadings:

	Age	RB	p16	DLK	Nanog	C.Myc	EZH2	IGF.2
Age								-0.171
RB				-0.173			0.962	
p16	0.382		0.745					
DLK				0.971		-0.211		
Nanog	0.475				0.391			
C.Myc	0.931		0.280			-0.225		
EZH2	0.614		-0.115			0.345		
IGF.2	0.767		0.350				0.188	

	Factor1	Factor2	Factor3
SS loadings	2.226	1.750	1.365
Proportion Var	0.278	0.219	0.171
Cumulative Var	0.278	0.497	0.668

Test of the hypothesis that 3 factors are sufficient.

The chi square statistic is 8.03 on 7 degrees of freedom.

The p-value is 0.33

A more thorough analysis of this data would require that we additionally research the roles of these identified genetic markers and then try to understand why they appear to be linked, as we identified in this statistical analysis. Additional examination of this example is continued in Exercise 8.4.

For a second example of factor analysis, let us look at the hamburger data given in Table 1.6. We first try runs of `factanal` with two and then three factors. Output 8.3 contains excerpts of the output from R.

The loadings of Factors 1 and 2 are almost identical in both of these factor analyses. Specifically, loadings for Factor 1 are chiefly `CalFat`, `Fat`, and `SatFat`. The loadings for Factor 2 are almost entirely `Carbs`, in both cases. The loadings for Factor 3 are all small and we interpret this to be mostly noise.

If we only concentrate on the *p*-values in Output 8.3, then we might conclude that two factors is just barely adequate in summarizing the data. The *p*-value is 0.065 for two factors and 0.7 for three factors. We already noted that the third factor does not have a reasonable interpretation beyond a measure of noise in the data. The message in this example, then, is we cannot rely entirely on *p*-values to identify the correct model, and we must also work at interpreting the output carefully.

Factor analysis is a powerful tool. As with many statistical methods, it also requires that we do our homework to interpret the results of the computer output. Historically, it has been well known that this method can yield misleading conclusions, and a small change in the data values can bring about further chaos. Armstrong (1967) presents an educational and elementary case of misuse of factor analysis.

8.6 Exercises

- 8.1 (a) In the biplot of Fig. 8.2, notice that Legg Mason (LM) and Harris (HPB) appear at the top and Highmount (HC) appears at the bottom. Why is that? What does the second principal component in the vertical axis represent?
- (b) Use R to find the eigenvalues and eigenvectors of the correlation matrix of the investment recommendation data of Table 1.5. Show that the eigenvectors represent the variances of the principal components of the correlation matrix with the code

```
sqrt(eigen(cor(invest))$values)
```

and verify that these are same the values obtained from principal components using the code

```
princomp(invest, cor = TRUE)
```

Output 8.3: Abbreviated output of a factor analysis for the hamburger data

```
> burger <- read.table(file = "burger.txt", header = T)
> factanal(burger[, -1], factors = 2) # Omit burger number

. . .

Loadings:
  Factor1 Factor2
CalFat  0.964  0.230
Cal     0.755  0.606
Fat     0.950  0.303
SatFat  0.912 -0.121
Sodium  0.634  0.347
Carbs      0.997
Protein  0.717 -0.111
. . .

Test of the hypothesis that 2 factors are sufficient.
The chi square statistic is 14.7 on 8 degrees of freedom.
The p-value is 0.0652

> factanal(burger[, -1], factors = 3) # Now try three factors

. . .

Loadings:
  Factor1 Factor2 Factor3
CalFat  0.960  0.226 -0.126
Cal     0.752  0.611
Fat     0.949  0.301
SatFat  0.940 -0.131  0.308
Sodium  0.654  0.348  0.248
Carbs      0.980
Protein  0.724 -0.117
. . .

Test of the hypothesis that 3 factors are sufficient.
The chi square statistic is 1.43 on 3 degrees of freedom.
The p-value is 0.699
```

- 8.2 The dataset `Harmon23.cor` in the `datasets` package is a correlation matrix of eight physical measurements made on 305 girls between the ages of 7 and 17.

- (a) Perform a factor analysis of this data using the command

```
factanal(factors = m, covmat = Harman23.cor)
```

where `m` is the number of factors.

- (b) Vary the number of factors to find an adequate fit of the model and interpret the resulting factor loadings.

- (c) Does the principal component analysis produce different conclusions when the correlation matrix (`cor = TRUE`) option is used? Which analysis do you prefer?

- 8.3 Consider a principal components analysis on the dataset appearing in Table 1.4. This table lists rates of individual cancer types (and overall rates) for each of the 50 US states plus DC.

- (a) Begin by examining the standard deviations of each cancer type, including the overall rates.

- (b) Perform a principal components analysis on this data and look at the biplot. Interpret the loadings on the first two principal components. Are these heavily weighted towards the largest standard deviations found in part (a)?

- (c) Repeat the principal components analysis on the scaled correlation matrix of the cancer rate data. How do you interpret this biplot?

- (d) Which analysis do you find more useful: the scaled or unscaled principal components analysis for this data?

- 8.4 How robust is the factor analysis procedure against outliers in the data?

- (a) Examine the marginal distributions of genetic markers in the hemangioma data of Table 8.2. Which of these appear to be normally distributed? Identify both large and small outliers. Are there transformations of the form (5.5) that make these distributions more normal looking?

- (b) Repeat the factor analysis along the lines of the method described in Sect. 8.5. Are your conclusions the same or how do these differ? Which conclusions do you prefer?

8.5 Examine the `USJudgeRatings` data in the `datasets` library. This dataset contains the ratings of 43 US Superior Court judges by attorneys. Each of the judges is evaluated on each of 12 attributes such as demeanor, preparation for trial, sound rulings, and the number of contacts each attorney had with that judge. See the `R` help file for more information on this dataset.

(a) Examine the pair-wise scatterplot for this data (with the `pairs` command) to reveal that some variables are very highly correlated.

(b) Perform a principal components analysis for this data. The first two components explain 94 % of the variability. The second component is almost entirely the number of contacts, and the first component is essentially all other variables, all given the same weight. Interpret this result.

8.6 Six different tests of intelligence and ability were administered to 112 people. The covariance matrix (but not the original data) of the test results is given in `ability.cov` in the `datasets` library. The six tests are called general, picture, blocks, maze, reading, vocabulary, and reading. More information is given in the `R` help file.

(a) Perform a factor analysis on the covariance matrix with

```
factanal(factors = 2, covmat=ability.cov)
```

Use the loadings to identify those variables that group together within the first two factors. Interpret these factors.

(b) Perform a principal components analysis using the covariance matrix

```
> summary(pc <- princomp(ability.cor))
> pc$loadings
```

and identify the variables making the largest contributions to the first two principal components. How do you interpret these principal components?

(c) Do you think it is more appropriate to examine the covariance or the correlation in a principal components analysis of this data?

(d) The `cov2cor` function efficiently converts covariances into correlation matrices. That is

```
> ability.cor <- cov2cor(ability.cov$cov)
> princomp(ability.cor)
> princomp(ability.cor)$loadings
```

Table 8.3: Mechanistic causes of death and rates for 50 states

State	All	Cut	Drown	Fall	Fire	Firearm	MotorVeh	Poison	Suffocate
AL	74.5	1.0	2.0	4.2	2.1	16.9	19.4	14.1	5.3
AK	87.1	NA	5.1	6.1	1.7	18.8	8.7	21.8	7.9
AZ	72.0	1.1	1.6	11.9	0.7	14.2	12.4	17.7	5.5
⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮
WI	57.8	0.7	1.3	14.4	0.8	8.1	9.9	12.3	5.1
WY	84.5	NA	1.3	9.5	NA	16.7	21.0	16.7	7.2

Source: National Vital Statistics System, <http://www.cdc.gov/nchs/deaths.htm>

obtains the correlation and performs the principal components analysis. Examine the loadings and interpret the first two principal components. Compare this data summary with parts (a) and (b) How do these differ? How are they similar?

8.7 The academic score data appears in Table 1.2 and is examined in Exercise 2.5.

(a) Perform a principal components analysis of this data. Notice that the first principal component accounts for much of the variance. What do the factor loadings suggest? Do the loadings differ if you use the covariance matrix or the correlation matrix?

(b) Look at the correlation matrix of this data. What does the correlation matrix say about this data? Is this consistent with conclusion of the principal components analysis of part (a) and Exercise 2.5?

8.8 Table 8.3 lists the mechanistic (as opposed to natural) causes of death, by state, for the years 1999–2010, as reported by the Centers for Disease Control. Rates are per 100,000 persons and include both accidental and intentional. There are a number of NAs listed where estimates are unreliable due to small numbers. Consider replacing these with a small number such as 0.2.

(a) Plot the data and identify any remarkable states. Explain these. In which states do deaths following falls seem unusually common?

(b) Perform a principal components analysis. Should the “All” category be included in this? Show that states with high rates of motor vehicle deaths also have high rates of mortality associated with firearms. Poisoning is important also but seems to be independent of these other two causes.

- 8.9 The `tree` dataset in the `datasets` library has three measurements on each of 31 black cherry trees: girth (diameter, in inches, measured at breast height); height in feet; and timber volume in cubic feet index-trees.
- Draw a `pairs` plot to identify strong correlations and any outliers.
 - Perform a principal components analysis of this data. Use the biplot to show how the first principal component captures the strong correlation in part a. Again, identify any outliers in this data.
- 8.10 A psychological study was conducted at Northwestern University on 160 subjects. Each subject was assessed on a variety of standard psychological measures. Then each subject was shown one of four different movies (comedy, horror, nature, and documentary) and then assessed again. The variable `affect` in the `psych` library contains this data. Look at the help file to see details on the variables, published references, and several summary displays of this data in R. Develop a few displays of your own for this data and interpret your findings.
- 8.11 The Synthetic Aperture Personality Assessment (SAPA) Project is a web-based psychological data collection.² A subset of the data is available in R as `bfi` in the `psych` library. This subset contains data on three demographic variables and 25 personality items submitted by 2800 volunteers. As examples of these items, we have:

- I know how to comfort others.
- I waste my time.
- I make friends easily.

Each item is rated on a scale of 1–7, on whether the respondent feels that he or she agrees with the statement a lot, disagrees a lot, or falls somewhere in between. See the `bfi` help file for more details.

- Use the `complete.cases()` command to remove individuals in `bfi` with any missing values.
- Use factor analysis to group together items of a similar nature. Try to interpret the nature of items that cluster together. This is a useful exercise in psychology. The chi-squared test of the adequacy of the number of factors may not be appropriate with such a large sample size.

²You can learn more and take the assessment at <https://sapa-project.org/>.

Table 8.4: Statistics on oil consuming nations in 2011

Nation	Daily consumption		Population in millions	Annual per capita		Production/ consumption
	1000 bbl	1000 m ³		bbl	m ³	
United States	18,835.5	2994.6	314	21.8	3.47	0.51
China	9790.0	1556.5	1345	2.7	0.43	0.41
Japan	4464.1	709.7	127	12.8	2.04	0.03
India	3292.2	523.4	1198	1.0	0.16	0.26
Russia	3145.1	500.0	140	8.1	1.29	3.35
Saudi Arabia	2817.5	447.9	27	40.0	6.40	3.64
Brazil	2594.2	412.4	193	4.9	0.78	0.99
Germany	2400.1	381.6	82	10.7	1.70	0.06
Canada	2259.1	359.2	33	24.6	3.91	1.54
South Korea	2230.2	354.6	48	16.8	2.67	0.02
Mexico	2132.7	339.1	109	7.1	1.13	1.39
France	1791.5	284.8	62	10.5	1.67	0.03
Iran	1694.4	269.4	74	8.3	1.32	2.54
United Kingdom	1607.9	255.6	61	9.5	1.51	0.93
Italy	1453.6	231.1	60	8.9	1.41	0.10

Source: US Energy Information Administration

- (c) Identify those questions that have a preponderance of extreme agree and/or disagree responses. Similarly, identify suspected outliers such as persons who appear to respond in an extreme fashion. That is, persons who tend to strongly agree and or disagree with a majority of the questions.
- 8.12 Table 8.4 summarizes oil consumption in the largest importing and exporting nations for the year 2011. Consumption is expressed both as a daily figure and per capita. These are expressed in barrels (bbl) and cubic meters. The ratio of production to consumption is given as well.
- Perform a principal components analysis on this data and draw the screeplot and biplot. How does the biplot group similar nations together?
- 8.13 The `bodyfat` data frame in the `TH.data` library lists 10 anthropomorphic measurements made on 71 healthy women. A key feature of this data is the method of measuring their total body fat with great precision but also at great cost. Use principal components to summarize this data. Show that the data can be well summarized using only two principal components.

Chapter 9

Multivariable Linear Regression

LINEAR REGRESSION is probably one of the most powerful and useful tools available to the applied statistician. This method uses one or more variables to explain the values of another. Statistics alone cannot prove a cause and effect relationship, but we can show how changes in one set of measurements are associated with changes of the average values in another.

Notice how this approach is different from that taken in principal components analysis. In principal components, all variables are associated with each other and the statistical analysis attempts to uncover groups of variables that vary together. In contrast, in linear regression, the data analyst specifies which of the variables are to be considered explanatory and which are the responses to these. This process requires a good understanding of the data. Sometimes we have a cause and effect relationship where some conditions are under our control. More often, we have jointly observed data and we want to express the behavior of some variables for given conditions of the others. A cause and effect relationship is difficult to demonstrate. The interested reader is referred to Pearl (2009) for a detailed description of the issues involved.

The methods in this chapter assume linear relationships between all the dependent and independent variables. In Sect. 10.5, we consider regression tree models for nonparametric settings where we can assume monotone, but not necessarily linear, relationships between these variables.

Let us begin by considering the `mtcars` data set in the `datasets` package. This `data.frame` contains 11 measurements on each of 32 model cars that were available in 1973–1974. These 11 measurements are listed in Table 9.1.

Table 9.1: Measures on 32 cars in the `mtcars` data set

Name	Definition	Design or empirical
<code>mpg</code>	Miles/(US) gallon	E
<code>cyl</code>	Number of cylinders	D
<code>disp</code>	Displacement (cu.in.)	D
<code>hp</code>	Gross horsepower	E
<code>drat</code>	Rear axle ratio	D
<code>wt</code>	Weight (lb/1000)	E
<code>qsec</code>	1/4 mile time	E
<code>vs</code>	cylinders form a “V” or are in a straight line	D
<code>am</code>	Transmission (0 = automatic, 1 = manual)	D
<code>gear</code>	Number of forward gears	D
<code>carb</code>	Number of carburetors	D

Some characteristics could be considered *design features* that might not be readily observed unless one were to open the hood, or perhaps dismantle an assembly and count the teeth on the various gears. These design features include the number of cylinders, displacement, rear axle ratio, “V” arrangement of cylinders, number of forward gears, and the number of carburetors.

Other features in this list are *empirical* and readily experienced by a driver. This list includes the miles per gallon, horsepower, weight, and quarter mile time. The casual driver would not know the exact weight or horsepower, of course, but in relative terms, these would be experienced in comparison to other cars with markedly different values. In this example we will classify the type of transmission (manual or automatic) as a design feature, although it might be considered an empirical feature, as well.

In this chapter we will develop mathematical models that use the design features to explain differences in the empirical features. The mean value of each empirical feature is modeled as a linear function of all the design features. The multivariable approach is to do this for all empirical features and then examine whatever is left over from that modeling process, i.e., the residuals. These multivariate residuals are used to determine if the empirical features remain correlated after having taken into account the linear effects of the design features.

9.1 Univariate Regression

The goal of linear regression is to attempt to explain the different values of one variable in terms of others. This idea is not to predict but rather to make a statement about the typical or mean value under specified conditions.

To begin, let's build a linear regression to explain the miles per gallon (mpg) values from the design features. The plan is not to predict mpg values but rather attempt to reasonably explain the values we have already observed. There is a danger of extrapolation: We cannot make any intelligent statement about combinations or values that are beyond the range of our experience. Within the range of observed data, we will be able to say something about which design features are more closely associated with mpg values.

We denote by Y_i a random variable with a distribution that depends on a vector of known explanatory values \mathbf{x}_i . The functional form is

$$Y_i = \boldsymbol{\beta}' \mathbf{x}_i + e_i \quad (9.1)$$

where the independent, normally distributed errors e_i have zero means and constant variances σ^2 . The regression coefficients $\boldsymbol{\beta}$ are parameters that need to be estimated from the observed data (y_i, \mathbf{x}_i) . In the present example, y_i is the observed, empirical feature (such as mpg) of the i th car, and \mathbf{x}_i is the vector of values of all the design features of that car.

The linear model of one variable in terms of another is motivated by the properties of the multivariate normal distribution with conditional mean and variance given in (6.6) and (6.7), respectively. Specifically, the conditional means of the Y_i are linear in the explanatory variables, and the conditional variances are independent of the values of the explanatory variables.

Least squares methods are used to obtain fitted parameter values $\hat{\boldsymbol{\beta}}$ that estimate $\boldsymbol{\beta}$. Also useful are *fitted values*

$$\hat{Y}_i = \hat{\boldsymbol{\beta}}' \mathbf{x}_i$$

that are the estimated mean values anticipated by model (9.1).

The estimated parameters $\hat{\boldsymbol{\beta}}$ are those values minimizing the sum of squared residuals $\sum r_i^2$ where the residuals are the observed differences between the observed and expected values

$$r_i = y_i - \hat{\boldsymbol{\beta}}' \mathbf{x}_i .$$

Similarly, the $\hat{\boldsymbol{\beta}}$ are often referred to as least square estimates. Least squares estimates are also maximum normal likelihood estimates. Plots of the residuals r_i are instrumental in identifying lack of fit and deviations from the assumed linear model (9.1) as we will illustrate in this chapter.

In R, we can fit a linear regression, and also capture the residuals, estimated regression coefficients $\hat{\boldsymbol{\beta}}$, and fitted values. These appear in Output 9.1. This Output lists, in respective columns, the estimated regression coefficients $\hat{\boldsymbol{\beta}}$, their standard errors, t-test statistics, and p-values testing the null hypothesis that the corresponding population coefficient (β) is zero. The asterisks indicate the level of statistical significance.

Output 9.1: Output from the linear model fitting mpg values

```

> library(datasets)
> univ <- lm(formula = mpg ~ cyl + wt + am + carb, data = mtcars)
> fit <- univ$fitted.values
> resid <- univ$residuals
> summary(univ)

Call:
lm(formula = mpg ~ cyl + wt + am + carb, data = mtcars)

Residuals:
    Min      1Q  Median      3Q     Max
-4.5451 -1.2184 -0.3739  1.4699  5.3528

Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept) 36.8503    2.8694 12.843 5.17e-13 ***
cyl        -1.1968    0.4368 -2.740  0.0108 *
wt         -2.4785    0.9364 -2.647  0.0134 *
am          1.7801    1.5091  1.180  0.2485
carb        -0.7480    0.3956 -1.891  0.0694 .
---
Signif. codes:  0 *** 0.001 ** 0.01 * 0.05 . 0.1   1

Residual standard error: 2.5 on 27 degrees of freedom
Multiple R-squared:  0.8502, Adjusted R-squared:  0.828
F-statistic:  38.3 on 4 and 27 DF,  p-value: 9.255e-11

```

In this table of parameter estimates, we see the number of cylinders (`cyl`) and weight (`wt`) provide a great amount of explanatory value in describing mpg values. The number of carburetors (`carb`) has limited value, and the transmission type (`am`: automatic or manual) makes a minimal contribution. The estimated coefficients for cylinders and weight are negative because, intuitively, larger engines and heavier cars will get fewer miles per gallon.

The analysis of variance (ANOVA) expresses the total sum of squares:

$$\sum (y_i - \bar{y})^2 = \sum (y_i - \hat{y}_i)^2 + \sum r_i^2. \quad (9.2)$$

The total sum of squares of the observed y_i about their average \bar{y} is the total amount of variability in the dependent variable. This amount can be partitioned into the sum of squared values of the observed values about the fitted values plus the sum of squared residuals. The sum of squared residuals was minimized in order to estimate $\hat{\beta}$. The sum of squared residuals is referred to as the *error sum of squares* or the *unexplained sum of squares*.

The sum of squares about the fitted values \hat{y}_i is the amount of variability attributed to knowing the explanatory variables \mathbf{x}_i . This is often called the *explained* or *model sum of squares*. Ideally, we want the model sum of squares to be large relative to the error sum of squares. This difference is usually expressed as a ratio or, more specifically, the *F-statistic* given at the end of Output 9.1.

How did we decide on this subset of all design features to use in explaining the mpg values? It helps to have a good understanding of the nature of the data. In this case, we all have a basic understanding of how a car works. A little trial and error identified number of cylinders, weight, automatic/manual, and number of carburetors as useful. Useful explanatory variables are generally identified by extremely small p-values. The table of fitted coefficients in Output 9.1 prints *'s to guide our attention towards those explanatory variables that are most highly statistically significant.

For every parameter (coefficient) in the regression model, R provides an estimated value and a standard error of that estimate. The **t value** is the ratio

$$\text{t value} = \text{Estimate}/\text{Std.Error}$$

The corresponding statistical significance of this *t*-statistic appears under $\text{Pr}[>|\text{t}|]$. This tests the null hypothesis that the true, underlying population parameter is actually zero. A small p-value for this test indicates that the strong relationship between the variables could not have happened by chance alone.

The regression model with fitted parameter values is

$$\text{mpg} = 36.85 - 1.20 \text{ cyl} - 2.48 \text{ wt} + 1.78 \text{ am} - 0.75 \text{ carb} + \text{error}. \quad (9.3)$$

In words, increasing the cylinders, weight, and number of carburetors results in decreased estimates of the miles per gallon. The difference between manual and automatic transmissions is less than 2 mpg and not statistically significant. For a range of values within those contained in this data, given a set of values of cylinders, weight, transmission type, and number of carburetors, this last expression can be used to give a reasonable estimate of the average miles per gallon of a car with those characteristics. Ultimately, (9.3) is easily interpreted and agrees with our intuition about factors that influence mpg.

Output 9.1 includes an estimate of 2.5 for the standard deviation of the errors associated with the linear model. That is, the fitted model in (9.3) estimates the mpg with a standard deviation of about 2.5. To appreciate the value of the regression, let us compare this value to the standard deviation of the marginal mpg values,

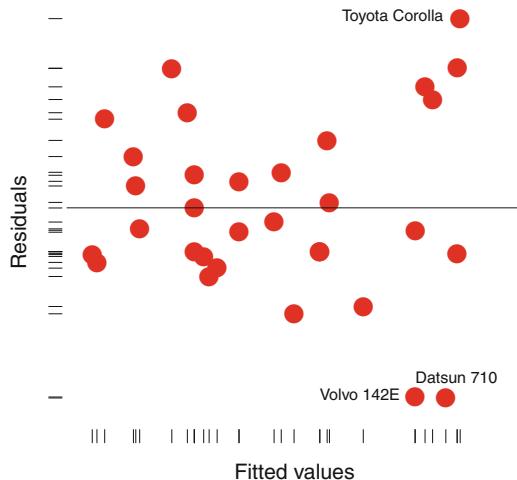


Figure 9.1: Fitted and residual values for the linear regression model (9.3) of mpg data

```
> sd(mtcars$mpg)
[1] 6.026948
```

illustrating the much higher variability associated without the use of the linear model.

We should always examine the residuals of the fitted model. The plot of residuals and fitted values is given in Fig. 9.1. The marginal distributions are displayed as rug fringes. A few unusual values are identified in this plot.

The rug fringe along the left marginal axis shows the residuals from this fitted model appear normally distributed. There are no extreme poorly fitting observations in the data. The three cars identified by name in the plot are notable. All three have high miles per gallon, as expected by the fitted model. Two models (Volvo 142E and Datsun—now Nissan 710) have much lower mpg than expected. The Toyota Corolla has much higher gas mileage than anticipated by the fitted model. The model assumptions seem to be reasonable in this example. In such plots we look for evidence of outliers, trends not accounted for by the model and nonconstant variability of the residuals.

Let us end this section with a brief discussion of the options R offers us in performing linear regression.

We use the `formula =` parameter to specify the linear model to be fitted. The notation

```
mpg ~ cyl + wt
```

for example, is shorthand for the model

$$\text{mpg} = \beta_0 + \beta_1 \text{cyl} + \beta_2 \text{wt}$$

where the tilde (\sim) takes the role of the equal sign in the formula.

To specify a model without an intercept β_0 , we would write

$$\text{mpg} \sim \text{cyl} + \text{wt} - 1$$

or equivalently

$$\text{mpg} \sim 0 + \text{cyl} + \text{wt}.$$

There are other options you can read about using `help(formula)` in R.

In addition to `lm()`, the `glm` and `aov` programs have a similar syntax. The `aov` program will be demonstrated in the following section. GLM is the abbreviation of *generalized linear model* and will be illustrated here.

To illustrate the use of `glm()`, we can write

```
> univ.glm <- glm(formula = mpg ~ cyl + wt + am + carb , data = mtcars)
> summary(univ.glm)
```

This produces similar output to that obtained using `lm`.

As with `lm`, the `glm` routine allows us to capture statistics about the fitted parameter values that appear in the output. Corresponding to Output 9.1, we can also write

```
> tt <- summary(univ.glm)
> print( tt$coefficients, digits=4)

      Estimate Std. Error t value Pr(>|t|)

(Intercept)  36.850    2.8694 12.843 5.172e-13
cyl        -1.197    0.4368 -2.740 1.075e-02
wt         -2.478    0.9364 -2.647 1.339e-02
am         1.780    1.5091  1.180 2.485e-01
carb       -0.748    0.3956 -1.891 6.941e-02
```

In this code, the variable `tt` contains a data frame with the values produced in `glm` and printed by `summary(univ.glm)`. The variable `tt$coefficients` contains the values produced by `summary`. We can then obtain separate values for the *t*-statistics and their *p*-values, for example, in addition to the estimated regression coefficients.

9.2 Multivariable Regression in R

The popularity of linear regression cannot be understated. It stands to reason that there are methods that generalize to more than one dependent variable. Such multivariable regression methods build upon the univariate linear regression of the previous section and then follow up with the principal components analysis described in Sect. 8.1. There are also multivariable analogies to the ANOVA called the *multivariable analysis of variance* or MANOVA, but this is not in common use today. See Hand and Taylor (1987) for more on the multivariate analysis of variance.

Multivariable linear regression is performed in two steps. First, we perform separate, univariate linear regressions for each of the dependent variables y and capture the residuals for each of these regressions. Each separate regression provides the estimated regression coefficients, regardless of how the various dependent variables are correlated with each other.

The second step is to perform a principal components or factor analysis on the residuals to see if there is additional information in the dependent variables, after having corrected for the effects of the explanatory x variables. We use graphical methods to check model assumptions and examine residuals for outliers and lack of fit.

The best way to illustrate the multivariable linear regression is to work through two examples in detail. In this section, we examine the characteristics of cars in the `mtcars` data set that was also examined in the previous section. In the following section, we will examine a much larger data set taken from a health survey.

In the `mtcars` example, Table 9.1 identifies the variables that we classified as *design features* and those that could be described as *empirical features* to be experienced by the owner.

We build a multivariable linear regression by explaining each of the empirical features (`mpg`, `hp`, `wt`, `qsec`) from the design features (`cyl`, `disp`, `am`, `drat`, `carb`, `vs`, `gear`). Four separate linear regressions for these empirical features were fitted using

```
univ.mpg <- aov(mpg ~ cyl + disp + am + carb , data = mtcars)
summary(univ.mpg)

univ.hp <- aov( hp ~ cyl + drat + am + gear + carb, data = mtcars)
summary(univ.hp)

univ.wt <- aov( wt ~ cyl + disp + drat + am + carb, data = mtcars)
summary(univ.wt)

univ.qsec <- aov( qsec ~ cyl + disp + drat + vs + am + gear, data = mtcars)
summary(univ.qsec)
```

producing four separate, marginal ANOVAs.

The fitted models are

```

mpg   =  30.19 - 0.657cyl - 0.0180disp + 3.599am - 1.19carb + error
hp    =  -100. + 27.7cyl - 3.98drat + 3.16am + 13.4gear + 13.8carb + error
wt    =  3.77 - 0.231cyl + 0.006659disp - 0.263drat - 0.647am + 0.195carb + error
qsec   =  26.3 - 0.804cyl + 0.000770disp - 0.362drat + 1.05vs - 1.38am
                    -0.623gear + error

```

The choice of explanatory variables is not the same in each of these regressions. These were chosen using a little trial and error to include only those with both intuitive explanatory value and statistical significance. The residuals from the four separate regressions can be captured and combined into a single `data.frame`:

```

> car.res <- cbind( univ.mpg$residuals, univ.hp$residuals,
+                     univ.wt$residuals, univ.qsec$residuals)
> colnames(car.res) <- c("mpg_res", "hp_res", "wt_res", "qsec_res")
> car.res <- data.frame(car.res)
> print(car.res, digits=2)

      mpg_res   hp_res   wt_res qsec_res
Mazda RX4      -1.2058 -52.749  0.0626  0.1024
Mazda RX4 Wag   -1.2058 -52.749  0.3176  0.6624
Datsun 710      -5.2311  26.952  0.2200 -0.3860

      . . .
      . . .

Maserati Bora      1.4107  46.675 -0.3407  0.2332
Volvo 142E       -5.2054  30.181  0.4665 -0.3118

```

Four separate, marginal plots of fitted and residuals are given in Fig. 9.2. A number of unusual and remarkable cars are identified by name. These are typically either economy makes (Toyota, Duster, and Datsun) or else large, luxury models (Maserati, Lotus, or Mercury).

A multivariate examination of these residuals begins with the matrix scatterplot presented in the top panel of Fig. 9.3. This figure includes the loess smoothing and does not identify any strong correlations between residuals that were not explained by the linear models. (See text for Fig. 3.16 for details on how we draw this figure in R.)

We can also perform a series of tests for the multivariate normal distribution of the residuals. The bottom panel of Fig. 9.3 is a QQ plot of the Mahalanobis distances from the centroid for the four-dimensional residuals.

The clear outlier (Mercury 230) is identified by name. The plot of univariate residuals in Fig. 9.2 identified this car model as having an unusually large quarter-mile time.

Formal statistical tests for the multivariate normal behavior of the residuals reflect what is observed in the QQ plot. Specifically, the code

```
> library(mvnormtest)
> mshapiro.test( t( car.res))

Shapiro-Wilk normality test

data: Z
W = 0.8389, p-value = 0.0002403
```

yields a p -value of 0.0002 indicating a poor correspondence to the multivariate normal distribution.

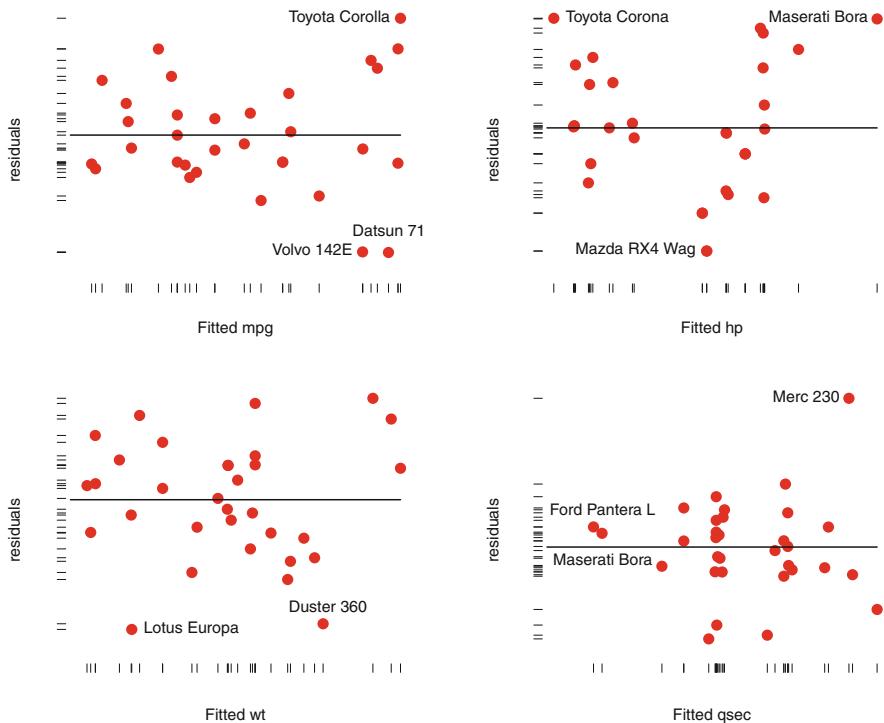


Figure 9.2: Fitted and residual values from four marginal linear regressions of car data

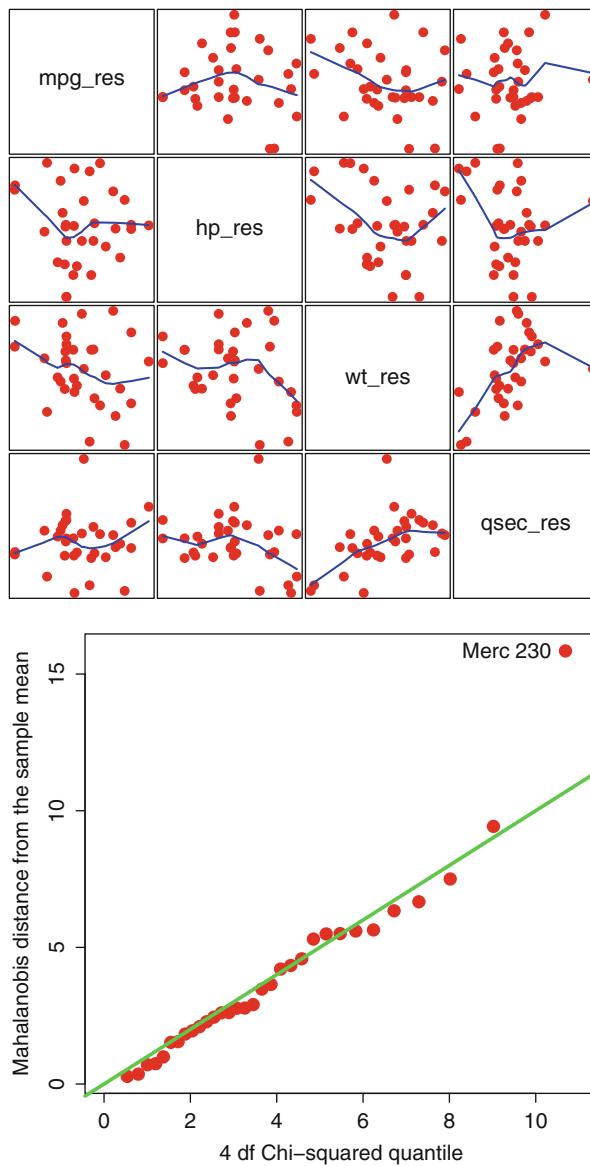


Figure 9.3: Scatter plot of residual values of car data with loess smooth (*top panel*) and QQ plot of Mahalanobis Distances (*bottom panel*)

We can omit the single observation with the largest Mahalanobis statistic in its residual:

```
> mah <- mahalanobis(car.res, colMeans(car.res), var(car.res))
> outi <- match(max(mah), mah) # index of outlier
> mshapiro.test( t( car.res[-outi,] ) )

Shapiro-Wilk normality test

data: Z
W = 0.9232, p-value = 0.02877
```

The fit to a multivariate normal distribution improves slightly, but is still suspect.

The next step in this multivariable linear regression is to perform a principal components analysis on these residuals. The object of this examination is to see if there is any additional information remaining between the four dependent variables (`mpg`, `hp`, `wt`, `qsec`) after accounting the linear effects of the explanatory variables (`cyl`, `disp`, `drat`, `vs`, `am`, `gear`, `carb`).

The principal components analysis in R is

```
> print(prcomp(car.res, scale = TRUE), digits = 3)

Standard deviations:
[1] 1.312 1.061 0.885 0.607

Rotation:
PC1      PC2      PC3      PC4
mpg_res  0.160 -0.864  0.277  0.388
hp_res   0.426  0.400  0.798  0.146
wt_res   -0.658  0.230  0.106  0.709
qsec_res -0.600 -0.199  0.524 -0.571
```

In the list of ordered standard deviations, we see all four principal components are comparable in magnitude; the largest is just slightly twice the size of the smallest. We interpret the loadings here to mean that the residuals of `hp`, `wt`, and `qsec` are all highly correlated with each. The `mpg` residuals are independent of these three.

The biplot for the first two principal components

```
biplot(prcomp(car.res, scale = TRUE), cex = c(.6, 1.2),
       col = c(3, 4), cex.lab=1.5,
       xlab = "First principal component",
       ylab = "Second principal component")
```

is given in Fig. 9.4.

The loadings of the first principal component shows that the residuals of weight and quarter second times are positively correlated with each other

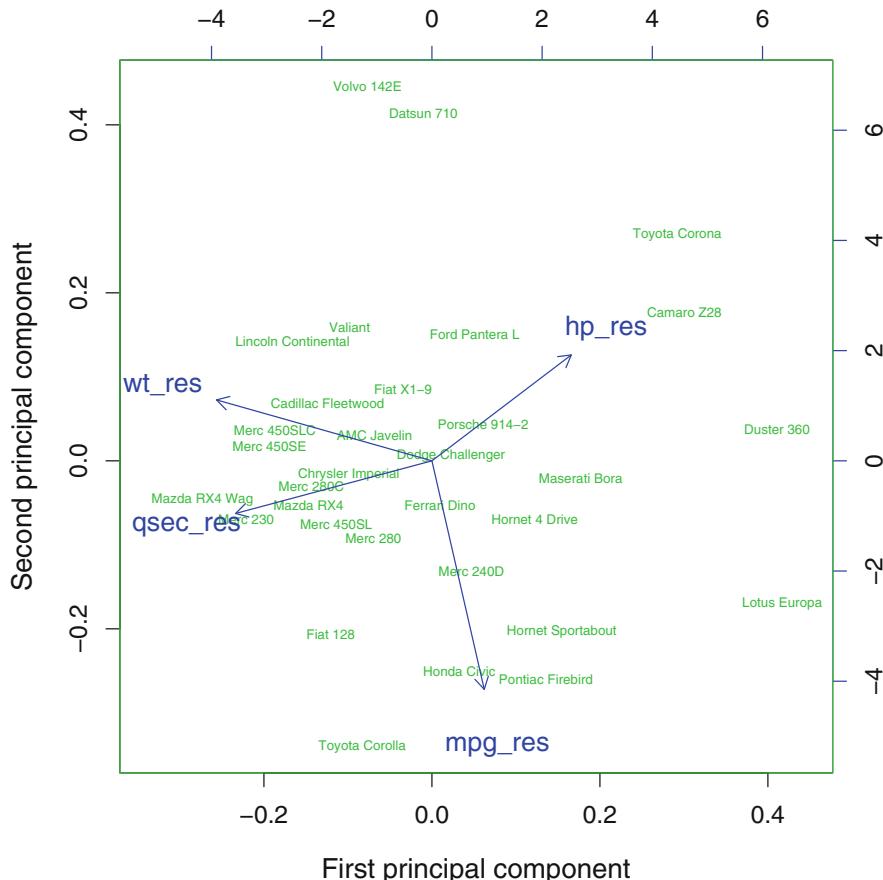


Figure 9.4: Principal component biplot of the residuals from the car data

and negatively correlated with `hp` residuals. The second principal component is composed almost entirely of the `mpg` residuals showing that these are independent of the other three.

In summary, the four individual linear regressions appear to capture much of the useful information about the four dependent variables. There are a few remarkable outliers. What is left over are residuals for `mpg` which appear independent of the other three sets of residuals.

9.3 A Large Health Survey

In this section, we examine a large data set and use it to further illustrate the uses of multivariable linear regression. The Behavior Risk Factor Surveillance System (BRFSS) is a large initiative sponsored by the Centers for Disease

Control (CDC) in Atlanta, Georgia. This is a telephone survey of individuals living in the largest metropolitan areas concerning their health, health behaviors, and individual risk factors. The survey is weighted towards reaching individuals who might not be easily identified in a traditional, straightforward sample. We will examine data from the survey taken in the year 2010. More details on these questions, other health-related questions, and surveys from other years are available on the SMART (Selected Metropolitan/Micropolitan Area Risk Trends) website given in Table 9.2.

Table 9.2 lists a number of survey items selected from the total. The items themselves form two separate types of measurements: behavioral and health outcomes. As examples, a report of binge drinking is a behavioral measure and a report of asthma is a health outcome. Some of these measures are not clearly one or the other such as BMI and health coverage. We will classify both of these measures as behavioral to simplify the discussion.

The object of the data analysis is to see if we can identify the behavioral risk factor's effects on the associated health outcomes. These associations are aggregate for cities, not individuals, so we can only infer properties of populations. For example, we cannot infer that the people who regularly see a dentist are less likely to have missing teeth, but, rather, populations with a large number of people seeing dentists are also populations with fewer missing teeth.

As another example of the shortcomings of this cross-sectional data, we are unable to tell if those individuals with asthma are more or less likely to be binge drinkers. Instead, we can only say something about the rates of asthma in cities with a high levels of binge drinking. One person is the binge drinker, but a different person in the same city develops asthma. Finally, the data examined here is only for 1 year (2010), so we are unable to determine if binge drinking has any long-term health effects or if binge drinking is on the rise.

The data set is too large for examining all possible pairs of scatter plots using `pairs()`. Instead, Fig. 9.5 plots `pairs()` for only those variables considered as outcomes. There are several highly correlated pairs of outcomes, including the perception of general health with each of having a heart attack, diabetes, and loss of any permanent teeth.

Let us illustrate how multivariable linear regression methods can help summarize the various patterns occurring in this data set. We begin by performing separate linear regressions for each of the eight outcome variables using all ten of the behavioral measures as explanatory variables.

The first examination asks which of these behaviors is associated with each of the different health outcomes. The second analysis asks how each of the health outcomes are related to each other after having corrected for all of the behavioral measures.

The separate linear regression for each of the eight health outcomes regressing on all of ten explanatory variables results in an 11×8 matrix of regression coefficients (including the intercepts). A simple way to examine all of these coefficients is to produce a *heatmap*, as in Fig. 9.6. The regression coef-

Table 9.2: The subset of the BRFSS data set summarizes the percentage of respondents answering positively to these items in each of 192 US metropolitan areas

Variable name	Description	Outcome or behavior
Binge	Regular binge drinking	B
Asthma	Reporting asthma	O
HeartAt	Ever had a heart attack	O
Colonosc	Adults 50+ who ever had a colonoscopy	B
Diabetes	Any diagnosis of diabetes	O
PregDia	Pregnancy-related diabetes	O
PreDia	Prediabetic or borderline diabetes	O
Disability	Limited activities due to disability	O
Exercise	Any exercise in the past month	B
Coverage	Any health care coverage	B
GeneralH	Self-reported general health of good or better	O
FluShot	Adults 65+ having a flu shot in the past year	B
Dentist	Visited a dentist in the past year	B
Teeth	Any permanent teeth extracted	O
BMI	BMI under 25 (not overweight)	B
PSA	Men 40+ with a PSA screen over the past year	B
Smokers	Current smokers	B
PAP	Women 18+ with a Pap test over the past 3 years	B

Source: <http://apps.nccd.cdc.gov/BRFSS-SMART/>

Every variable is classified as either behavioral (B) or health outcome (O)

ficients with the greatest statistical significance are in white, and those less so are in yellow, with red indicating no statistical significance. The `heatmap()` program reorganizes the rows (behaviors) and columns (outcomes) in order to visually group together regression coefficients with similar significance values. Heatmaps are discussed again in Sect. 11.3.

The red/yellow color pattern only indicates statistical significance of the estimated regression coefficient. These do not all correspond to good or bad health patterns because the explanatory variables are not all indicative of the same direction. Frequent binge drinking is (presumably) a bad health behavior and visiting a dentist is a good behavior. So in these two examples, a positive regression coefficients can have opposite interpretations. Similarly, smoking is highly correlated with any reported disability, but it is not clear from the heatmap whether this correlation is positive or negative. Further, it is not obvious why these two variables should be highly correlated.

The eight separate regressions create eight vectors of residuals. These different residuals represent the eight different health outcomes for each of 192 metropolitan areas after having corrected for each of the ten behavioral measures.

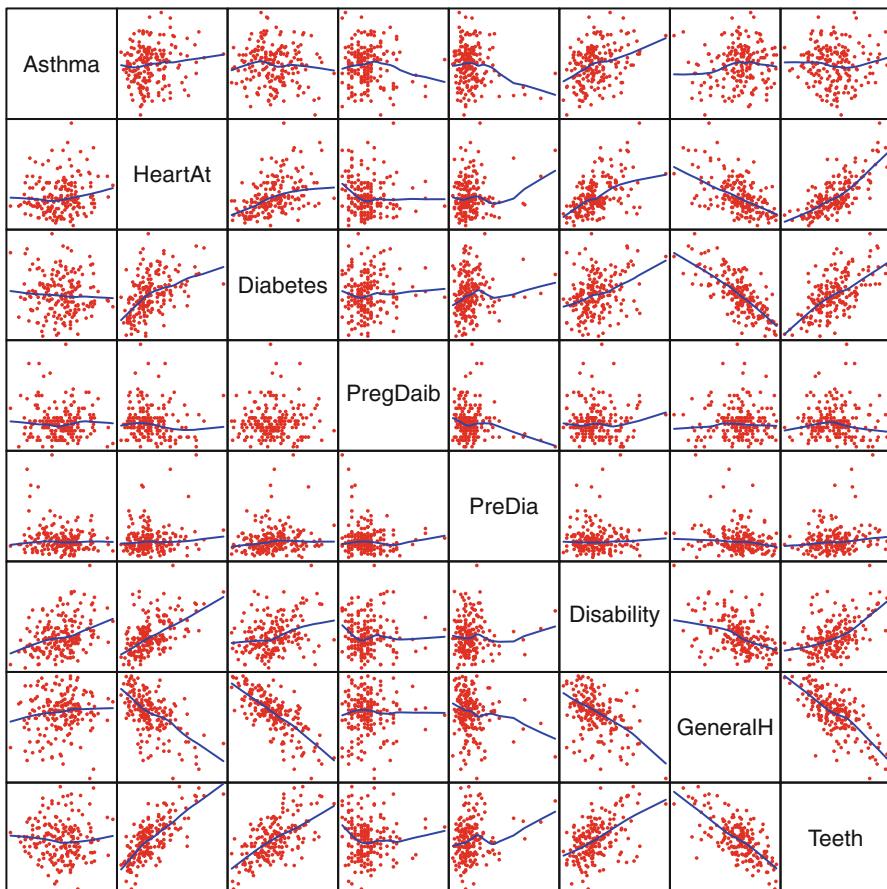


Figure 9.5: Matrix scatter plot and smooth fit of BRFSS health outcome variables

The 8×8 correlation matrix of the residuals appears in Output 9.2. Again, these are not the correlations between the various health outcomes in Table 9.5, but, rather, the correlations of the eight health outcomes after having corrected for each of the ten behavioral measures. The largest correlation is between the diabetes residuals and self-reported general health residuals. We interpret this to mean that the relationship between diabetes and general health at the population level is not accounted for by any of the behavioral measures.

This correlation is large (-0.493), but it is also true that diabetes is reported by less than 9 % of those surveyed. That is, the strong correlation may only reflect a small portion of those affected in the population. Similarly, there is also a large correlation (0.44) between the residuals of those reporting

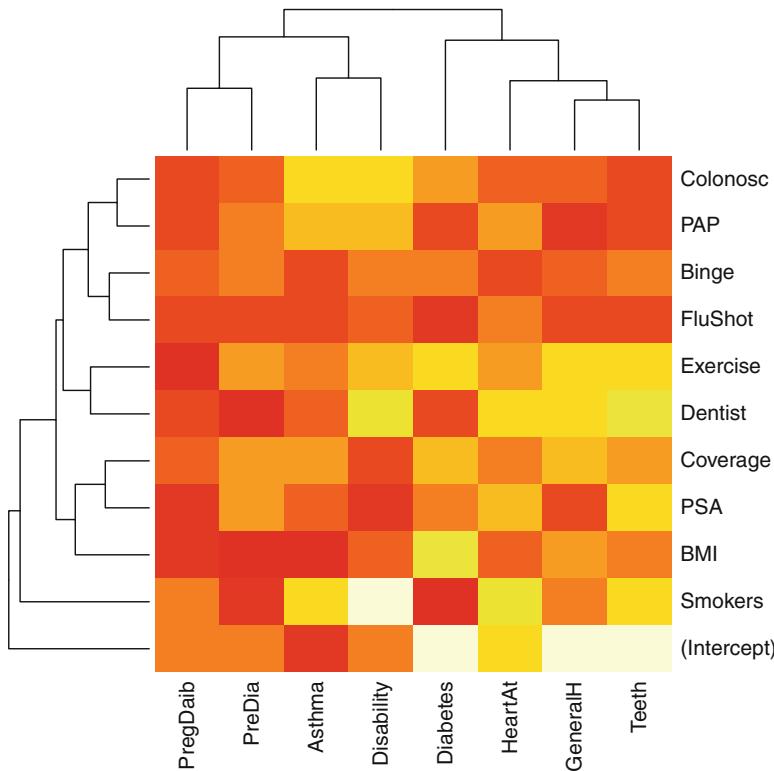


Figure 9.6: Heatmap of statistical significance for regression coefficients in BRFSS data

a heart attack and those reporting loss of adult teeth. Heart attacks were reported by only 4.3 % of those surveyed. In both of these examples (diabetes and heart attack), strong correlations only occur in small segments of the population.

The largest correlation we can identify among the residuals is a large negative and intuitive relationship between those of disability and perception of general health, after having corrected for all of the explanatory behavioral variables in the data set. The “any disability” question is reported by 21.3 % of those surveyed and is experienced by a larger portion of the population than either diabetes or heart attack (Fig. 9.7).

A scatterplot of “any disability” and “reported general health” is given in Fig. 9.8, both as raw data and as residuals after correcting for all of the behavior variables. These separate plots will again reinforce the difference between these different concepts. Noticeably, the residual plot is given on a smaller scale than that of the original data. In both plots, Huntington, West Virginia, exhibits a high level of individuals with a disability and low levels of

Output 9.2: Correlation matrix of BRFSS residuals

```

> cr <- cor(BRFSS.resid)
> print(cr, digits = 2)

          Asthma HeartAt Diabetes PregDaib PreDia
Asthma     1.000    0.12    0.054   -0.028 -0.153
HeartAt    0.118    1.00    0.121   -0.110  0.173
Diabetes   0.054    0.12    1.000    0.042  0.168
PregDaib  -0.028   -0.11    0.042    1.000 -0.121
PreDia     -0.153    0.17    0.168   -0.121  1.000
Disability 0.254    0.28    0.147    0.020  0.088
GeneralH  -0.056   -0.22   -0.493    0.061 -0.275
Teeth      -0.033    0.44    0.280   -0.069  0.272

          Disability GeneralH Teeth
Asthma      0.254   -0.056 -0.033
HeartAt     0.276   -0.220  0.445
Diabetes    0.147   -0.493  0.280
PregDaib   0.020    0.061 -0.069
PreDia      0.088   -0.275  0.272
Disability  1.000   -0.349  0.245
GeneralH   -0.349    1.000 -0.352
Teeth       0.245   -0.352  1.000

```

individuals with self-reported good or excellent general health. On the basis of the 2006 BRFSS survey, the CDC listed Huntington as one of the most unhealthy cities in the US.

In contrast, Fayette, Arkansas, appears to have a high level of self-reported health as a residual, after having corrected for health behaviors. This city does not appear unusual in the original, raw data. Fayette is a university town with an unusually large percentage of citizens with Master's and Ph.D. degrees. The Fayette metropolitan area includes Bentonville, home to many well-paid executives at the Walmart corporate headquarters.

A pairwise scatterplot of the eight sets of residuals is given in Fig. 9.7. There does not appear to be any obvious deviation from the assumption of a multivariate normal distribution. (See Exercise 9.2 for more details.) A principal components analysis of the residuals from these individual regressions completes the multivariate analysis. A portion of that analysis appears in Output 9.3.

From the standard deviations, we see that first few components contain most of the variability. In this case, the residual for loss of `Teeth` has almost all of the weight in the first component and seems to be independent of all

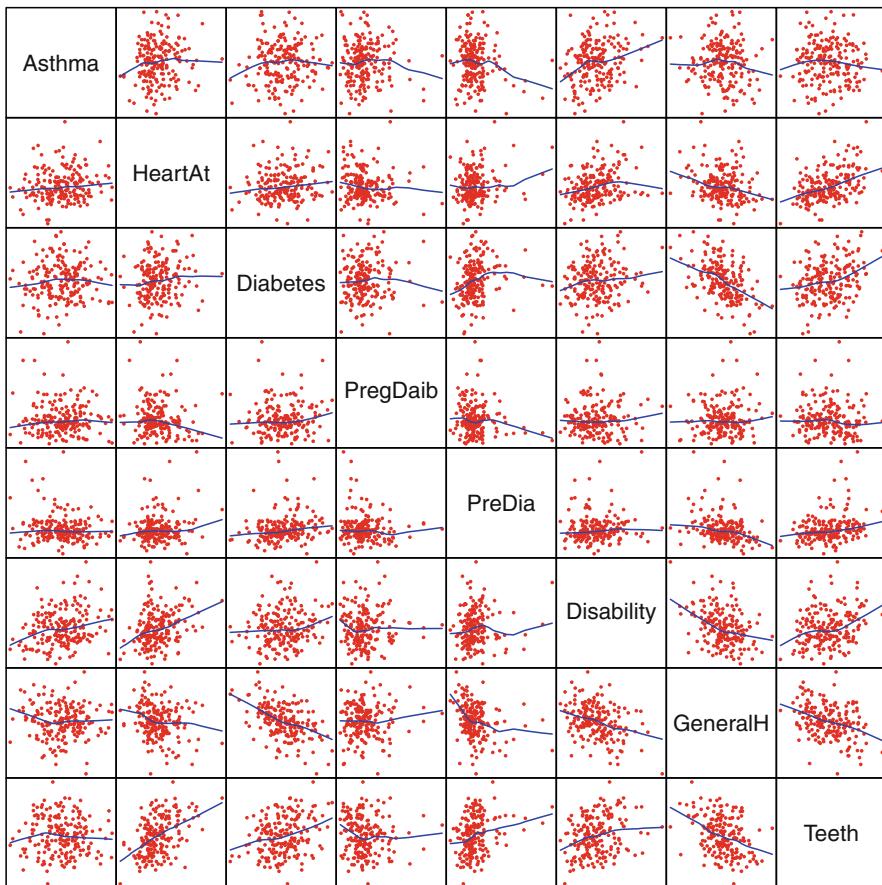


Figure 9.7: Matrix scatterplot and smooth fit of BRFSS residuals

other residuals. Similarly, the second component is almost entirely composed of the **Disability** residual. The third component is the **GeneralH** residual.

The biplot of this principal components analysis appears in Fig. 9.9. The largest contributors to health residuals appear to be loss of permanent teeth and the presence of a disability. These two outcomes, after having corrected for all of the behavior variables, are orthogonal to each other and appear to offer a large amount of explanatory value to the residuals from the multivariate regressions.

In summary, the multivariate regression of the large health survey yields a number of useful summary measures. Behavior variables such as having seen a dentist recently is a good explanatory measure of health outcomes, and the perception of one's health is a single standout determinant of other health outcomes across cities. Two cities appear as outliers at opposite ends of the

 Output 9.3: Principal components analysis for BRFSS residuals

Standard deviations:

```
[1] 4.609 2.943 2.057 1.727 1.127 0.839 0.740
[8] 0.476
```

Rotation:

	PC1	PC2	PC3	PC4
Asthma	0.0138	0.25499	0.17051	-0.9437
HeartAt	0.1009	0.02420	0.03981	-0.0453
Diabetes	0.1101	0.05205	-0.35152	-0.1134
PregDaib	-0.0070	0.00653	0.00677	0.0142
PreDia	0.0530	-0.00957	-0.08155	0.0738
Disability	0.2926	0.85581	0.30301	0.2882
GeneralH	-0.2549	-0.26160	0.84547	0.0591
Teeth	0.9078	-0.36152	0.18012	-0.0473

	PC5	PC6	PC7	PC8
Asthma	-0.0619	0.0341	-0.09833	-0.019658
HeartAt	-0.0794	-0.9342	0.31974	-0.065046
Diabetes	0.9171	-0.0713	0.01803	0.046964
PregDaib	0.0610	0.0912	0.08302	-0.990321
PreDia	-0.0282	-0.3118	-0.93550	-0.108811
Disability	0.0707	0.0409	-0.01358	0.016743
GeneralH	0.3727	-0.0595	-0.07430	0.017944
Teeth	-0.0174	0.1010	0.00252	0.000187

health scale. Tooth loss and having any disability remain highly variable even after taking into account the effects of the explanatory variables.

9.4 Exercises

- 9.1 Table 1.1 lists some cost of living statistics for each of the 50 states plus DC. The three costs are apartment rents, costs of houses, and the cost of living index. Perform a multivariable linear regression to explain these three metrics in terms of the state populations and average incomes. Are these explanatory variables useful for each of the cost variables? Capture the residuals from the three separate linear regressions and perform a principal components analysis. Is there anything left over that the regressions fail to capture? Are there outliers that should be noted?

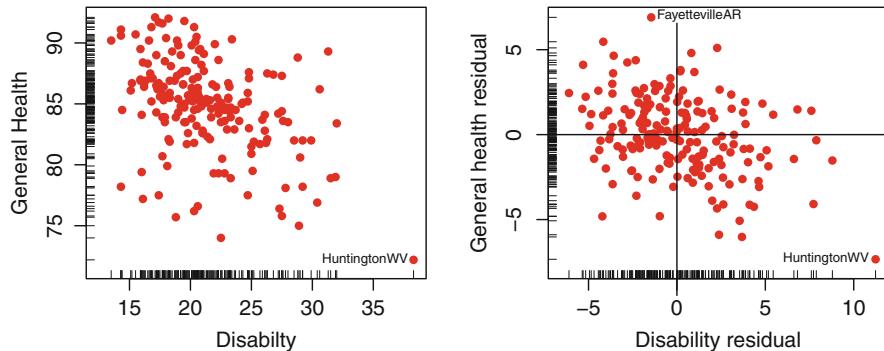


Figure 9.8: Scatterplot of disability and general health, both as raw data and as residuals corrected for all of the behavioral measures

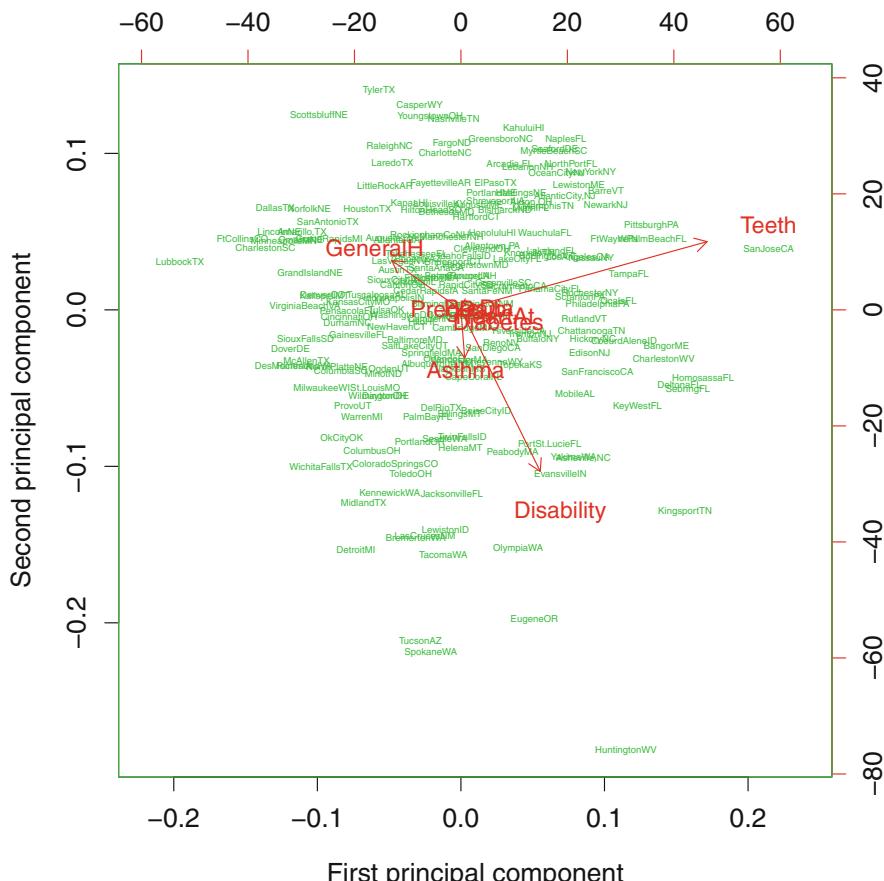


Figure 9.9: Biplot for principal components analysis of BRFSS residuals

Table 9.3: Personal health care expenditures by Medicare patients, listed by functional status for the years 1992–2007

Year	All	No disability	Any physical limitation	Any IADL limitation	1–2 ADL's	3–6 ADL's
1992	6550	2980	3468	5770	7373	17,058
1993	7063	3101	3841	6240	7949	18,782
1994	7730	3355	3783	6396	8349	22,994
⋮	⋮	⋮	⋮	⋮	⋮	⋮
2005	13,218	7577	8975	12,363	16,489	33,663
2006	14,448	8847	9520	14,353	17,759	34,751
2007	14,842	7664	10,009	15,641	17,725	38,809

Source: MCBS

- 9.2 Test the BRFSS residuals for multivariate normality using the tests introduced in Sect. 7.7. Are the outliers highlighted in Fig. 9.8 large enough to lead us to question multivariate normality using these tests? Do the tests have markedly different outcomes if we delete the residuals from these two cities?
- 9.3 The Medicare Current Beneficiary Survey (MCBS) is an ongoing, representative, nation-wide survey of all persons who were Medicare recipients during any part of the current year. The data in Table 9.3 reports all health care goods and services that were purchased directly by the Medicare recipient. Recipients were contacted by telephone to assess their (self-reported) disability status. Physical disabilities were classified as essential activities of daily living (ADL) such as bathing, dressing, eating, and as instrumental ADL (IADL) such as preparing meals, shopping, and answering the telephone. Another examination of this data appears in Exercise 12.4.
- Fit separate linear regressions using the year as the explanatory variable. Choose your dependent variables (disability categories) carefully because some of these include others. Do discontinuous jumps occur in the annual expenditures? These may be attributed to policy changes.
 - Plot the residuals for each regression by year and comment on any apparent lack of independence from one year to the next.
 - Does a principal components analysis reveal any remarkable years?

Table 9.4: Coal mining workers and fatalities by year

Years	Miners	Fatalities
1900	448,581	1489
1901	485,544	1574
1902	518,197	1724
⋮	⋮	⋮
2010	135,500	48
2011	143,437	21
2012	137,650	20

Source: MSHA

- 9.4 Table 9.4 lists the annual number of coal miners and the number of deaths for the industry as reported by the US Department of Labor. The deaths and number of workers have decreased dramatically during the time period covered by this data. In Fig. 9.10, we see the death rate is falling faster than the number of miners. Perform a multivariable regression using year as the explanatory variable. Consider taking logs of the two response variables. What additional information would you like to see in order to draw useful conclusions from this data analysis?
- 9.5 Elston and Grizzle (1962) present the data in Table 9.5 on measurements of Ramus (jaw) bones on 20 boys at four different ages. The explanatory variable is age. We should expect correlations of the four measurements within each boy.
- (a) Fit a regression model using Age as the explanatory variable. Examine residuals graphically and identify outliers. Does a principal components analysis provide additional insights?
 - (b) Are the variances the same at every age?
- 9.6 Many investors in stocks are looking for dividends to be paid out of future profits. Table 9.6 lists a number of the largest technology companies and information of their financial status, as of September 2010. The outcome variables to explain are current and future dividends. See what models you can develop from market capitalization, net cash, and cash flow. You can also create new measures that are nonlinear functions of other explanatory variables such as the ratio of cash flow and market capitalization.
- 9.7 Stepwise regression automates the model-building process. The program

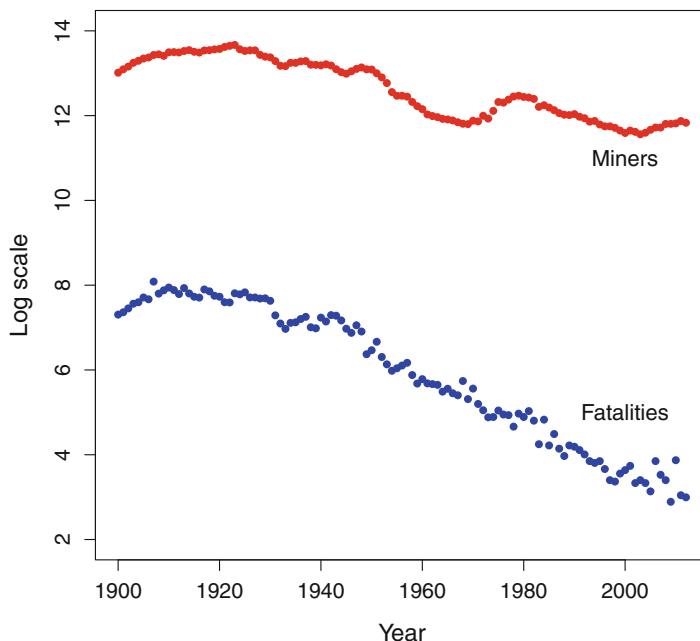


Figure 9.10: US coal miners and fatalities, on a logarithmic scale

```
library(datasets)
library(MASS)
data(mtcars)
univ <- lm(mpg ~ cyl + disp + hp + drat + wt + qsec +
            vs + am + gear + carb, data = mtcars)
backward <- stepAIC(univ)
summary(backward)
```

begins with a linear model containing all of the explanatory variables and removes one at a time. This *backward stepwise regression* allows every explanatory a chance to contribute to the model and uses AIC to eliminate those that do not make a significant contribution.

The AIC is equal to twice the log-likelihood, less 2 times the number of parameters. Unlike the likelihood, AIC charges a “penalty” for every parameter in the model, forcing every parameter to make a contribution to the model. AIC was developed for times series models with many parameters and is described in Sect. 12.2.

Does the final fitted model from this program coincide with our intuition? What are the advantage and disadvantages of having the computer decide on the model for us?

Table 9.5: Measures of jaw bones on 20 boys at four different ages

	Age in years			
	8	8.5	9	9.5
1	47.8	48.8	49.0	49.7
2	46.4	47.3	47.7	48.4
3	46.3	46.8	47.8	48.5
⋮	⋮	⋮	⋮	⋮
19	46.2	47.5	48.1	48.4
20	46.3	47.6	51.3	51.8
Mean	48.7	49.6	50.6	51.5

Source: Elston and Grizzle (1962)

Table 9.6: Characteristics of several high-tech companies as of September 2010. Dollar amounts are in \$Million

Company	Market cap	Net cash	2009 cash flow	Cash flow as % of cap	Cash+cash flow as % of cap	Current dividend rate	Dividend at 60 % payout
Adobe	\$17,254	\$1370	\$1118	6.48 %	14.42	0.0 %	3.9 %
Amazon	66,336	5070	3293	4.96	12.61	0.0	3.0
Apple	252,664	45,800	10,159	4.02	22.15	0.0	2.4
Cisco	125,246	23,700	10,173	8.12	27.05	0.0	4.9
Dell	24,153	8800	3906	16.17	52.61	0.0	9.7
eBay	31,361	6720	2908	9.27	30.70	0.0	5.6
Google	153,317	30,300	9316	6.08	25.84	0.0	3.6
Hewlett-Packard	90,280	6400	13,379	14.82	21.91	0.8	8.9
Intel	105,625	22,100	11,170	10.58	31.50	3.4	6.3
Microsoft	219,195	38,450	24,073	10.98	28.52	2.1	6.6
Oracle	127,578	9914	8681	6.80	14.58	0.8	4.1
Qualcomm	67,370	2870	7172	10.65	14.91	1.8	6.4
Symantec	11,793	1040	1693	14.36	23.17	0.0	8.6
Texas Instruments	30,560	3557	2643	8.65	20.29	1.9	5.2
Yahoo!	19,132	7230	1310	6.85	44.64	0.0	4.1

Source: StreetAuthority (www.StreetAuthority.com) and David Sterman. Used with permission

9.8 The program

```
influence(univ)
```

produces a large number of diagnostics for the regression model. These include `$hat` which is a measure of the influence each observation has on its fitted value. The `$coefficients` estimates how much each estimated regression coefficient is changed when that observation is omitted and the model is refitted. Omitting each observation, in turn, is a method called the *jackknife*. Similarly, `$sigma` estimated the change in estimated standard deviation of the residuals changes when this observation is jackknifed.

Plot some of these diagnostics for the `mtcars` data. Are influential observations also those with unusually large residuals?

- 9.9 Examine `glmrob` in the `robustbase` library, to perform *robust* linear regression. Does the robust fitted model in the `mtcars` data differ from the least squares regression model we fitted here? A larger set of data on more recent cars is available as `car.test.frame` in the `mypart` library.

Chapter 10

Discrimination and Classification

IF WE HAVE multivariate observations from two or more identified populations, how can we characterize them? Is there a combination of measurements that can be used to clearly distinguish between these groups? It is not good enough to simply say that the mean of one variable is statistically higher in one group in order to solve this problem because the histograms of the groups may have considerable overlap making the discriminatory process only a little better than guesswork. To think in multivariate terms, we do not use only one variable at a time to distinguish between groups of individuals, but, rather, we use a combination of explanatory variables.

The difference between discriminant analysis and principal components analysis is that in discriminant analysis, we begin by knowing the group membership. In discriminant analysis we try to identify linear combinations of several variables that can be used to distinguish between the groups. In principal components, by contrast, it is not clear if there are separate groups. If principal components identify groups, then there is no confirmatory step because we may not be aware of separate groups *a priori*. Similarly, in the following chapter, we assume that there are groups within the data but do not identify these in advance.

10.1 An Introductory Example

Let us begin by introducing an example and then carry it through this chapter. Data on three varieties of wine cultivars is given in the data set `wines` (Forina et al. 1988). The entire data set is also available online along with additional information on the variables and a list of references to other,

Table 10.1: List of variables measured on three cultivars of Italian wine grapes

	Variable name	Description
1	Class	Which of three cultivars of wine grapes
2	Alcohol	Alcohol content
3	Malic	Malic acid: provides a sour taste
4	Ash	Ash content
5	Alcal	Alcalinity of ash
6	Mg	Magnesium content
7	Phenol	Total phenols: compounds found in drugs and plastics
8	Flav	Flavanoids: compounds found widely in plants
9	Nonf	Nonflavanoid phenols
10	Proan	Proanthocyanins: tannins which affect color and aging
11	Color	
12	Hue	
13	Abs	Ratio of light absorption at two different frequencies
14	Proline	Proline, an amino acid

published analyses of this data. There are 178 different wines examined. A list of the 14 variables in this data set are listed in Table 10.1.

We can read this data directly from the website using

```
wines <- read.table(
  "http://archive.ics.uci.edu/ml/machine-learning-databases/
  wine/wine.data",
  sep = ",")
```

The `pairs()` matrix scatterplot is given in Fig. 10.1. The R code that produces this figure is

```
colors <- c("green", "red", "blue")[wines[ , 1]]
newwine <- cbind(  # new dataframe with jittered Class
  variable
  jitter(as.integer(wines[ , 1])),
  wines[ , -1])
names(newwine)[1] <- names(wines)[1]  # old name to new
variable
pairs(newwine, pch = 16, cex = .3, gap = 0, col = colors,
  xaxt = "n", yaxt = "n")
```

Table 10.2: Group means for each variable in the wine data. In every row, the statistical significance is smaller than 10^{-4} testing equality of group means

Name	Means		
	Class=1	Class=2	Class=3
Alcohol	13.74	12.28	13.15
Malic	2.01	1.93	3.33
Ash	2.46	2.24	2.44
Alcal	17.04	20.24	21.42
Mg	106.34	94.55	99.31
Phenol	2.84	2.26	1.68
Flav	2.98	2.08	0.78
Nonf	0.29	0.36	0.45
Proan	1.90	1.63	1.15
Color	5.53	3.09	7.40
Hue	1.06	1.06	0.68
Abs	3.16	2.79	1.68
Proline	1115.71	519.51	629.90
Sample			
sizes	59	71	48
codes	Green	Red	Blue

The `Class` variable is jittered to make it easier to view. The `pairs()` command uses options to remove the axes and spaces between individual panels. These instructions create a new data frame called `newwine` in which the integer values of `Class` variable have been jittered.

Discriminant analysis helps us identify distinguishing characteristics of the different groups. One approach is to examine each of the individual measurements separately in a univariate, marginal analysis. In the top row and left column in Fig. 10.1, we can identify individual variables that demonstrate how individual variables differ across the three groups of wines. We can quantify these individual relationships in terms of a separate one-way analysis of variance for each. Specifically, we can perform a hypothesis test that the means of each of the variables are the same across the three groups. If we do this, we find that the one-way analysis of variance demonstrates an extreme level of statistical significance for every variable in the data set. The individual group means are given in Table 10.2 for each variable in the data set.

This marginal approach is intuitive for identifying group means, but it fails to identify discriminatory characteristics for individuals. One individual cultivar may have a high or low value for a specified measurement, but the histograms of the three groups may exhibit considerable overlap, making assessment of group membership difficult. This overlap is readily apparent in

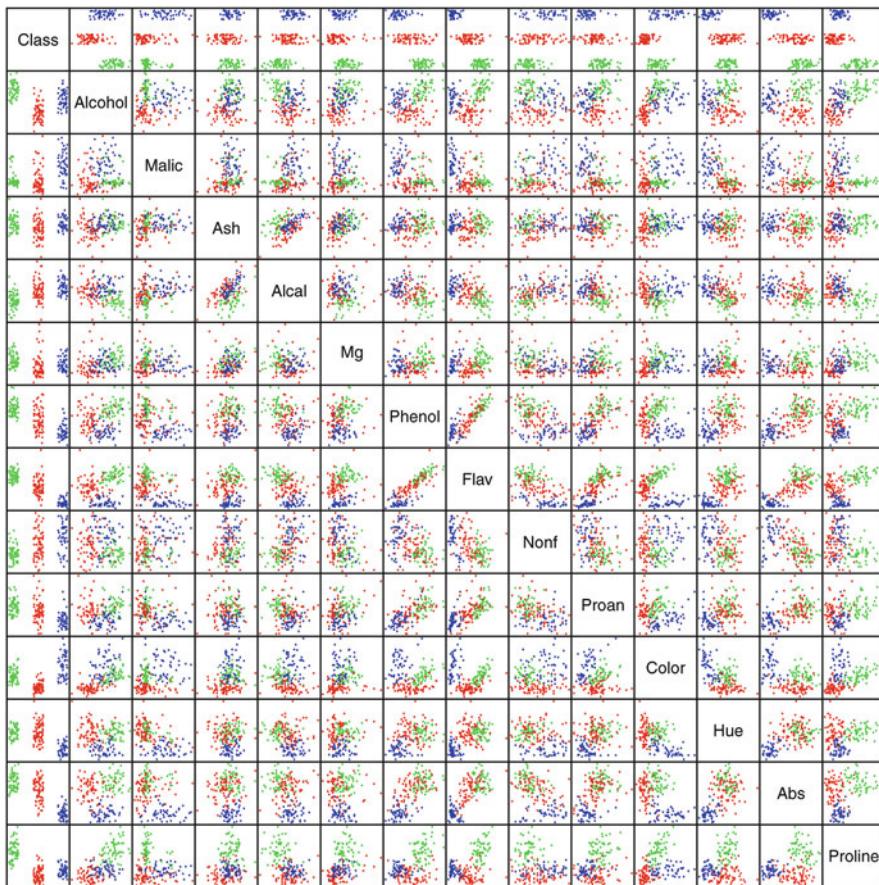


Figure 10.1: Matrix scatterplot for wine data. The *colors* correspond to the three cultivars

the parallel coordinate plot given in Fig. 10.2. Not all variables are included in this figure. The choice of axes in this figure was subjective and performed with a little trial and error. Parallel coordinates were introduced in Sect. 3.5.

The univariate approach fails to include correlations between the individual measurements. There may be combinations of variables that provide a much higher level of discriminatory precision between the three cultivars than this univariate approach.

Figure 10.1 suggests another way of distinguishing the three cultivars. A number of plotted pairs are useful in identifying and discriminating between the three cultivars in Fig. 10.1. These include (Abs, Proline), (Alcohol, Hue), and (Color, Flav) as examples. The object of discriminant analysis is to identify distinguishing characteristics between the different groups.

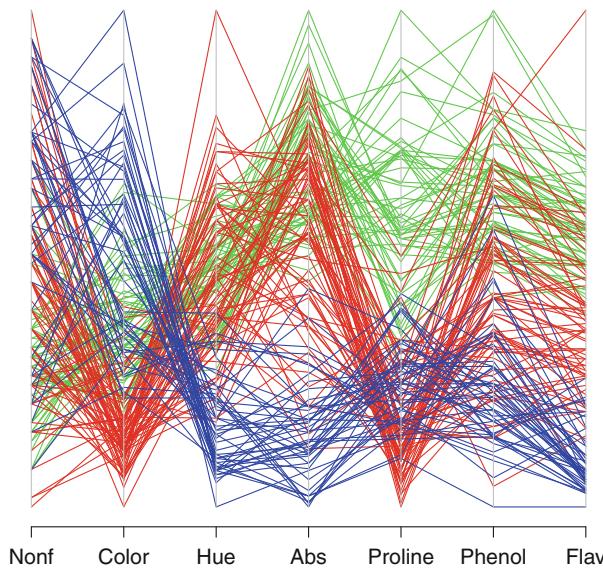


Figure 10.2: Parallel coordinate plot for wine data. The *colors* correspond to those in Fig. 10.1

Even though there are many small plots in the figure, the use of color helps us identify those pairs of variables that have high value in discriminating between the three cultivars.

The following two sections describe discriminatory methods based on linear combinations of all variables in this data set. The support vector approach, described in Sect. 10.4, identifies specific observations that help define regions of high discriminatory value and do not necessarily seek linear combinations to achieve these goals.

10.2 Multinomial Logistic Regression

The reader may already be familiar with the closely-related univariate discriminant method called *logistic regression* in which we use regression methods to distinguish between two different groups. This classification criteria is based on a probabilistic statement about the group membership of each observation. Let us begin with a brief review of this method.

In linear logistic regression, we assume that group membership is expressible as a binary-valued response, $y = 0$ or 1 , conditional on a vector of explanatory variables \mathbf{x} . The data on the i -th observation is then (y_i, \mathbf{x}_i) . The model is expressed as a probability statement about the distribution of a future observation y and any arbitrary value of \mathbf{x} . This model gives us a mathematical statement of the probability that $y = 0$ or 1 for any given value of \mathbf{x} .

Specifically, the model of logistic regression is

$$\log \left(\frac{\Pr[y = 0 \mid \mathbf{x}]}{\Pr[y = 1 \mid \mathbf{x}]} \right) = \boldsymbol{\beta}' \mathbf{x} \quad (10.1)$$

or the log-odds that $y = 0$ versus $y = 1$ is a linear function of the explanatory variables \mathbf{x} . Logistic regression makes no assumption about the distribution of the explanatory variables \mathbf{x} .

We can solve (10.1) for $\Pr[Y = 1]$ in terms of \mathbf{x} :

$$\Pr[Y = 1 \mid \boldsymbol{\beta}' \mathbf{x}] = \exp(\boldsymbol{\beta}' \mathbf{x}) / \{1 + \exp(\boldsymbol{\beta}' \mathbf{x})\}.$$

We can estimate the parameter vector $\boldsymbol{\beta}$ using maximum likelihood and perform statistical inference on it, much as we did in the previous chapter. Intercepts are typically included in these regression coefficients. We interpret each β parameter as the log-odds change in $\Pr[Y = 1]$ for each unit change in the corresponding explanatory variable x .

We next describe the generalization of this model when there are more than two groups that we want to discriminate between. The most commonly used approach selects one category as a reference or baseline and compares all other categories to it. This approach performs a pairwise comparison between each of the categories to the single baseline, reference category. This approach has a useful interpretation when there is an obvious baseline standard, and it makes sense that all categories should be compared to it. In the case of the wine cultivar data, there is no obvious comparison group, and we will arbitrarily set Class=2 as the reference.

The generalization of (10.1) to model the three categories for the wine data is the pair of simultaneous equations

$$\log \left(\frac{\Pr[\text{Class} = 1 \mid \mathbf{x}]}{\Pr[\text{Class} = 2 \mid \mathbf{x}]} \right) = \boldsymbol{\beta}_1' \mathbf{x}$$

$$\log \left(\frac{\Pr[\text{Class} = 3 \mid \mathbf{x}]}{\Pr[\text{Class} = 2 \mid \mathbf{x}]} \right) = \boldsymbol{\beta}_3' \mathbf{x}.$$

In this pair of equations, probabilities $\Pr[\text{Class} = 1]$ and $\Pr[\text{Class} = 3]$ are separately compared to the reference category $\Pr[\text{Class} = 2]$ with respective regression coefficients $\boldsymbol{\beta}_1$ and $\boldsymbol{\beta}_3$.

We next see how to estimate the regression coefficients $\boldsymbol{\beta}_1$ and $\boldsymbol{\beta}_3$ in R. The program and output appear in Output 10.1. This code begins by defining the new variable **rClass** as type **factor** and then sets the reference category.

These regression coefficients are the pairwise comparisons between Class=1 and =3 with the reference category. The fitted coefficients represent log-odds ratios of the change on classification probabilities when

Output 10.1: Multinomial logistic regression for the wine data

```

> require(nnet)
> wines$Class <- as.factor(wines$Class) # create factor
  categories
> wines$rClass <-
+   relevel(wines$Class, ref = 2)      # set reference category
> winelogit <- multinom(rClass ~ Alcohol + Ash + Alcal + Abs +
  Proline,
+                           data = wines, maxit = 200)

# weights:  21 (12 variable)
initial  value 195.552987
iter  10 value 38.789908
...
iter 170 value 13.330023
final  value 13.325689
converged

> print(ws <- summary(winelogit), digits = 4)

Call:
multinom(formula = rClass ~ Alcohol + Ash + Alcal + Abs + Proline,
  data = wines, maxit = 200)

Coefficients:
            (Intercept) Alcohol     Ash     Alcal     Abs Proline
1      -124.00     6.213  22.849 -3.3478  10.354  0.029383
3      -46.46     2.927   6.192   0.3032 -7.483  0.005955

Std. Errors:
            (Intercept) Alcohol     Ash     Alcal     Abs Proline
1       0.1139    1.6304  0.1403  1.0161  0.2612  0.032351
3       0.3588    0.4539  2.8564  0.2566  1.8766  0.003968

Residual Deviance: 26.65138
AIC: 50.65138

> tratio <- ws$coefficients / ws$standard.errors
> # two tailed p values from the t with $edf = effective df
> print( 2 * (1 - pt(abs(tratio), df = ws$edf)), digits = 4)

            (Intercept) Alcohol     Ash     Alcal     Abs Proline
1           0 2.482e-03 0.00000  0.006404 4.308e-14  0.3816
3           0 3.169e-05 0.05101  0.260270 1.802e-03  0.1592

```

the independent variable changes by one unit. This is the same interpretation as with binary response logistic regression.

The models are specified by

```
rClass ~ Alcohol + Ash + Alcal + Abs + Proline
```

in the `multinom` routine, using notation similar that we used to specify linear models in the previous chapter.

Following some trial and error, we found that this choice of covariates provided a good fit. Output 10.1 ends by showing how to test the statistical significance of these regression coefficients and computes two-tailed p-values using a t-distribution with *effective df* determined by `edf`.

The fitted multinomial distribution for each observation is obtained as follows:

```
ws$fitted.values
      2           1           3
1  6.405531e-18 1.000000e+00 2.109756e-21
2  3.942623e-16 1.000000e+00 1.247350e-20
3  3.273230e-11 1.000000e+00 2.887328e-12
...
176 3.195637e-03 2.996409e-10 9.968044e-01
177 3.295305e-03 4.418253e-09 9.967047e-01
178 2.347762e-05 3.582232e-15 9.999765e-01
```

Every row of these fitted values sums to one (or within rounding error of one). Each row is the estimated probability of class membership for this wine.

Let us introduce some graphical diagnostics for this model. Figure 10.3 plots the fitted model and standardized residuals using `wine$Class=2` as the reference category. Fitted values only appear below the diagonal because $\Pr[Y = 1]$ and $\Pr[Y = 3]$ must sum to less than one. A perfect fit would have all of these values in each of the corners of the triangle: green (for Class=1) in the lower right, red (Class=2, the reference category) at the origin in the lower left, and blue (Class=3) at the upper left.

Let us define standardized residuals for this model:

$$(obs - \hat{p}) / \sqrt{\hat{p}(1 - \hat{p})} . \quad (10.2)$$

There are three residuals for each observation in the wine data. The three \hat{p} values are obtained from `ws$fitted.values`, above. The obs is the indicator of observed group membership for each category. In the wine data, with three categories, an observation in Class=3 will have $obs = (0, 0, 1)$.

The residuals are standardized to have zero means and unit variances. We should not expect these to look normally distributed because obs is binary

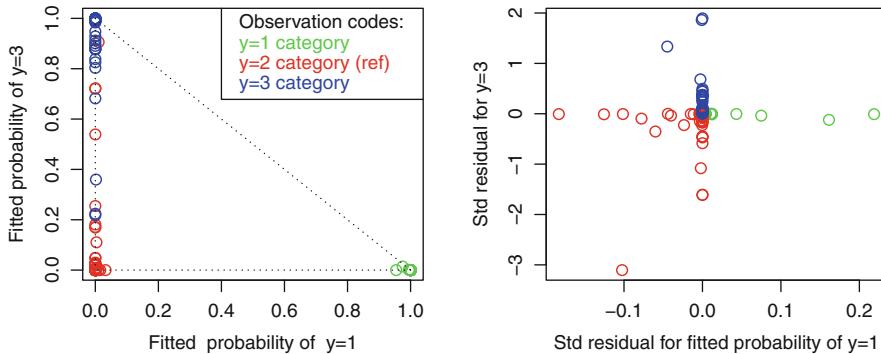


Figure 10.3: Fitted and standardized residuals in multivariate logistic model wine data using `Class=2` as the reference category. These plots use the same color codes as in Figs. 10.1 and 10.2

valued so residual values equal to zero are not possible. Every observation will yield one residual for every category so every cultivar will have three residuals. Figure 10.3 shows the scatterplot of residuals for the `Class=1` and `=3` categories. The residuals of observed values all fall into different orthants, again because the `obs` values are either zero or one. Specifically, when one of the three residuals is positive valued, then the other two must be negative. There is one extreme residual with an absolute value of five and only a few with values greater than three, so we conclude that the model contains few outliers.

Let us conclude this section with a brief discussion of this generalization of logistic regression to more than two categories. Multinomial logistic regression does not have a large collection of diagnostics unlike logistic regression for binary-valued responses. We described a set of residuals in this section.

An advantage to the approach of comparing all categories to a reference is that it supports the *independence of irrelevant alternatives*. Specifically, if observations from a new category are added then the results remain unchanged. Similarly, if observations from a non-reference category are deleted, then, again, the results remain unchanged. Independence of irrelevant alternatives follows from the approach of performing a series of pairwise comparisons with a baseline category. See Exercise 10.9 for another approach to generalizing logistic regression to multinomial data.

10.3 Linear Discriminant Analysis

Linear discrimination analysis allows us to identify a linear combination of variables that can be used to clearly identify the group membership of all individuals. Unlike logistic regression which makes no assumption about the

Output 10.2: Code to produce Fig. 10.4

```

library(MASS)
ld <- lda(Class ~ ., data = wines)
loading <- as.matrix(wines[ , 2 : 14]) %*% ld$scaling

plot(loading, col = c(6, 2, 4)[wines[ , 1] ],
     pch = 16, cex = 1.25,
     xlab = "First linear discriminator",
     ylab = "Second linear discriminator")
for (i in 1 : 3)                      # add class number to
  each centroid
{
  centx <- mean(loading[wines[,1] == i, ] [ , 1] )
  centy <- mean(loading[wines[,1] == i, ] [ , 2] )
  text(centx, centy, i, cex = 2)
}

```

explanatory variables \mathbf{x} , linear discriminant analysis assumes that the \mathbf{x} s have multivariate normal distributions with different means for each group but the same covariance across all groups. These assumptions will be made clear again below, when we develop the methodology for this approach.

In Fig. 10.4 we apply the linear discrimination analysis to the wine data and plot the resulting groups in colors and identifying Class number. The `lda()` function is the program we need. The code that performs the analysis in R and produces Fig. 10.4 is given in Output 10.2.

The first and second discriminators are linear combinations of variables that best discriminate between the three cultivars of wines. The linear weights are listed as `LD1` and `LD2` in Output 10.3. The loadings are the linear combinations of the explanatory variables, calculated in the code and plotted in Fig. 10.4. This figure illustrates a clear distinction between the three cultivars.

The fitted (posterior) estimated probabilities of group membership can be obtained as `predict(ld)$posterior`. The plot of these appears in Fig. 10.5. This plot is much better than the corresponding Fig. 10.3 for the multinomial logistic regression.

The remainder of this section introduces some methodology and shows how the mechanics of linear discrimination work. As we work out the theory, we will refer to an idealized example of discriminating between a mixture of two normal distributions depicted in Fig. 10.6. Then we will return to the example of the three wine cultivars.

Suppose we have K different populations (for some $K = 2, 3, \dots$) and each population is expressible as a p -dimensional normal population with re-

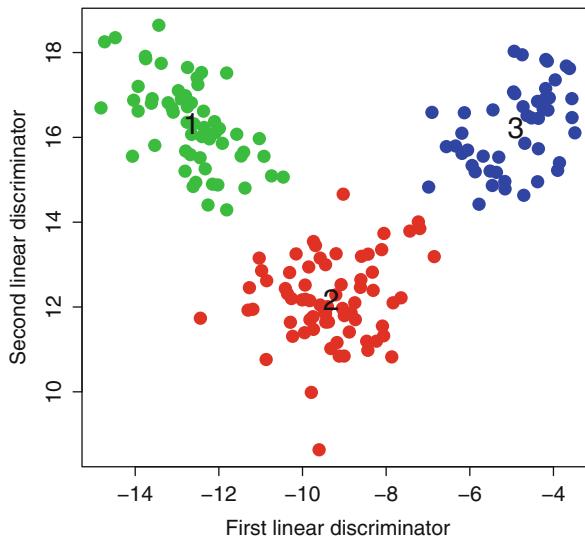


Figure 10.4: Linear discrimination for wine data using the same color codes as in Figs. 10.1 and 10.2

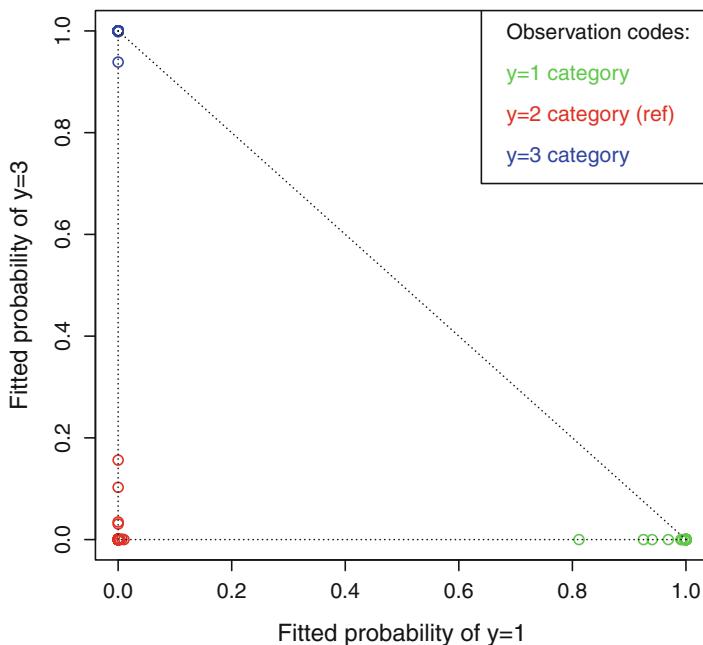


Figure 10.5: Fitted linear discrimination posterior probabilities for wine data using the same color codes as in Figs. 10.1 and 10.2

Output 10.3: Linear discriminant analysis `lda` for the wine data

Prior probabilities of groups:

1	2	3
0.3314607	0.3988764	0.2696629

Group means:

	Alcohol	Malic	Ash	Alcal	Mg	Phenol
Flav						
1	13.74475	2.010678	2.455593	17.03729	106.3390	2.840169
	2.9823729					
2	12.27873	1.932676	2.244789	20.23803	94.5493	2.258873
	2.0808451					
3	13.15375	3.333750	2.437083	21.41667	99.3125	1.678750
	0.7814583					
Nonf	Proan	Color	Hue	Abs	Proline	
1	0.290000	1.899322	5.528305	1.0620339	3.157797	1115.7119
2	0.363662	1.630282	3.086620	1.0563380	2.785352	519.5070
3	0.447500	1.153542	7.396250	0.6827083	1.683542	629.8958

Coefficients of linear discriminants:

	LD1	LD2
Alcohol	-0.403274956	0.8718833272
Malic	0.165185223	0.3051811048
Ash	-0.368792093	2.3459219420
Alcal	0.154783909	-0.1463931519
Mg	-0.002162757	-0.0004611477
Phenol	0.617931702	-0.0324979420
Flav	-1.661172871	-0.4916834144
Nonf	-1.495756932	-1.6303752589
Proan	0.134093115	-0.3070371492
Color	0.355006846	0.2530559406
Hue	-0.819785218	-1.5182643908
Abs	-1.157612096	0.0512054337
Proline	-0.002690475	0.0028540202

Proportion of trace:

LD1	LD2
0.6875	0.3125

spective means $\boldsymbol{\mu}_j$ ($j = 1, \dots, K$) and all with the same covariance matrix $\boldsymbol{\Sigma}$. (It will be useful to review the functional form of the multivariate normal distribution (7.2) at this point.) We also have mixing probabilities π_j representing the probability that a randomly selected observation is sampled from Population j .

The parameters π_j are called *prior probabilities* because they represent characteristics of the population that are known to us before any data is observed. Of course, these can be estimated from the data, as is frequently the case in practice. In Output 10.3, for example, these prior probabilities are the observed sample proportions of the three wine cultivars. The means $\boldsymbol{\mu}_j$ and the covariance $\boldsymbol{\Sigma}$ common to all populations will be assumed to be known, but, in practice, these will also be estimated from the data.

Given a p -dimensional observation \mathbf{x} we can express the prior probabilities

$$\Pr[\text{Population } j] = \pi_j$$

that a randomly selected observation is sampled from Population j .

The conditional density function of \mathbf{x} given that it was sampled from Population j is

$$f(\mathbf{x} \mid \text{Population } j) = f(\mathbf{x} \mid \boldsymbol{\mu}_j, \boldsymbol{\Sigma})$$

for a multivariate normal density function given in (7.2) with mean $\boldsymbol{\mu}_j$ and variance $\boldsymbol{\Sigma}$.

As an example, Fig. 10.6 displays the density function of a mixture of two bivariate normal distributions. Population 1 occurs with (prior) probability $\pi_1 = 0.6$ and Population 2 occurs with $\pi_2 = 0.4$. By *prior probability* we mean that, before having observed any data, we will guess that there is a 60% chance that data will be sampled from Population 1. In these illustrations, the two population means are $\boldsymbol{\mu}'_1 = (-1, -1)$ and $\boldsymbol{\mu}'_2 = (1, 1)$. Both populations have the same variance matrix

$$\boldsymbol{\Sigma} = \begin{pmatrix} 1 & -0.4 \\ -0.4 & 1.2 \end{pmatrix}.$$

This example is illustrated in Fig. 10.6, both as a perspective and as contour plots. The front/left normal (with $\pi_1 = 0.6$) is a little taller than the second population with $\pi_2 = 0.4$. Both distributions exhibit slight elliptical orientations from the upper left to lower right. Given a sampled observation $\mathbf{x} = (x_1, x_2)$, we want the best way to distinguish which of the two distributions it was sampled from. We will come back to this example again as we develop the mathematical background.

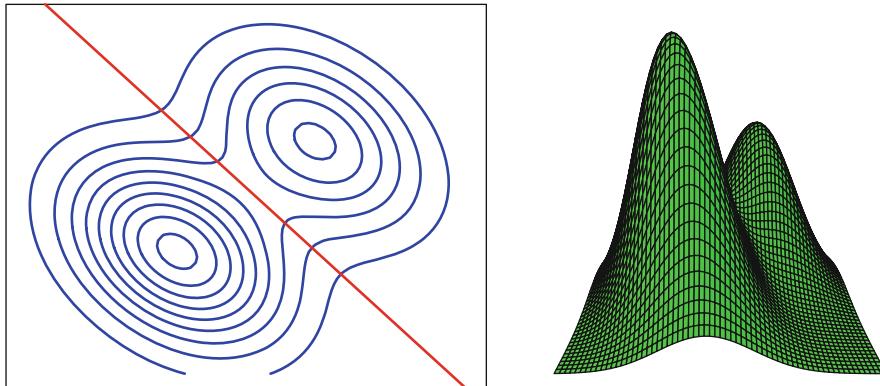


Figure 10.6: A mixture of two bivariate normal density functions plotted as contours and perspective. The *red line* is the boundary of the linear discriminator, given at (10.6)

Getting back to the general setting, the joint density of observing \mathbf{x} from Population j is

$$f(\mathbf{x} \text{ was sampled from Population } j) = \pi_j f(\mathbf{x} \mid \boldsymbol{\mu}_j, \boldsymbol{\Sigma})$$

That is, we have to select the j th population and also observe \mathbf{x} from it.

The marginal density for a value \mathbf{x} sampled from an unspecified population

$$f(\mathbf{x}) = \sum_j^K \pi_j f(\mathbf{x} \mid \boldsymbol{\mu}_j, \boldsymbol{\Sigma})$$

is the sum over all possible population values of $j = 1, \dots, K$.

The *posterior probability density* of sampling from Population k for a given observation \mathbf{x} is

$$f(\text{Population } k \mid \mathbf{x}) = \pi_k f(\mathbf{x} \mid \boldsymbol{\mu}_k, \boldsymbol{\Sigma}) \left/ \sum_j^K \pi_j f(\mathbf{x} \mid \boldsymbol{\mu}_j, \boldsymbol{\Sigma}) \right. . \quad (10.3)$$

This is the basic formula needed to estimate the population that observation \mathbf{x} was sampled from. The *maximum a posteriori* (MAP) estimator \hat{k} directs us to choose the value of k that makes the probability in (10.3) as large as possible. Intuitively this makes sense. We want to identify the most likely population. The *mode* is one way to estimate this. The `lda()` routine in R calculates the K different values of (10.3) for us. The remainder of the

mathematical development provides the detail of the computation when the data \mathbf{x} is sampled from one of K different multivariate normal populations.

Notice the denominator of (10.3) is the same for every value of k so the MAP estimator of k

$$\hat{k} = \text{Value of } k \text{ that maximizes } \pi_k f(\mathbf{x} \mid \boldsymbol{\mu}_k, \boldsymbol{\Sigma}).$$

is the value that maximizes the numerator of (10.3).

The value of k that maximizes $\pi_k f(\mathbf{x} \mid \boldsymbol{\mu}_k, \boldsymbol{\Sigma})$ will also maximize the logarithm of this quantity.

We next need to use the mathematical form of the multivariate normal density f . Recall from (7.2) that the p -dimensional multivariate normal distribution with mean $\boldsymbol{\mu}_k$ and variance $\boldsymbol{\Sigma}$ has density function

$$f(\mathbf{x}) = \frac{1}{2\pi^{p/2}\text{Det}(\boldsymbol{\Sigma})^{1/2}} \exp\left\{-1/2(\mathbf{x} - \boldsymbol{\mu}_k)' \boldsymbol{\Sigma}^{-1}(\mathbf{x} - \boldsymbol{\mu}_k)\right\}.$$

Then we can write

$$\log\{\pi_k f(\mathbf{x} \mid \boldsymbol{\mu}_k, \boldsymbol{\Sigma})\} = \log(\pi_k) - \log\{(2\pi)^{p/2}\text{Det}(\boldsymbol{\Sigma})^{1/2}\} - 1/2(\mathbf{x} - \boldsymbol{\mu}_k)' \boldsymbol{\Sigma}^{-1}(\mathbf{x} - \boldsymbol{\mu}_k).$$

The second term involving $(2\pi)^{p/2}$ and $\text{Det}(\boldsymbol{\Sigma})$ does not depend on either k or the data \mathbf{x} , so this term can be ignored and will be omitted from further discussion.

We next want to find the value of k to maximize

$$\begin{aligned} \log(\pi_k) - 1/2(\mathbf{x} - \boldsymbol{\mu}_k)' \boldsymbol{\Sigma}^{-1}(\mathbf{x} - \boldsymbol{\mu}_k) \\ = \log(\pi_k) + \mathbf{x}' \boldsymbol{\Sigma}^{-1} \boldsymbol{\mu}_k - 1/2 \boldsymbol{\mu}_k' \boldsymbol{\Sigma}^{-1} \boldsymbol{\mu}_k - 1/2 \mathbf{x}' \boldsymbol{\Sigma}^{-1} \mathbf{x} \end{aligned}$$

after we expand the quadratic form in \mathbf{x} .

The last term in $\mathbf{x}' \boldsymbol{\Sigma}^{-1} \mathbf{x}$ does not depend on the choice of k and can also be ignored.

Finally, the discriminant function, defined by

$$\delta_k(\mathbf{x}) = \mathbf{x}' \boldsymbol{\Sigma}^{-1} \boldsymbol{\mu}_k - 1/2 \boldsymbol{\mu}_k' \boldsymbol{\Sigma}^{-1} \boldsymbol{\mu}_k + \log(\pi_k),$$

is the function we need to evaluate in order to choose the appropriate population that \mathbf{x} was sampled from. Our MAP estimate of k is that value which maximizes $\delta_k(\mathbf{x})$. We only have to evaluate these K functions $\delta_k(\mathbf{x})$ and pick the largest.

Only the first term in $\delta_k(\mathbf{x})$ depends on the data \mathbf{x} . This is a linear function of \mathbf{x} , leading us to use the name, *linear discrimination*. In practice, the parameters $(\boldsymbol{\mu}_k, \boldsymbol{\Sigma})$ are replaced by their usual estimators. The `lda()` function in R calculates the $\delta_k(\mathbf{x})$ and evaluates the posterior probability (10.3) for every observation in the data.

Let us be specific and ask how the linear discrimination process distinguishes between two different populations denoted j and k . The *boundary* of this process occurs for values of \mathbf{x} for which

$$\delta_j(\mathbf{x}) = \delta_k(\mathbf{x}).$$

That is, the solutions to this equation is a set of hypothetical data values \mathbf{x} that would provide equal amounts of evidence for both of these different populations.

The solutions of the equation $\delta_j(\mathbf{x}) = \delta_k(\mathbf{x})$ occur for values of \mathbf{x} in which

$$\log(\pi_k/\pi_j) - 1/2 (\boldsymbol{\mu}_k + \boldsymbol{\mu}_j)' \boldsymbol{\Sigma}^{-1} (\boldsymbol{\mu}_k - \boldsymbol{\mu}_j) + \mathbf{x}' \boldsymbol{\Sigma}^{-1} (\boldsymbol{\mu}_k - \boldsymbol{\mu}_j) = 0 \quad (10.4)$$

or more simply,

$$\text{Constant} + \mathbf{x}' \boldsymbol{\Sigma}^{-1} (\boldsymbol{\mu}_k - \boldsymbol{\mu}_j) = 0 \quad (10.5)$$

where the Constant depends on j and k but not on \mathbf{x} .

If we return to the parameter values in the example of normal mixtures, (10.4) becomes

$$0.40546 + (x_1, x_2)'(-3.08, -2.69) = 0$$

or

$$x_2 = 0.1506 - 1.1428x_1. \quad (10.6)$$

This last equation is plotted as the red line in Fig. 10.6 and clearly provides a good dividing line to discriminate between the two mixed populations.

We can generalize this example by examining the linear function of \mathbf{x} in (10.5). Specifically, the *Fisher linear discriminant function* between populations j and k is

$$L_{jk}(\mathbf{x}) = \mathbf{x}' \mathbf{S}^{-1} (\hat{\boldsymbol{\mu}}_k - \hat{\boldsymbol{\mu}}_j). \quad (10.7)$$

Parameter values in (10.5) have been replaced by their usual estimates in (10.7) and the constant term has been ignored. Specifically, population means $\boldsymbol{\mu}_k$ are replaced by the sampled within-group means. The covariance matrix $\boldsymbol{\Sigma}$ is replaced by the sample covariance matrix \mathbf{S} assuming that the covariance is the same in all groups. The discriminator in (10.7) is a scalar-valued, linear function of a vector of data values, \mathbf{x} . More generally, when discriminating between K groups, there will be (at most) $K - 1$ linear discrimination functions. Two linear discriminant functions are plotted in Fig. 10.4 for the three wine cultivars.

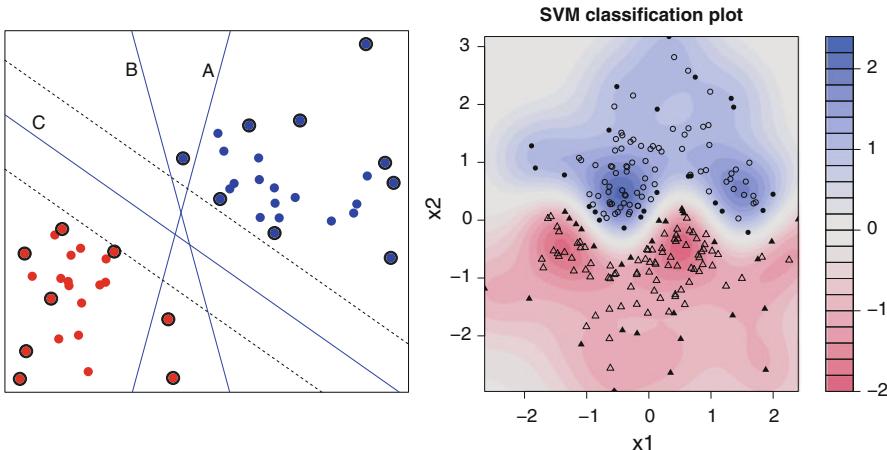


Figure 10.7: Examples of support vector methods: linear and kernel classifiers

We next describe a method that allows the computer to identify a more general classification rule between groups of individuals. This rule does not begin with any pre-specified functional form.

10.4 Support Vector Machine

The support vector machine (SVM) is a group of classification algorithms that include a variety of parametric and nonparametric models. Parametric models include straight lines and similar regression methods. The nonparametric methods contain a variety of kernel smoothing techniques. The programs in R include features that estimate the classification probabilities using cross validation as well as training samples in machine learning.

Two examples are presented in Fig. 10.7. The left panel illustrates a linear SVM classifier. Line A does not completely classify the red and blue groups of samples. Line B classifies correctly but has small margins for misclassification. Line C, the product of a SVM, provides the largest possible margins. These margins are given with dotted lines.

Clearly, those observations that are closest to the margins are most important to the determination of the classification regions. Such observations are referred to as *support vectors*. The support vectors in this figure are plotted with black circles. Observations that define and lie on the periphery of the regions of different colored points are support vectors, as well. Support vectors will be discussed again below.

The right panel of Fig. 10.7 is the result of a SVM with a kernel smoothing classifier. Kernel smoothing is closely related to the *loess* fits in Fig. 3.16 and in the kriging map of altitudes of US cities in Fig. 3.14. Unlike the linear

classification regions assumed in the previous two sections of this chapter and in the left panel of Fig. 10.7, kernel smoothing on the right panel of this figure makes no assumption on the shape of the regions.

The kernel smooth produced by SVM classifies future observations with confidence based on the intensity of the plotted color. The lighter-colored regions have low confidence and white represents complete indifference, as in the wavy region across the center. A functional form for the boundary between these two regions is not specified, but the SVM program clearly locates it.

Note that the upper corners of this figure are also plotted as white. If any future observations were to fall in either of the extreme top corners, then SVM would not automatically classify these as the blue type. There have not been any known observations of that type appearing in either of these regions, so there is no reason to classify new observations one way or the other with any degree of certainty. The concept of classifying new observations is described in the discussion of *training samples* and *test samples* below.

The data in the right panel of Fig. 10.7 was generated as 250 pairs of correlated normal random variates. We omitted a small number of observations near a sine wave region running through the data. The groups above and below this sine wave are plotted as circles and triangles, respectively. Those observations are identified as support vectors. These are critical to estimating the boundaries plotted in solid. The search for support vectors is similar to observations located on the convex hull, except that the classification regions are not necessarily convex. (An example of a plotted convex hull appears in Fig. 3.11.) The SVM algorithm, then, includes a search for classification regions as well as those observations that bound and determine the regions.

The right panel of Fig. 10.7 was produced by the R code in Output 10.4. In this code, we begin by generating 250 pairs of bivariate normals. The sine-wave shaped classification region is called `wavy`. The code removes all observations that are close to this region. A `data.frame` is created, and only `group` membership is identified to the `ksvm` program. The first and second index are reversed in the `data.frame`. By default, plotted SVM output puts the axis for the second variable on the bottom and the axis for the first variable on the left. This is contrary to the usual way this is done in R.

The index of the support vectors is obtained and the support vector in the original data is available in R using

```
svi <- alphaindex(sv)[[1]]  
all[svi, ]
```

This code was used to identify and highlight the support vectors in the left panel of Fig. 10.7.

The SVM works well for these two artificial examples. Before we apply the SVM to the wine data, let us introduce a method of testing the accuracy of a classification model called *cross validation*.

Output 10.4: Create a nonlinear classification and identify the support vectors in Fig.10.7

```

library(kernlab, mvtnorm)           # for ksvm and
                                    rmvnorm
x <- rmvnorm(n = 250, mean = c(0, 0),
              sigma = matrix(c(1, .1, .1, 1), 2, 2))
wavy <- sin(pi * x[,1]) / 2        # wavy boundary
include <- (abs( wavy - x[,2]) > .25 )# 2x width of
                                         boundary
x <- x[include, ]                  # include those
                                         inside
wavy <- wavy[include]               # the wavy
                                         boundary
group <- 1 + (x[,2] > wavy)        # above or below
                                         boundary?
all <- data.frame(x = x[,c(2, 1)],
                  group = group)           # build a data.frame
colnames(all) <- c("x2", "x1", "group")

sv <-ksvm(group ~., data = all, type = "C-svc")
plot(sv, data=all)

```

j

As with any classification method, we are deluding ourselves if, after fitting the model to some data, we then claim how well the model appears to predict all of the observations the data. The model was built around the data so such a claim is hollow. A much stronger claim would be to see how well the model correctly classifies some future observations that were not part of the model building process. We rarely have access to additional data so the idea of cross validation is to fit the model and then test it with different parts of the existing data.

Cross validation, then, is a method for allowing us to fit and then test on different portions of the data set. Specifically, an n -fold cross validation randomly partitions a data set into n nearly equally sized sets. (Typically, n is an integer in the range between 5 and 10.) One set, called the *testing data set*, is omitted. Then the model is fitted using the remaining $n-1$ sets. These are referred to as the *training data set*.

One training data set is fitted and then cross validation examines how well the resulting model classifies the observations in the omitted, testing data set. The cross-validation process then systematically replaces the omitted data and removes a different set. This process is repeated, separately fitting and testing n different models. Cross validation produces a more reliable estimate of the fitting accuracy. We can also compare the n different fitted

models to examine the consistency of the model building process.

The process of cross validation produces an estimate of the accuracy of the model but also has a hidden benefit, referred to as *machine learning*. In the process of producing an n -fold estimate of the classification error, the SCV also had to fit n different models. Some of these models may have better properties than the original model fitted from the entire data. In this manner, the SVM appears to learn about better models.

Some useful R code for the wine example includes

```
> (svw <- ksvm(Class ~ ., data = wines,
+    type = "C-svc", cross = 5))

. . .

Cross validation error : 0.01127
```

illustrates how we obtain an estimate of the five-fold cross-validation error. See Exercise 10.10 for more on the fold parameter when performing a cross validation.

The `alphaindex()` command produces three separate lists of support vectors: one for each of the three cultivars. There may be some duplication when support vectors are on the boundary for more than one of the three groups. We can combine these lists and remove duplicates as follows

```
> svi <- ( c(alphaindex(svw)[[1]], alphaindex(svw)[[2]],
+           alphaindex(svw)[[3]]))  # master list of
+                               support vectors
> svi <- svi[!duplicated(svi)]  # remove duplicates
```

using the `duplicated()` function in R.

We can use this code to identify and plot the support vectors in the wine data. The original data has 178 observations on three cultivars. In Fig. 10.8, only the support vectors are plotted, using the same colors as before. There are 69 support vectors plotted in this figure, a considerable simplification over the corresponding plot in Fig. 10.1. This approach would also be beneficial with a much larger sample size and each panel would be overwhelmed with data.

The SVM will also produce estimated multinomial prediction probabilities of individual observations belonging to each of the different groups. In the case of the wine cultivar data, we have

```
> svw <- ksvm(Class ~ ., data = wines, type = "C-svc",
+   prob.model = T)
> print(predict(svw, wines[,-1], type="probabilities"),
+   digits=2)
```

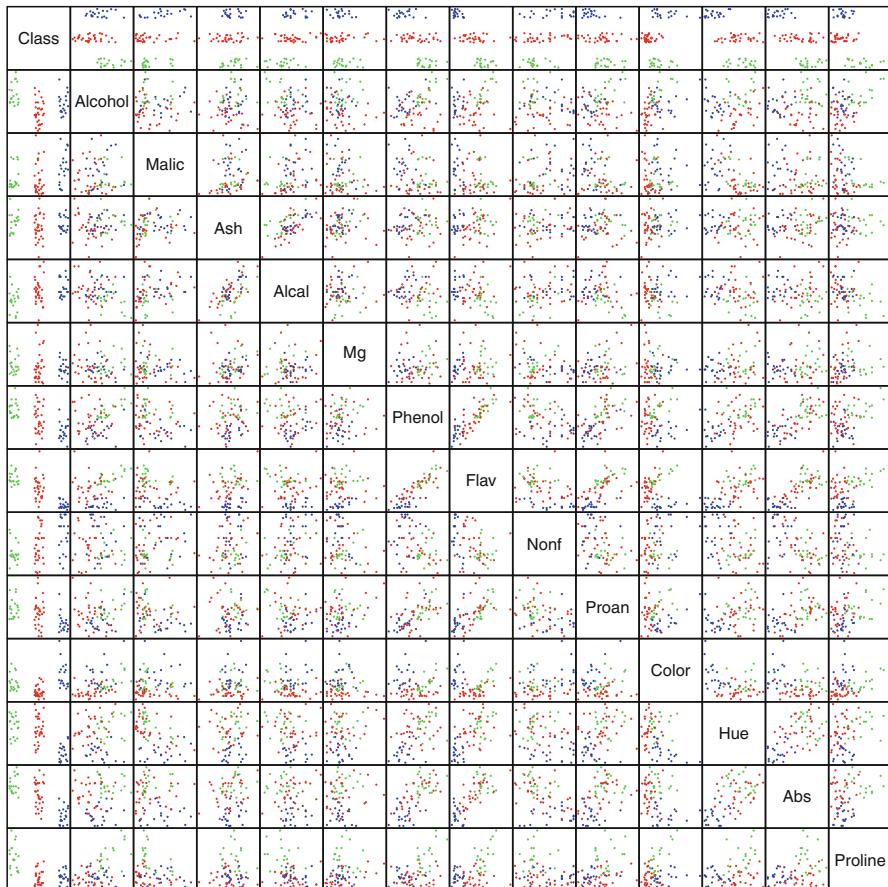


Figure 10.8: SVM classifier for the three wine cultivars. Only the support vectors are shown

```

      1      2      3
[1,] 0.99129 0.00280 0.0059
[2,] 0.98174 0.00977 0.0085
      .      .
[177,] 0.00826 0.00470 0.9870
[178,] 0.00690 0.00451 0.9886

```

where each row sums to one and estimates the probability that this observation belongs to the three different cultivars.

From these estimated multinomial probabilities, we can plot the fitted and residual values, with analogy to Fig. 10.3. Again, we use the second category as reference and continue to use the same color codes for the three classes in this example.

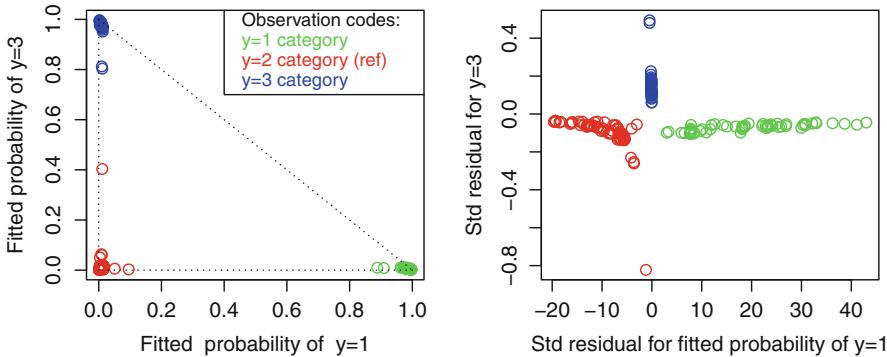


Figure 10.9: SVM fitted probabilities and residuals for the wine cultivars

The SVM fit in Fig. 10.9 is clearly accurate: The fitted probabilities for the three cultivars place them squarely in the three corners of the triangle-shaped figure, just as we would expect of a well-fitting model. There is no overlapping of fitted categories as visible in Fig. 10.3 showing that SVM produces a much better fit. However, the residual plot is not useful and exhibits a distorted horizontal scale, owing to the small probabilities involved.

There is much more that can be said about SVM including the many options and different kernel smoothing functions available, but this is a good place to stop and review.

What are the good and bad features of the different discrimination methods described so far in this chapter? Figure 10.9 illustrates an excellent discrimination of the three wine cultivars. This figure illustrates a much better fit to the data than the corresponding plot that multinomial logistic regression provides us in Fig. 10.3. Unfortunately, SVM produces estimates but no model that can be expressed as a mathematical formula. Conversely, SVM is extremely flexible and able to detect the wavy boundary in Fig. 10.7 without any additional specification on our part.

Linear discrimination provides both a mathematical form and a useful diagram in Fig. 10.4. The two axes of this figure are made of linear-weighted composite measures that lack a simple explanation. Similarly, multinomial logistic regression also expresses discrimination functions on the basis of linear combinations of the data values.

We next describe a classification method that combines the regression models of the previous chapter with a classification tree.

10.5 Regression Trees

We can also build classification rules based on hierarchical trees. These methods will work well for classifying groups based on a continuous outcome (see Exercise 10.16), but we will concentrate on discrete group membership in

this section. The methods of this section are also referred to as *recursive partitioning* and as *computer-aided regression trees (CART)*.

Let us look at a regression tree for the wine data. The regression tree appearing in Fig. 10.10 was built using the R code:

```
winetree <- mpart(Class ~ . , data = wines, method =
"class", size = 4)
```

The R program `mvpart` (in the library of the same name) was used to draw this picture. At the tips of the leaves, this program draws a small histogram of the three different categories of wines. The R program `rtree` (also in a library of the same name) has a similar function.

The `mpart` program has a syntax that is identical to that of the regression program specifying the dependent variable (`Class`) and a list of the explanatory variables to be considered in the model. The period in the notation `Class ~ .` is shorthand for a list of all variables in the data frame. The `size` variable specifies the number of leaves on the tree. The program will choose a value for you if this number is not included. Diagnostics for choosing the size of the tree will be discussed below.

The printed tree in Fig. 10.10 can be described in words. The first split on Proline separates mode of the `Class=1` wines. The second split on Flavonoids removes a small number of the other two classes from this initial split. The branch on `Abs` segregates the `Class=2` and `3` wines. At the bottom of the tree, there is a summary of several diagnostics that we will describe next in a larger example.

Let us introduce another data set to explain CART in more detail. The `crabs` data set in the `MASS` library lists five dimensions made on each of 200 crabs *Leptograpsus variegatus*, 50 each of the combinations of two sexes and two color variants (blue or orange). The five measurements (in mm) and symbols are frontal lobe size (`FL`), rear width (`RW`), carapace length (`CL`), carapace width (`CW`), and body depth (`BD`). We will use the regression tree approach to classify the four categories of sex and color on the basis of these five measurements.

The program in Output 10.5 creates four group categories and appends these to the original `crab` data, producing a new data frame called `cp`. The groups of sex/color combinations are coded as 1–4 and also using character symbols indicating color (`B` and `O`) and upper/lower case for M/F. This code prints out one observation from each of the four groups before and after this transformation. Printing out some data allows us to see if this is being done correctly. This is a good programming habit to develop.

The regression tree for the crab data appears in Fig. 10.11. Sometimes, the regression tree can grow to unmanageable complexity so the maximum number of branches is specified by the `size =` option in the `mpart` statement in Output 10.5. Every branch ends with a set of the frequencies of the four categories of crabs and plots a small histogram. The symbol of the modal

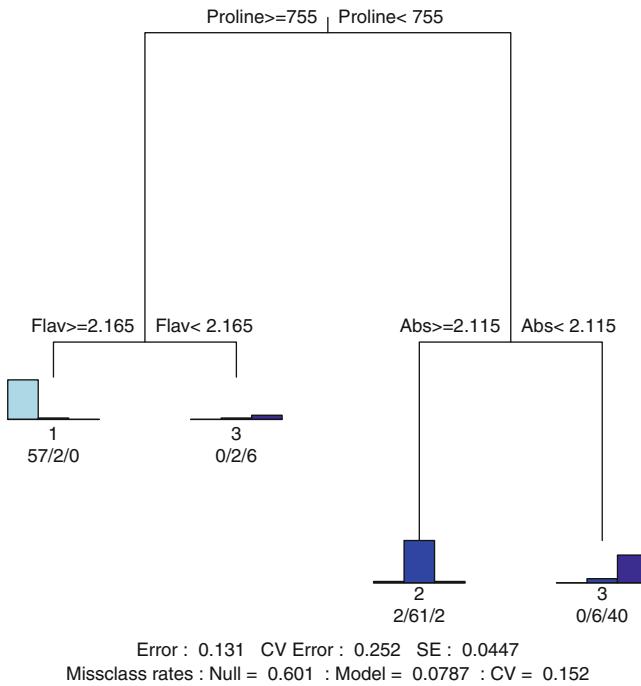


Figure 10.10: Regression tree of wines

category is also printed for us. The first split, for example, is made on large values (≥ 13.95 mm) of rear width RW and this branch segregates a majority (35) of the orange female crabs from all others.

There are a number of useful diagnostics available to us that help guide us to identify an optimal tree size and to estimate the predictive value of the tree. As with many statistical models, there is a trade-off between complexity and precision. A tree with more branches will fit the data better but suffers from the additional burden of its complexity. Similarly, a tree that was built from a data set will appear to classify those values well. Ideally, we would like to make a statement about how a given tree predicts some new set of additional data.

A useful way to approach the competing goals of prediction and complexity is to consider cross validation, a topic introduced in Sect. 10.4. Specifically, a number of the observations are omitted and a new regression tree is built based on the remaining observations. Then we measure how well the resulting tree classifies the omitted values.

We can perform a cross validation simulation of the regression model method by fitting a large tree with many splits and then computing statistics on each of the smaller sized trees. In R we do this for the crab data as follows:

Output 10.5: Program to create four groups of crabs and produce Fig. 10.11

```

> library(MASS)
> data(crabs)
> crabs[c(1, 51, 101, 151),]           # look at some raw data
   sp sex index  FL  RW  CL  CW  BD
1   B   M     1 8.1 6.7 16.1 19.0 7.0
51  B   F     1 7.2 6.5 14.7 17.1 6.1
101 0   M     1 9.1 6.9 16.7 18.6 7.4
151 0   F     1 10.7 9.7 21.4 24.0 9.8

> group <- 1 + 2 * (crabs[,1] == "0") + (crabs[,2] == "F")
> groupch = c( "B", "b", "0", "o")[group]
> cg <- cbind(crabs, group, groupch)
> cg[c(1, 51, 101, 151),]           # look at the appended data
   sp sex index  FL  RW  CL  CW  BD group groupch
1   B   M     1 8.1 6.7 16.1 19.0 7.0     1     B
51  B   F     1 7.2 6.5 14.7 17.1 6.1     2     b
101 0   M     1 9.1 6.9 16.7 18.6 7.4     3     0
151 0   F     1 10.7 9.7 21.4 24.0 9.8     4     o

> library(mvpart)                  # draw the regression tree
> crabtree <- mvpart(groupch ~ FL + RW + CL + CW + BD, data = cg,
+                      method = "class", size = 7)



---


crabtree <- mvpart(groupch ~ FL + RW + CL + CW + BD,
                     data = cg, method = "class", size = 20)
crabcp <- printcp(crabtree)

```

The `printcp()` program produces cross-validated errors on models up to the size specified by the `size` parameter in `mvpart()`. This program also calculates a complexity parameter (*CP*) that takes into account the size of the tree in addition to its predictive value. These values are plotted in Fig. 10.12 for the crab data.

The cross-validation errors (left scale) and CP statistic (right scale) decrease with model size. The largest gains appear among the smallest models. There is much slower improvement in models with more than five splits. This figure was used to choose the model size in Fig. 10.11.

Finally, it is possible to completely automate the model building process. For example, we can specify that the regression tree continues branching until no additional splits result in a specified improvement in the CP statistic.

Some colorful language has also been developed among those who study this methodology. Reducing the complexity of an existing tree is called, appropriately enough, *pruning* and the many random trees resulting from cross-validation studies are often referred to as a *forest*.

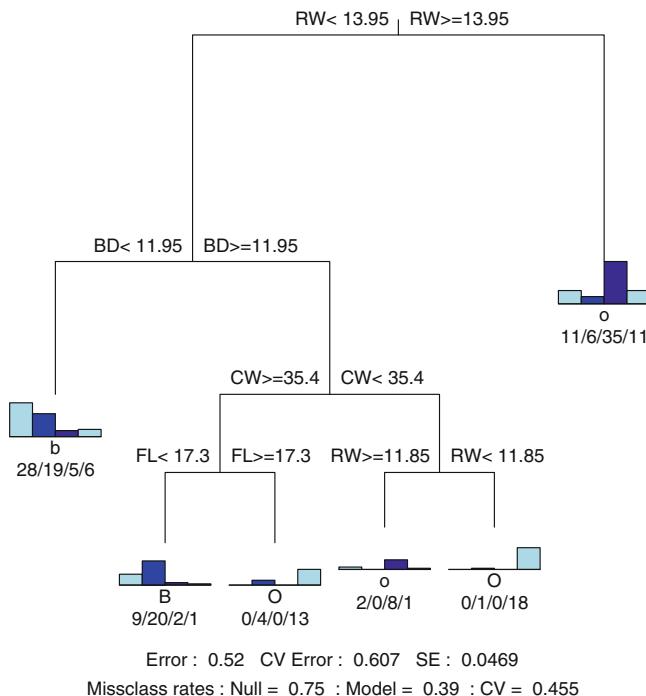


Figure 10.11: Regression tree classification of 200 crabs

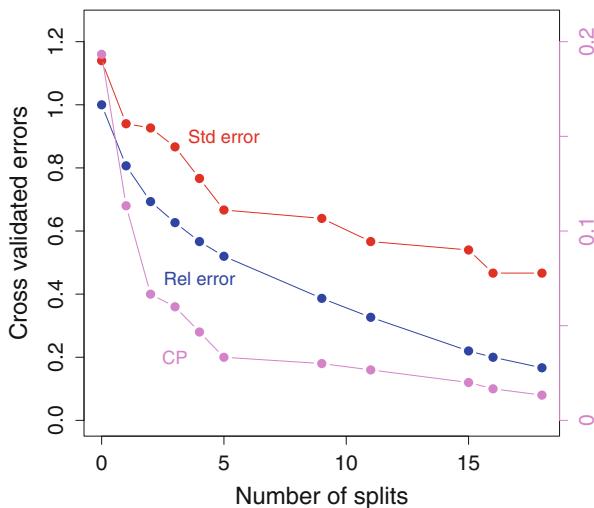


Figure 10.12: Diagnostics of crab regression tree

10.6 Exercises

Exercises 10.5 through 10.8 refer to the analysis of large data sets. The data is available in the `kernlab` library in R and also in the University of California at Irvine Machine Learning Repository. This repository is located at

<http://archive.ics.uci.edu/ml/index.html>

and is an excellent resource for other data sets.

- 10.1 In times of stress, the body undergoes a process called vasoconstriction in which blood vessels at the extremities are closed, forcing blood to the central organs. Vasoconstriction can also occur after taking a deep breath. The data set `vaso` in the `robustbase` library summarizes the vasoconstriction (or not) of subjects' fingers along with their breathing volumes and rates.
 - (a) Plot the breath rates and volumes using different colors for those with and without vasoconstriction. Perform any of the discrimination methods and see how well these distinguish between the two groups.
 - (b) Repeat your analysis of part (a) but first take logs of the explanatory variables. Which analysis do you prefer?
- 10.2 The human leukocyte antigen system (HLA) is a group of genes on chromosome 6 that are linked to the immune system. The data set `hla` in the `gap` library contains HLA data on six markers for 177 schizophrenia patients and 94 matched healthy controls. How can we use these six markers to distinguish between the patients and their controls?
- 10.3 The data set `skulls` in the `HSAUR2` library lists four-dimensional measurements made on ancient Egyptian skulls from five different epochs, hundreds of years apart. Differences are attributed to interbreeding with different immigrant populations. Even though the epochs are ordered in times, do you see a break in the ordering, equivalent to a major change in the genetic mix?
- 10.4 The data set `iris` has four measurements on three different species of 150 irises. Figure 3.21 shows the parallel coordinate plot of this data. Describe the factor loadings from a discriminant analysis and try to reconcile these with what you see in this figure.
- 10.5 The `musk` data set in the `kernlab` is an example of a discrimination problem on a large data set. In this data set there are 476 molecules: 207 are classified as a musk and the remaining 269 are not. The goal

is to identify a classification of the musks from non-musks using any combination of the 166 explanatory variables. These explanatory variables measure molecular distances in different directions. The original data appears at

[https://archive.ics.uci.edu/ml/datasets/Musk+\(Version+1\)](https://archive.ics.uci.edu/ml/datasets/Musk+(Version+1))

with additional information including a complete description of the explanatory variables. The UCI website contains a list of other methods that have been tried on this data.

- 10.6 The **promotergene** data set in the **kernlab** is another example of a discrimination problem in a large data set. This data set contains 106 gene sequences, classified as being either promoters or not. The explanatory variables are the lists of DNA base values preceding the gene of interest. The base values take the values a, c, g, or t corresponding to adenine, cytosine, guanine, or thymine, respectively. Use the base values to find a rule for discriminating between promoters and non-promoters. Additional information on this data can be found on the UCI website.
- 10.7 The **spam** data set in the **kernlab** library was gathered in an attempt to distinguish emails that are advertisements (spam) from non-spam. There are 4601 email messages collected by Hewlett-Packard and of these, 1813 are classified as spam and 2788 are non-spam. There are 57 explanatory variables that measure the frequency of various words such as “free” or “credit.” Other explanatory variables count the frequency of different punctuation symbols or the length of strings of all capital letters. See the help file for a detailed explanation of the variables in this data set. Can you find a good rule to distinguish spam from non-spam?
- 10.8 The UCI data set at

<https://archive.ics.uci.edu/ml/datasets/Post-Operative+Patient>

lists outcomes of 90 postoperative patients and several attributes such as blood pressure, body core temperature, and oxygen saturation. The object is to classify where patients should be sent from the postoperative recovery area. There are three choices: intensive care, regular hospital floor, and discharge. Use any of the methods discussed in this chapter to build a suitable model that classifies patients.

- 10.9 Another approach to generalizing logistic regression to multinomial data has been developed by McFadden (1974). This method compares each category to all others, combined. McFadden, an economist, was concerned with modeling consumer choices, made to the exclusion of all other options. This explanation motivates models of the form

$$\log \left(\frac{\Pr[y = i \mid \mathbf{x}]}{\Pr[y \neq i \mid \mathbf{x}]} \right) = \boldsymbol{\beta}'_i \mathbf{x}$$

for each choice i .

- (a) Solve for $\Pr[y = i]$ and show that this model is over-parameterized. (What happens when you add the same vector to all $\boldsymbol{\beta}$ s?) One solution to this problem is to restrict $\boldsymbol{\beta}_1 = \mathbf{0}$.

- (b) Compare this restricted model to the approach taken in Sect. 10.2 where the reference category corresponds to $y = 1$. Are these two approaches the same? How are they different?

- (c) Does this approach support independence of irrelevant alternatives?

- 10.10 How large should n be in an n -fold cross validation? Try different values of n to see how much these error estimates vary. Useful code may include

```
(sv <- ksvm(group ~., data = mydata, type = "C-svc",
            cross = 5))
cross(sv)
```

using the `cross()` function to capture the cross-validation error estimate. Plot these estimates for different values of n and comment on the effect of changing the sample size.

- 10.11 The `GlaucomaM` data frame in the `TH.data` library contains 62 measurements on 196 eyes in two classes: normal and glaucomatous. The subjects in the two groups were matched by age and sex to provide balance. This represents a large number of measurements on each eye. Use the methods described in this chapter to identify a much smaller set of measurements that can be used to characterize the two groups.

- 10.12 The data frame `stagec` in the `rpart` library summarizes observations made on 146 men treated for Stage C prostate cancer. There are eight measurements made on each patient including whether or not the cancer has progressed. Use regression tree methods to indicate important prognostic measures on whether the cancer will progress from this data.

- 10.13 Kyphosis is a severe curvature of the spine. The **kyphosis** data frame in the **rpart** library presents history of 81 children who had corrective spinal surgery and whether this resulted in kyphosis. The data frame includes three additional variables indicating the extent of the surgery and the child's age in months.
- (a) Use regression trees to identify risk factors for kyphosis.
 - (b) Similarly, use logistic regression to build a linear model of the log-odds risk of kyphosis.
 - (c) Discuss these two different approaches to modeling kyphosis. Which model is more intuitive? Which is easier to explain and use?
- 10.14 The data set **mammoexp** in the **TH.data** library describes a survey of 412 women's attitudes to and experiences with mammography. Among the data are the respondent's perceived benefits of mammography and whether a close female relative had been diagnosed with breast cancer. A suitable response to these measurements is the variable **ME** that measures the time since the woman had her last mammography. The categorical responses to this variable are never, within a year, and over a year ago. Use a regression tree approach to model the time since last mammography. If you were a public health official in charge of educating the public about the importance of periodic mammography examinations, what is the most effective message that you can give?
- 10.15 A *haplotype* is a strand of genetic material on one chromosome that is inherited as an intact gene from one parent. Lander et al. (2011) collected and examined the lengths of haplotypes at 27 loci on 1915 beech trees (*Fagus sylvatica*) in France. The authors of this study examined historical data to verify that these stands of trees existed at least 200 years ago. The trees were growing in three geographically separated areas, referred to as East, South, and West in the data. The data is available for download at

<http://dx.doi.org/10.5061/dryad.q98202jk>

Use linear discriminant analysis to show that the East and South populations can be clearly distinguished but the West population overlaps both of these.

- 10.16 Regression trees are not limited to classifying individuals into discrete groups. These methods will also estimate cut points in continuous measurements and thereby create groups of data. Build a regression tree to model the mpg values in the car data introduced in Table 9.1. Show that the most important classification is the number of cylinders and, to a smaller degree, the displacement.

Chapter 11

Clustering

CLUSTERING is a nonparametric method of arranging similar observations together, often in a graphical display that can be used to detect patterns of grouping and outliers. The approach is usually considered nonparametric because there is no specified underlying distribution or model that we need to assume. R offers great flexibility in graphical capability that makes these methods possible. The largest difference between these methods and those considered in the previous chapter is that in this chapter we do not know group membership *a priori*, or whether in fact there are different groups at all. Similarly, part of the methods discussed here include estimates of the number of dissimilar groups present in the data.

11.1 Hierarchical Clustering

Consider the statistics on the number of health care workers in Canada given in Table 11.1. This table lists the number and type of health care workers per 100,000 population in each Canadian province or territory.

Figure 11.1 depicts a hierarchical cluster representation of this data. This figure is interpreted as a tree or *dendrogram*. The root is at the top and the observations are represented as leaves towards the bottom. The vertical scale of the branches indicates how far individual observations and groups of observations are from each other using a distance metric that we will discuss later in this section.

This representation is different from a regression tree or CART, as in Fig. 10.11. In regression trees there is a single variable of greatest interest. In Fig. 10.11, for example, we model the species and/or sex of the crabs. In contrast, in Fig. 11.1, the variables are of equal importance; our goal is to identify provinces with similar characteristics overall.

Table 11.1: Numbers of Canadian health care workers per 100,000 residents in 2006, listed by province or territory

Province or territory	Doctors	Nurses	Psychologists	Social workers	Other
Newfoundland and Labrador	137	1149	45	179	1843
Prince Edward Island	97	1203	22	101	2153
Nova Scotia	153	1066	47	141	2268
New Brunswick	115	1121	53	172	2215
Quebec	142	825	95	150	2259
Ontario	127	825	45	166	1874
Manitoba	121	1061	36	197	2421
Saskatchewan	114	992	42	179	2354
Alberta	131	989	54	149	2096
British Columbia	134	584	45	134	1956
Yukon	331	1110	50	348	1722
Northwest territories	97	1047	61	207	1595
Nunavut	85	648	34	222	801
Canada, overall	132	881	58	157	2052

Source: Statistics Canada

Yukon is identified as very different from all others because of the huge number of doctors (331) per unit population. (In 2001, this figure was only 70, so something has clearly changed during that 5-year period.) Manitoba and Saskatchewan are similar in many ways and form the tightest cluster between any pair. The maritime provinces (Newfoundland, Nova Scotia, New Brunswick, and Prince Edward Island) also appear close together in this figure.

The R code that produces Fig. 11.1 is as follows:

```
Cmed <- read.table(file = "Canmed.txt",
  header = TRUE, row.names = 1)
Cmed <- Cmed[-14, ]      # omit "Canada total" row
d <- dist(scale(Cmed))  # distances between provinces
clust <- hclust(d)      # build hierarchical cluster
plot(clust, xlab = "", sub = "", main = "", ylab = "",
  yaxt = "n")
```

Another example of clustering appears in Fig. 11.2. The statistics on the three species of iris flowers are summarized in terms of their Euclidean distances from each other. This data also appears in Fig. 3.21 using another clustering method.

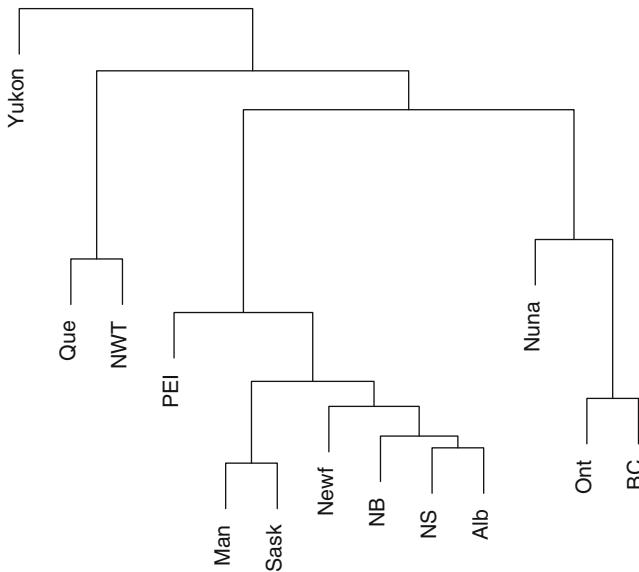


Figure 11.1: Clustering dendrogram of Canadian provinces and territories of data in Table 11.1

The branches of the dendrogram summarize the distances between each flower's observations. The leaves at the end of each branch are color coded according to the three different species. The resulting dendrogram shows the relative distances of the various clusters. These distances determine how far back from the leaves we have to go to obtain the junction with a different branch. Branches are joined with other branches, farther apart, until the tree is joined at a single root. The method is called *hierarchical* because each branch depends on all previous branches leading to it.

In Fig. 11.2 we see that the algorithm does a reasonable job of grouping together the individual species into three separate regions of the tree. There is some overlap of the species seen in this figure, of course. However, we made no assumptions or specifications. The Euclidean distances between every pair of irises were the only criteria used to construct the tree. Unlike CART, the algorithm does not have the species information when constructing the tree. At completion of the clustering, these values were used to draw the final figure.

The program that creates this figure is as follows:

```

id <- dist(scale(iris[, 1 : 4])) # find euclidean distances
fit <- hclust(id) # build the tree
library(ape) # graphics for trees
plot(as.phylo(fit), type="phylogram", cex = .5, label =
  offset = .1,
  tip.col = c(rep("red", 50), rep("blue", 50), rep("green",
  50)))

```

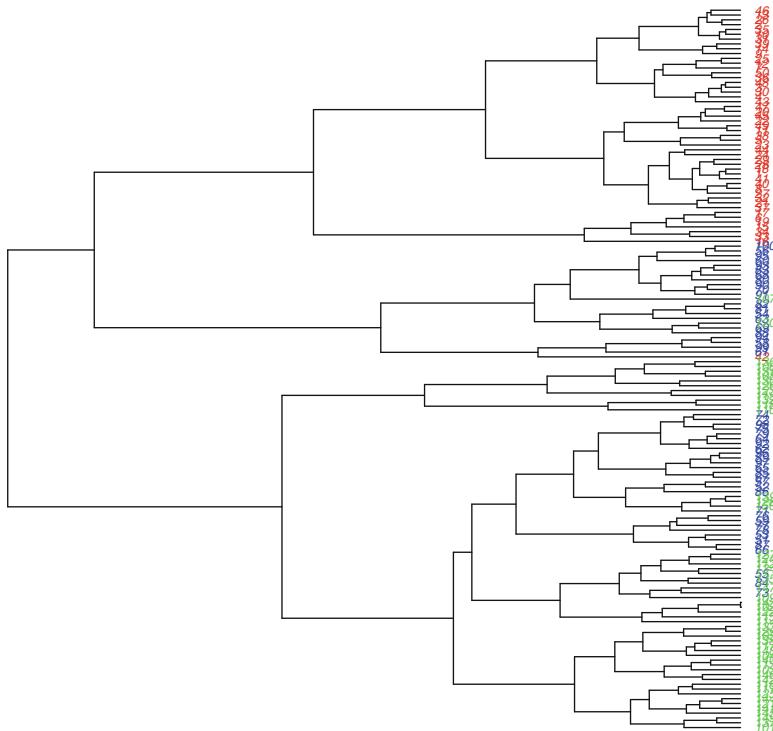


Figure 11.2: Clustering dendrogram of iris data

When we begin, the data columns are usually scaled to have the zero means and unit variances. This is done so that no one variable dominates the others simply by nature of having greater variability. See Exercise 11.1 for details.

The `dist()` program calculates the Euclidean distance between every pair of observed flowers. That is, the whole data set was reduced to a set of pairwise comparisons specifying the distance between observations. Euclidean distances are the default, but there are other options, and these are discussed at the end of this section. The clustering tree is built by R in `hclust` from the matrix of distances. The `ape` library offers a number of options to present these trees.

Let us consider a more detailed example and use it to illustrate some of the many additional graphical options available to us. The data in Table 11.2 summarizes the records of all major league teams in 1986, attendance totals, and average 1987 salaries. There are two leagues (American and National) and two divisions (East and West). Teams are ranked within each of the four combinations of leagues and divisions. The number of wins has a strong negative correlation with the number of losses, but this correlation is not perfect because not all teams played the same number of games.

The top four panels in Fig. 11.3 are produced using

Table 11.2: Baseball team records for 1986 and total attendance in 1000s

Name	League	Division	Rank	Wins	Losses	Attendance		Average salary
						At home	Away	
NYMets	N	E	1	108	54	2768	2178	\$527
Phi	N	E	2	86	75	1933	1721	541
StL	N	E	3	79	82	2472	1696	445
⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮
Min	A	W	6	71	91	1255	1707	432
Sea	A	W	7	67	95	1029	1559	186

Source: <http://lib.stat.cmu.edu/datasets/baseball.data>

The 1987 average salary data is in \$1000s

```
d <- dist(scale(baseball[,c(-1,-2)])) # scale numerical values
library(ape) # offers plotting options
fit <- hclust(d)
plot(fit, main = "Plain dendrogram", hang = -1, cex = .8,
     xlab = "", ylab = "", sub = "", axes = FALSE)
plot(as.dendrogram(fit), type = "triangle",
     main = "Triangle branches", cex = .8, axes = FALSE)
plot(as.phylo(fit), type = "unrooted", cex = .8,
     main = "Unrooted tree")
plot(as.phylo(fit), type = "fan", cex = .8,
     main = "Leaves spread in a circle")
```

The bottom panels of Fig. 11.3 were produced using the R code in Output 11.1. In the iris data, this method appears to confirm our understanding of the data. Identical species of flowers have much in common. However, in the case of the baseball data, it is not obvious why some teams appear to cluster. For example, the two New York teams and Boston always appear in the same tight cluster, but except for their geographic proximity, it is not clear why these teams belong together. (This, despite the long-standing rivalry between Red Sox and Yankees fans.) Clearly, R can demonstrate the clusters, but it remains for us to interpret the resulting figure.

As a final example in this section, let us point out that some data sets lend themselves to the tree-like structure and are stored in R as such. The `chiroptera` data set in the `ape` library is a *supertree*, a composite tree constructed from many different sources, describing the complete phylogeny of 916 species of bats (Mammals of the order *Chiroptera*). This data is best displayed as a tree, and two versions appear in Fig. 11.4. The R code that produces this pair of figures is

```
library(ape)
data(chiroptera)
plot(chiroptera, type = "r", cex = .1)
```

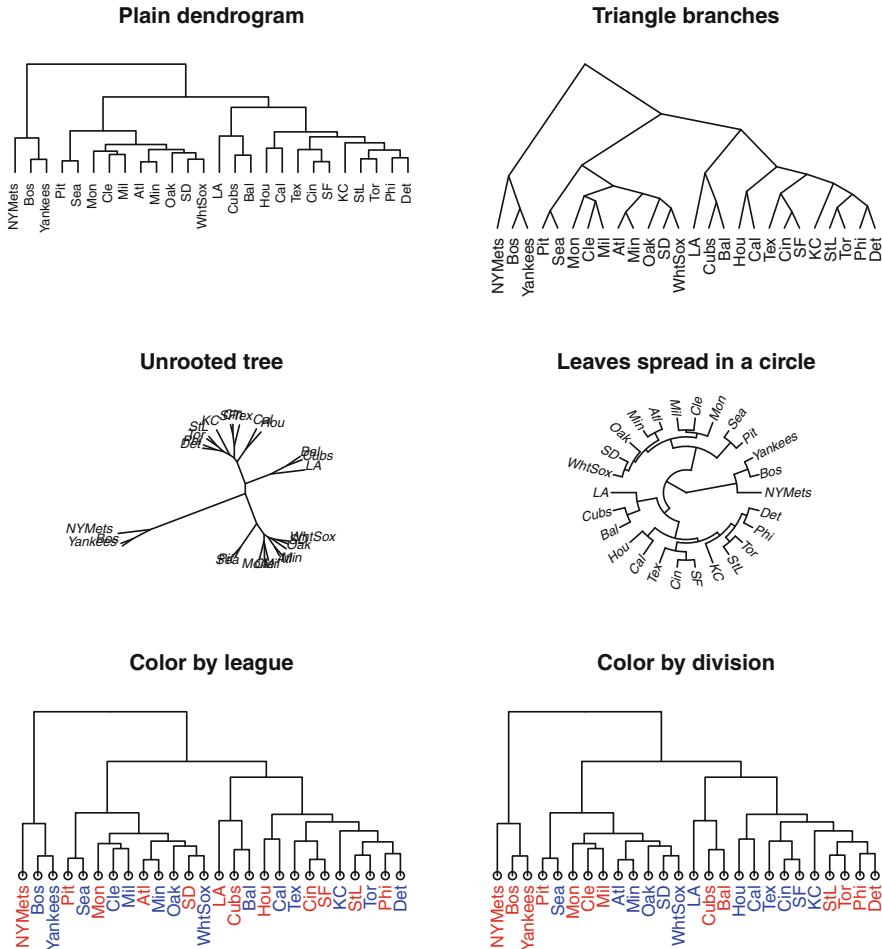
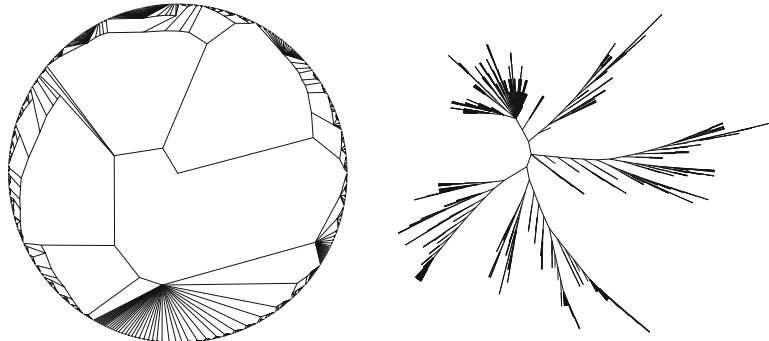


Figure 11.3: Hierarchical clustering of baseball teams using a variety of displays

```
plot(chiroptera, type = "u", cex = .1)
```

Similar tree structures for birds are available as `bird.orders` and `bird.families`, both in the `ape` library.

Let us end this section with a discussion of options for the distance between two observations. In a `data.frame`, it usually makes sense to start by scaling or normalizing the columns (different variables) to have the same variances. Otherwise a column (variable) with a large variance will dominate any reasonable distance, and a column with a small variance will tend to be ignored. That is, we should usually employ the template

Figure 11.4: Two displays of the `chiroptera` data

```
d <- dist(scale(mydata))
```

when using `dist`.

The `dist` function will calculate the distance between every pair of observations (rows) in a `data.frame`. Consider, then, two observations (rows in a `data.frame`) denoted by the vectors $\mathbf{x}' = (x_1, \dots, x_n)$ and $\mathbf{y}' = (y_1, \dots, y_n)$. There are several useful options available, depending on how we define distance.

The most popular distance is the Euclidean distance

$$\text{Euclidean distance}(\mathbf{x}, \mathbf{y}) = \sqrt{\sum (x_i - y_i)^2}$$

that is the default distance for the `dist` function.

The Euclidean length of a vector was introduced in (4.4). It corresponds to the length of the shortest, straight line connecting \mathbf{x} and \mathbf{y} .

The *maximum* or *supremum norm*

$$\text{Maximum norm}(\mathbf{x}, \mathbf{y}) = \max_i |x_i - y_i|$$

is the largest component-wise difference.

The *Manhattan norm*,

$$\text{Manhattan distance}(\mathbf{x}, \mathbf{y}) = \sum_i |x_i - y_i|$$

is calculated as though we had to walk along rectangular, city blocks.

The *Minkowski norm*¹ is

$$\text{Minkowski distance}(\mathbf{x}, \mathbf{y}) = \left\{ \sum_i |x_i - y_i|^p \right\}^{1/p}$$

¹Hermann Minkowski (1864–1909). Mathematician and mathematical physicist, lived in Germany.

for power $p > 0$ includes the Euclidean norm for $p = 2$, the Manhattan for $p = 1$, and the maximum norm for large values of p . These norms are available as options in the `dist` program, including the choice of the p parameter in the Minkowski distance.

Finally, there is the *Gower distance*, available in the `daisy` program of the `cluster` library. The Gower metric first standardizes each variable by its range so that all data values fall between zero and one. The Gower distance also generalizes to allow us to cluster interval-valued data.

Output 11.1: R program to produce the plots with colored leaves in Fig. 11.3

```

colLab <- function(n)          # function on dendograms
{
  if (is.leaf(n))             # to get colored labels
  {
    a <- attributes(n)        # when we find a leaf...
    teamn <- match(a$label, row.names(baseball)) # capture its attributes
                                                # which team number is it?
    teamtype <- c("red", "blue")[teamn]           # color for league or division
    leafcolor <- teamtype[teamn]                   # assign new attributes to leaf
    attr(n, "nodePar") <- c(a$nodePar, lab.col = leafcolor)
  }
  return(n)                      # return the dendrogram
}

league <- baseball[, 1]
division <- baseball[, 2]
d <- dist(scale(baseball[, c(-1, -2)])) # scale numerical values
library(ape)                          # offers plotting options
fit <- hclust(d)
teamtype <- league                  # leaf color by league
colfit = dendrapply(fit, colLab)     # dendrapply to tree
plot(colfit, main = "Color by league",
     cex = .8, axes = FALSE)

teamtype <- division                # leaf color by division
colfit = dendrapply(fit, colLab)
plot(colfit, main = "Color by division",
     cex = .8, axes = FALSE)

```

Sourced, in part from: <http://www.gastonsanchez.com>

Table 11.3: Characteristics of 11 Japanese smokers

Age	Height in cm	Weight in kg	Nicotine	Tar	Age start	Cigarettes per day	Years smoking	Pack years
1	36	168	50	0.7	8	20	15	16
2	41	170	64	0.7	8	20	20	21
3	35	169	65	0.8	10	20	30	15
4	55	177	68	1.0	12	20	20	35
5	21	172	80	0.7	10	16	15	5
6	46	165	53	1.4	17	20	20	26
7	38	167	57	0.1	1	20	10	18
8	37	165	58	0.1	1	20	20	17
9	40	156	53	0.4	5	18	20	22
10	36	172	55	0.5	6	20	20	16
11	39	168	65	0.7	8	16	10	12

Source: Takahashi et al. (2013)

11.2 *K*-Means Clustering

The *K*-means clustering algorithm is based on the principle that there are a specified number, *K*, multivariate normal populations present in the data and these differ only in terms of their means. The cluster members and their mean are estimated in such a way as to minimize the within-cluster variability. The algorithm uses an analysis of variance (ANOVA) approach to estimate the *K* different multivariate means as well as the group membership of each observation. The ANOVA approach also suggests the clustering algorithm proposed by Hartigan and Wong (1979). The algorithm determines the group membership of each observation so that the program minimizes the sums of squares within each group.

Let us begin with a small example. Table 11.3 gives the characteristics of 11 male Japanese cigarette smokers who participated in a larger study of the health effects of smoking. The data in this table includes demographic variables (age, weight, height), characteristics of their cigarette brands (nicotine, tar), and smoking history (age at start, cigarettes per day, and pack-years).

The *K*-means program is in the `stats` library. The program that fits *K* = 4 clusters and produces Fig. 11.5 is as follows:

```
require(graphics, stats)
(cl <- kmeans(smokers, centers = 4))
plot(smokers[,c(3, 9)], xlab = "Weight in kg",
     ylab = "Pack years", pch = 16, col = cl$clust, cex = 2.5)
text(smokers[,3], smokers[,9], labels = row.names(smokers),
     pos = 2)
```

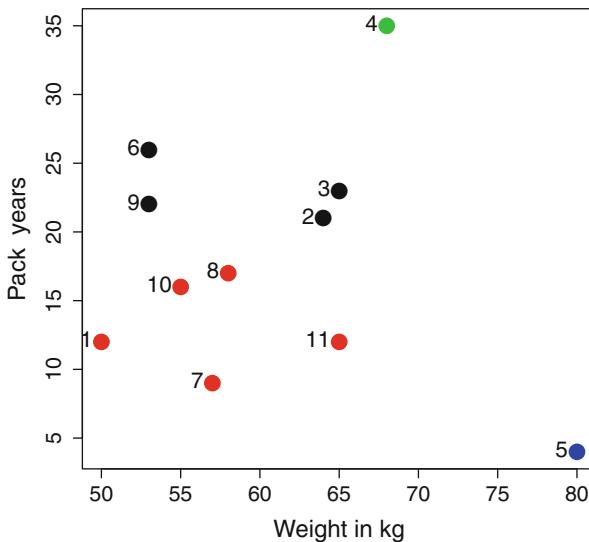


Figure 11.5: K-means clustering of 11 Japanese smokers

Figure 11.5 plots the four different clusters by color by their pack-years and weights. This figure identifies two unusual individuals: a low-smoking, obese man (#5) in the lower, right-hand corner of this plot; and a heavy smoker (#4) at the top of the figure. The remaining nine individuals are either classified as five light smokers (red) or four heavy smokers (black).

Let us begin with the choice of axes in this plot. These were chosen with a combination of interpretation and visual appeal. The visual appeal works because the clusters separate nicely and do not overlap in this display. The interpretation also aligns with our sense of the overall health effects of smoking. Unfortunately, useful axis choices in this figure are found by trial and error, so the user will have to do some experimenting in order to produce an appealing display.

A graphical display can help us choose an appropriate value of K . The ANOVA has an interpretation that we can use here and is introduced in (9.2). The simple idea of the ANOVA is that the total sum of squares can be decomposed as

$$\text{Total sum of squares} = \text{Between cluster sum of squares}$$

$$+ \text{Within cluster sum of squares}$$

or, more simply, the total sum of squares is the sum of *explained sum of squares* plus the *unexplained sum of squares*.

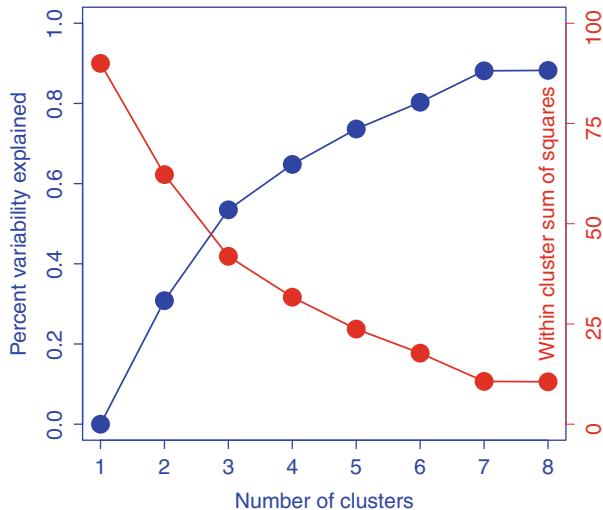


Figure 11.6: Percentage of variability explained (blue) and within cluster sum of squares (red) in K-means clustering of 11 Japanese smokers

The total sums of squares is the same for every choice of K . We can examine the within-cluster variability which will decrease as K increases. Another reasonable summary of how well we are doing is to examine the percent of explained variability. That is,

$$\text{Percent variability explained} = \frac{\text{Between group sum of squares}}{\text{Total sum of squares}}$$

and this will decrease as K is increased.

These two summary measures represent a trade-off and can be compared to each other. Figure 11.6 plots these two summaries for different values of K .

This figure confirms our intuition that the percentage of explained variability increases with the number of clusters, K . Similarly, the within-cluster variability decreases with the number of clusters. At $K = 1$, the data is estimated to have originated from one population and nothing is explained. At the other extreme, if K is equal to the sample size, then 100 % of the variability is explained by having each observation in its own cluster, but nothing is learned. We look at Fig. 11.6 to see if we can identify a compromise. The percent variability explained increases steeply up to $K = 4$ and then starts to level off for larger values of K . This choice of K is somewhat arbitrary and $K = 3$ might also have done a good job.

Let us compare K-means with hierarchical clustering. We begin by introducing the `milk` data set in the `robustbase` library. This data set consists of

Table 11.4: Variable names and their definitions in the `milk` data

<code>dens</code>	Density
<code>fat</code>	Fat content
<code>prot</code>	Protein content
<code>casein</code>	Casein content
<code>Fdry</code>	Cheese dry substance measured in the factory
<code>Ldry</code>	Cheese dry substance measured in the laboratory
<code>drysub</code>	Milk dry substance
<code>cheese</code>	Cheese product

eight measurements on each of 86 separate containers of milk. The variables are labeled `X1` through `X8` in the original. Table 11.4 renames these and gives their definitions.

In the first panel of Fig. 11.7, a clear outlier (observation #70) appears in the hierarchical clustering method. In the second, middle panel, this observation has been removed and the `hclust` has been repeated, indicating two distinct clusters of observations. These two clusters are largely determined by the values of casein, although other variables could provide similar discrimination. In the middle panel, values of casein over 25.5 are in blue, others in red.

The third panel in this figure plots the percent variability explained in terms of the number of K-means clusters. This third panel illustrates a big change for $K = 2$ and $K = 3$ but larger values of K yield only small improvements.

Figure 11.8 is the `pairs()` plot of the K-means clusters for milk data with values of $K = 2$ in the lower panels and $K = 3$ in the upper panels. In this figure we see a strong linear relationship between each of the pairs of variables `prot`, `casein`, `Fdry`, and `Ldry`. Both K-means clustering indicate evidence that clusters appear along the lengths of these lines.

Figure 11.8 was produced using the R code in Output 11.2. In this code, we begin by omitting the outlier, renaming the variables and identifying the color schemes for 2 and 3 K-means. The `panel.up` function tells the `pairs()` program how to process separate scatterplots. In this case, we use it to provide separate, colored plots in the panels above and below the diagonal. Specifically, the `upper.panel=` is an option on `pairs` that can be assigned the value of this function. There are other analyses that can be done with this data. See Exercise 11.6 for some suggestions.

The K -means clustering, then, is a simple and intuitive method for clustering data and is dependent only on the user's choice of K . To complete our illustration of the method, let us try a small simulation to show the effect of mis-specification of K .

Consider a simulation in which we generate 100 samples from each of three different multivariate normal populations with different means and a slight negative correlation. These samples are plotted at the top of Fig. 11.9 with different colors for each of the three populations. The plot of percent variance explained seems to indicate that $K = 3$ clusters should be appropriate and little is to be gained using larger values.

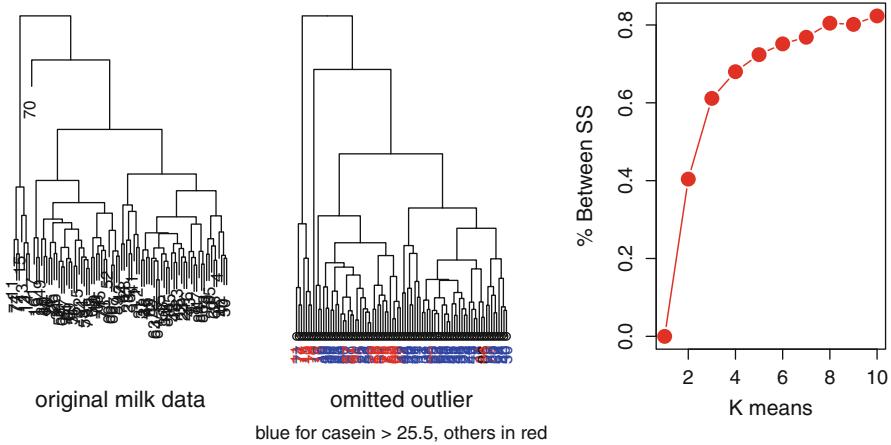


Figure 11.7: Milk data as hierarchical cluster: original and with omitted outlier. Color is determined by low (red) and high (blue) values of casein. The third panel is percent variability explained in K-means

The next four graphs in Fig. 11.9 summarize the results of using different values of K . The plot with $K = 2$ clearly misses one group by combining the two dissimilar groups at the bottom. The $K = 3$ plot closely reproduces the original figure, albeit with different colors. Plots with larger values of $K = 4$ and 5 tend to pull apart clusters that may seem adequate to our eyes. Exercise 11.4 asks the reader to further explore what can go wrong if the specified value of K is not appropriate.

In summary, what can we say about the K -means clustering algorithm? The approach is not limited to small data sets. The choice of K can be estimated from graphics such as Fig. 11.6. The interpretation of the K clusters is up to us. A useful plot such as Fig. 11.5 requires us to identify appropriate choices for the axes and, again, requires that we are able to interpret the resulting figure. In the following section we describe methods for assessing the quality of the clusters identified by these algorithms.

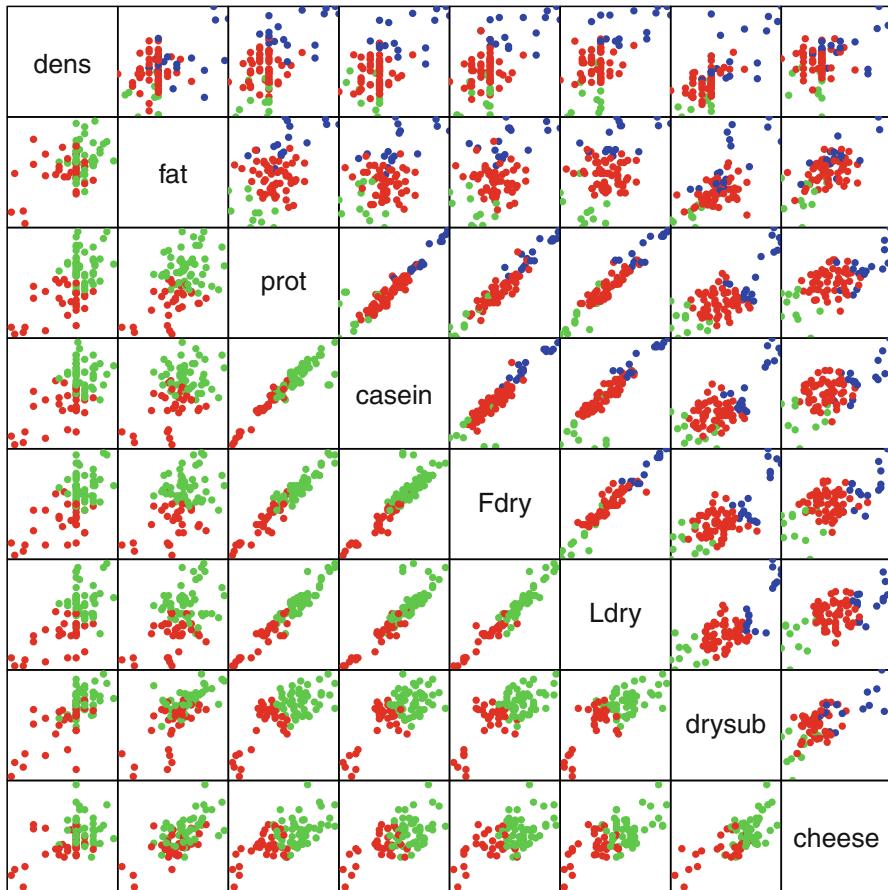


Figure 11.8: K-means for milk data with $K = 2$ (below) and $K = 3$ (above)

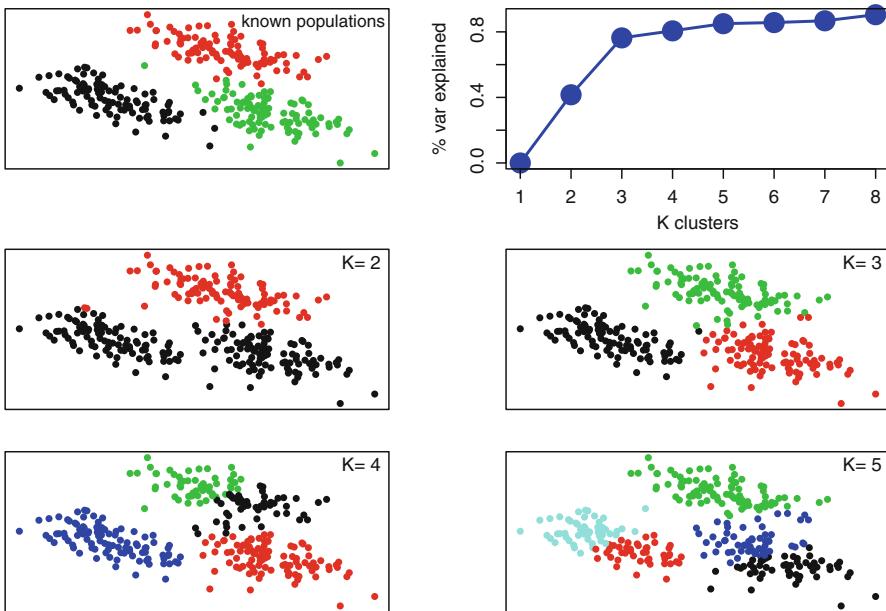


Figure 11.9: Simulation of K-means clustering

11.3 Diagnostics, Validation, and Other Methods

Clustering algorithms provide a data diagnostic to help our exploration. Figure 11.6 has shown us that this illustration can be an aid in identifying the number of clusters in a K-means procedure. It is reasonable to see a clustering figure and then ask whether such a diagram could have occurred by chance alone. Will a set of randomly generated data values naturally appear to cluster into two or more groups? The clustering procedures are nonparametric, so it is reasonable to retain this model-free approach in any study of validation.

Two popular methods to assess the quality of a clustering procedure are jittering and bootstrap resampling. Jittering adds a small amount of random noise to the data and then repeats the clustering procedure. The bootstrap randomly samples from the observed data before repeating the clustering procedure. Both methods are repeated several times. The goal is to check the stability of the outcomes. (Jittering also appears as a graphical tool in Fig. 3.6.)

Clustering, most generally, breaks the sample into subsets of the total. We will then need a way to compare the results of two different clustering processes. There are three popular measures of agreement in clustering of

Output 11.2: R code to produce Fig. 11.8

```

library(robustbase)                      # library with the milk dataset

milk2 <- milk[-70, ]                      # omit outlier
colnames(milk2) <- c("dens", "fat", "prot", "casein", "Fdry",
  "Ldry", "drysub", "cheese")             # supply new names
                                         # color schemes for K-means
colorlow <- rainbow(3)[kmeans(scale(milk2), centers=2)$cluster]
colorup <- rainbow(3)[kmeans(scale(milk2), centers=3)$cluster]

panel.up <- function(x, y, ...)
{
  {                                         # function to produce scatterplot in pairs()
  usr <- par("usr")                      # save par() values
  on.exit(par(usr))                      # set par() at end
  par(usr = c(max(y), min(y), max(x), min(x))) # set bounds
  points(y, x, col = colorup, pch = 16)    # plot data points
}

pairs(milk2, pch = 16, gap = 0, xaxt = "n", yaxt = "n",
  col = colorlow, upper.panel = panel.up)

```

sets. These are attributed to Jaccard, Dunn, and Rand.

Let us introduce a measure of similarity between two sets. Let S and T be finite sized sets. The *Jaccard Index*² is defined as

$$J(S, T) = \frac{\text{\# of elements in } (S \cap T)}{\text{\# of elements in } (S \cup T)}.$$

If S and T are both empty, then $J = 0$.

Clearly, $0 \leq J \leq 1$ with larger values indicate a greater percentage of agreement. The relevance here is to compare a set S identified by a clustering algorithm based on the observed data with a set T obtained from simulated data. The simulated measure J will then have a distribution. We will need to look at a summary of the randomly generated values such as its histogram or mean value. We don't assign a statistical significance to the value of the Jaccard index, but it is possible to do so. See Exercise 11.7 for details.

A commonly used measure of cluster quality is the Dunn Index (Dunn 1973). The Dunn Index is the ratio of the smallest distance between clusters divided by the diameter of the largest cluster. Ideally, we want small clusters that are located far apart, so larger values of the Dunn Index are better. Of course, there are many possible definitions of distance, as we pointed out

²Paul Jaccard (1868–1944). Swiss professor of botany and plant physiology.

in Sect. 11.1, so there are many variations on how the Dunn Index may be defined. The general idea of this measure is similar to other metrics that are frequently encountered in applied statistics. See Exercise 11.7 for details.

Another general measure of agreement is the Rand Index (Rand 1971). Suppose we have two sets of sets $\mathbf{X} = \{\mathbf{x}_1, \dots, \mathbf{x}_n\}$ and $\mathbf{Y} = \{\mathbf{y}_1, \dots, \mathbf{y}_m\}$ that both make up partitions of the sampled observations. Imagine taking all possible observations, two at a time. The Rand Index counts the proportion of times these observations occur in the same \mathbf{x}_i and same \mathbf{y}_j or else in different \mathbf{x} s and different \mathbf{y} s. See Exercise 11.7 for more on this.

The R program `prediction.strength()` in the `fpc` library provides a cross-validated measure of the quality of a cluster. This program randomly divides the data into two equal sized number of observations, called A and B . The set A is used to estimate the k clusters and then records the percent of times that observations in B are clustered into the same clusters as in the original, full data. The procedure is then reversed, fitting B and predicting A . The simulation is repeated for different partitions of A and B and then for different values of k . The prediction strength will generally decrease with k , and the authors of this method recommend that we choose values of k that result in a prediction strength over 0.8 or 0.9. An example of this simulation appears in Fig. 11.10, below.

Now let us examine a larger and more complex data set involving genetic markers measured using an Affymetrix DNA microarray. In this example, three sets of mouse mesenchymal cells from each of two anatomic structures (mesodermal and neural crest) were examined. Mesenchyme are cells that can develop into a variety of different tissues including bone, cartilage, and parts of circulatory and lymphatic systems. Many genetic markers were measured in the original data, but only those 147 that exhibited a large difference between the mesodermal and neural crest cells are included here.

A portion of this data is obtained and displayed

```
> library(clValid)
> data(mouse)
> print(mouse, digits = 4)

      ID      M1      M2      M3      NC1      NC2      NC3          FC
1 1448995_at  4.707  4.528  4.326  5.568  6.915  7.353 Growth/Differentiation
2 1436392_s_at  3.868  4.052  3.475  4.996  5.056  5.184  Transcription factor
3 1437434_a_at  2.875  3.380  3.240  3.877  4.460  4.851  Miscellaneous
...
145 1417129_a_at  6.694  6.019  7.037  5.770  5.149  4.541  Transcription factor
146 1425779_a_at  6.109  5.960  5.999  4.537  4.068  4.251  Transcription factor
147 1450723_at   5.948  5.753  6.001  5.027  4.187  3.111  Transcription factor
```

The six cells are listed as M1, M2, M3 for the mesodermal and NC1, NC2, NC3 for the neural crest. The ID is the specific genetic address and FC refers

to the gene's functional class. There are nine different functional classes of genes in this data.

Notice that this data is presented transposed from our usual manner of displaying data: observations as rows and variables as columns. In our applications of clustering so far in this chapter, the object has been to cluster individuals. In this case the data is *wide* in the sense that there are many more variables than observations. Similarly, the present object of the clustering analysis in this data is to group similar genes together, rather than different cell samples.

Figure 11.10 includes a plot of the percent variability explained by cluster size and a dendrogram. The simulated prediction probability decreases with larger number of clusters. The dendrogram plots the functional class of each marker in a separate color but does not demonstrate a clear indication of homogeneity of these clusters. Together, the two panels in Fig. 11.10 suggest that there should be three cluster centers, maybe four at most.

The `clusterboot` program in the `fpc` library simulates cluster stability by simulating K-means clustering using a variety of methods including jittering or bootstrap methods. The mean Jaccard Index for $K = 3$ clusters in the `mouse` data using jittering yields

```
short <- mouse[ , 2 : 7]           #   remove text columns
cbj <- clusterboot(short, bootmethod = "jitter",
                    krange = 3, clustermethod = kmeansCBI)
cbj$jittermean
[1] 0.9960000 0.9957377 1.0000000
```

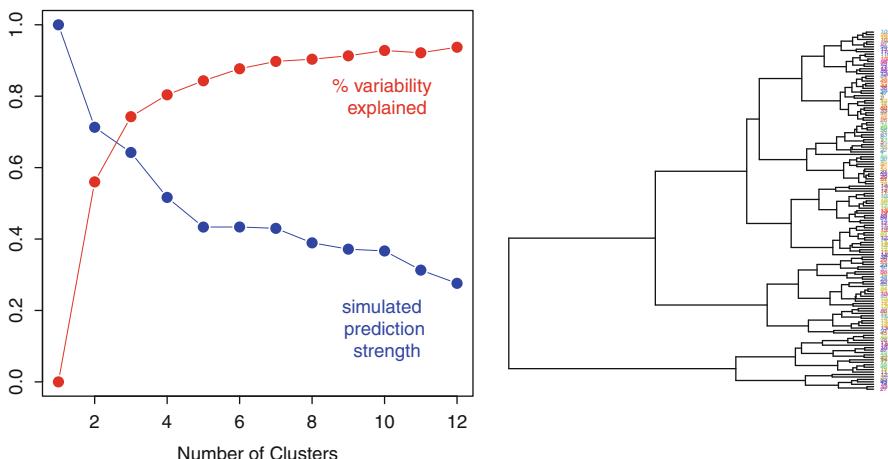


Figure 11.10: Clustering of genetic markers in mouse mesenchymal cells

The same simulation using a bootstrap gives

```
cbb <- clusterboot(short, bootmethod = "boot",
  krangle = 3, clustermethod = kmeansCBI)
cbb$bootmean
[1] 0.9170135 0.9179769 0.9026569
```

The authors of these programs suggest that average Jaccard Index values above 0.75 indicate stable clusters. Clearly, these simulations indicate that $K = 3$ clusters is a reasonable number.

A simulation with $K = 4$ on this data gives

```
> cbb$bootmean
[1] 0.5059524 0.8515681 0.6708926 0.4336492
> cbj$jittermean
[1] 0.8069331 0.9293281 0.8260002 0.8801505
```

These second sets of simulations yield somewhat ambiguous results. The bootstrap simulation provides much lower mean Jaccard values for $K = 4$ than we saw for $K = 3$, above. The jittered simulation provides lower mean values but these are considerably higher than those of the bootstrap and much closer to the values for $K = 4$. From these simulations we may conclude that $K = 3$ clusters is a reasonable conclusion, and there is weaker evidence that $K = 4$ is appropriate.

The Dunn Index for $K = 3$ clusters is 0.087, but we have no context to understand this value. We can perform a bootstrap simulation to examine the distribution of the statistic. The R code to perform this simulation is given in Output 11.3.

This simulation produces values presented in Fig. 11.11. The Dunn Index for the observed data is highlighted and appears near the center of a right-skewed distribution that may also have a bimodal distribution. It is also possible to perform a bootstrap simulation to describe the behavior of the Dunn Index assuming a model in which there are no clusters, with the data sampled from a single population. See Exercise 11.10 for details on this simulation.

A generalization of the single-linkage clustering is a simultaneous clustering of both rows and columns of a data matrix, also known as a *heatmap*. We used a heatmap in Fig. 9.6 to summarize the statistical significance of a large number of regression coefficients. Figure 11.12 displays clusters of mouse mesenchymal markers (by rows) and cells (by columns) in a way that blocks of high and low data values are grouped together. The data values are displayed by color, as hotter (larger) or colder (smaller) values. The blocks of colors are clear in this figure because the data only includes markers that exhibited large differences between the two cell types. The margins of this figure include separate dendograms. The colors along the left edge are the same as those used in Fig. 11.10.

Output 11.3: R code to perform bootstrap for K-means clustering

```

short <- mouse[ , 2 : 7]           # remove text columns
d <- dist(short)
cl <- kmeans(short, centers = 3)
dunn <- cluster.stats(d, cl$cluster)$dunn

n <- dim(short)[1]
for (i in 1 : 100)                 # number of bootstrap samples
{
  booti <- as.integer(1 + n * runif(n)) # bootstrap indices
  bd <- dist( short[booti, ] )      # distances of bootstrap sample
  clb <- kmeans(bd, centers = 3) # cluster bootstrap sample
  dunn <- c(dunn,                  # bootstrapped Dunn values
            cluster.stats(bd, clb$cluster)$dunn )
}

```

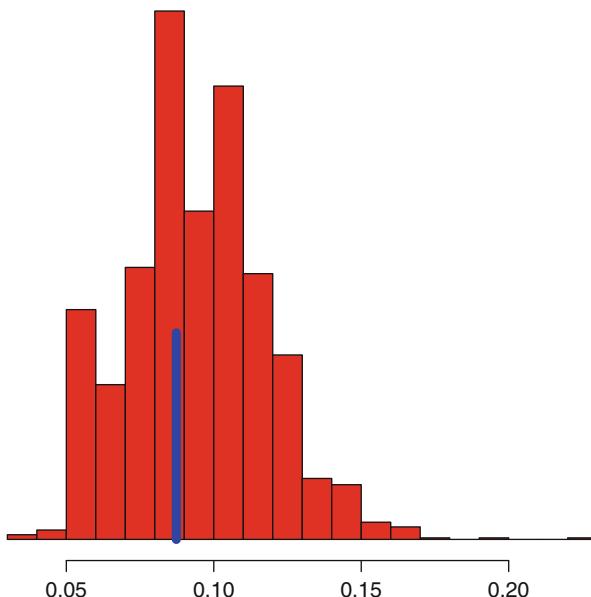


Figure 11.11: Bootstrap simulation of Dunn Index in `mouse` data. The value for the observed data is *highlighted*

This figure can be produced with the R code

```

library(ape)
library(clValid)

```

```

library(stats)
data(mouse)
iclass <- as.integer(mouse$FC) # integer categories
heatmap( as.matrix( mouse[, 2 : 7] ),
RowSideColors = rainbow(max(iclass))[iclass] )

```

This code begins by loading the three necessary libraries. The FC column of the `mouse` data contains the functional class as factor levels and the

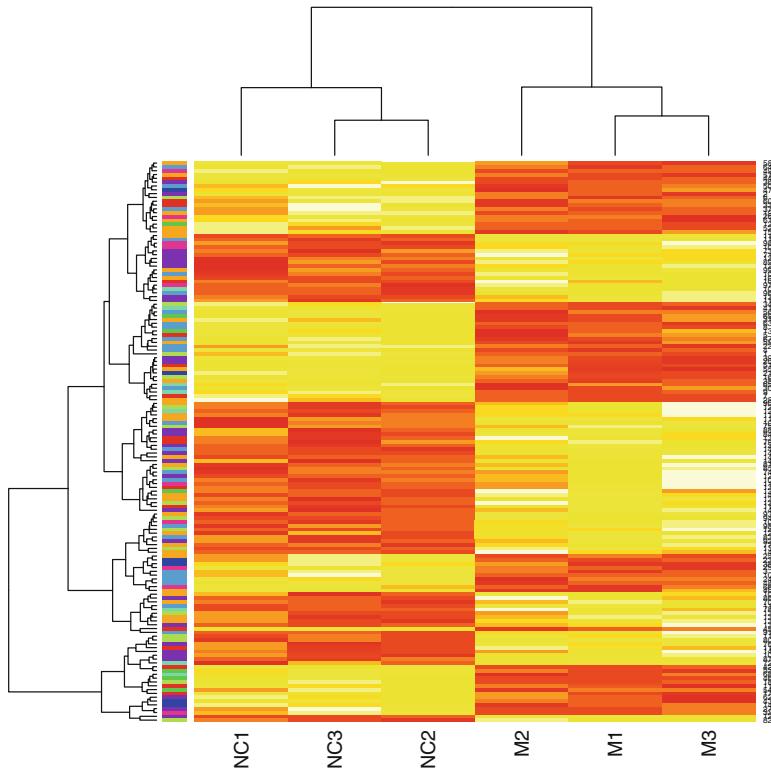


Figure 11.12: Heatmap for genetic markers in mouse mesenchymal cells

`as.integer` function recodes these as integer values. Columns 2 through 7 contain the numerical values of the gene expression data. The `heatmap` program operates on a matrix of numerical values so the `data.frame` also needs to be reformatted. The `RowSideColors` option adds colors corresponding to functional class of the genetic markers. There are many more options and enhancements available in the `heatmap.2` program in the `gplots` library.

Let us end this section by pointing the reader towards a number of other clustering methods that are available in R. The `cluster` package contains a number of useful programs including `pam()` which performs K-means using

a variety of metrics that are more robust than the within-group sums of squares. The `agnes()` program implements the popular unweighted pair group method with arithmetic mean algorithm. The `clara()` algorithm (also in `cluster`) uses a faster algorithm than `pam()` and is useful for large data sets. The `diana()` algorithm begins with all observations in a single cluster and successively peels away until each cluster contains only one item. The `fanny()` routine estimates a probability that each observation belongs to every cluster, rather than strictly assigning membership to only one cluster.

Neural networks assume that there are unobservable, intermediate models within the observed data. The self-organizing tree algorithm `sota()` in the `clValid` library uses neural networks. The self-organizing maps program `som()`, in the `kohonen` library, is useful for visualizing high-dimensional data and plotting in two dimensions.

A variety of clustering metrics have also been proposed. Many of these are discussed at length in the documentation for the `clValid` library in R. *Connectivity* is a measure that examines the number of “nearest neighbors” of each observation and counts how many of these occur in the same cluster partition.

The usual jackknife deletes individual observations (or rows of a `data.frame`) to assess variances or other properties of statistics measured on the full data set. Various stability measures of clustering are discussed in the `clValid` documentation that propose deleting variables (`data.frame` columns) of the data. Among these measures are the *average distance* between observations fitted in the same cluster with the full data and then with a column of data omitted. Similarly, the *average distance between means* measures the changes in cluster means when individual columns of data are omitted.

It is also possible to include biological information about clusters. Information about the functional class of the genetic markers in the `mouse` data, for example, should be included in any clustering of these markers. Some markers belong to more than one functional class. Measures of statistical clustering that include such biological information include the *biological stability index* and the *biological homogeneity index*, both available in the `clValid` library.

11.4 Exercises

11.1 How critical are the use of scaling and choice of distance metric in hierarchical clustering?

(a) Try different distance metrics on the `iris` data. Do these do better or worse than the plot in Fig. 11.2?

(b) Redraw Fig. 11.1 without using `scale` to transform the data columns to the same variances. Has the scaled figure changed? Which figure is easier to interpret: scaled or unscaled? Explain your rea-

Table 11.5: Government bond returns by issuer and duration

Issuer	1mo	3mo	6mo	8mo	1yr	3yr	5yr
USGovt	1.88	4.45	6.37	8.39	7.97	7.68	5.94
AustAsia	-0.19	9.47	4.94	5.52	13.93	10.46	9.13
Canada	2.22	3.98	5.48	7.30	7.07	7.27	5.20
Eurozone	2.42	2.73	4.30	5.92	6.55	6.92	4.11
Japan	0.66	2.20	3.08	3.14	3.94	3.01	2.04
Switzerland	2.18	2.89	5.06	6.64	8.59	7.00	3.61
UK	4.70	6.12	10.35	10.69	8.69	9.01	5.99

Source: ©2010 Morningstar, Inc., Morningstar Bond Market Commentary, September, 2010. All Rights Reserved.
Used with permission.

soning. Try different distance metrics. Do these yield very different appearing dendograms?

- 11.2 Look at the `swiss` data examined in Chap. 6 using clustering methods. Is there evidence that some cantons were making the demographic transition sooner than others?
- 11.3 Table 11.5 lists the annual returns to investors (as of Sept., 2010) of government bonds, listed by duration and issuer. These returns are influenced by the respective rates of inflation and strengths of the various currencies as well as market perceptions for these rates into the future. Perform a hierarchical cluster of these returns to identify countries with similar financial situations. Comment on how the dendrogram clusters countries in similar geographic regions, as well.
- 11.4 Repeat the example summarized in Fig. 11.9. What happens when the means of the sample populations are closer? What happens when the sample means are much further apart?
- 11.5 The `coleman` data set in the `robustbase` library lists summary statistics for 20 different schools in the northeast US. The six variables measured on each school include demographic information (such as percent of white-collar fathers) and characteristics of each school (such as staff salaries per pupil). Read the help file of `coleman` for the complete list of demographics and references to other's analyses of this data.
 - (a) A suggested analysis is a regression model explaining the variable Y , the mean verbal score of all sixth graders.
 - (b) Perform a hierarchical cluster of this data using all explanatory variables. Is there evidence of different types of schools?

- (c) Similarly, does a K -means clustering provide evidence of different types of schools?
- (d) Which of these four types of statistical analyses seems most appropriate for the data? Is there strong evidence that there are no clusters? What might such data look like?
- 11.6 Try some other examinations of the `milk` data. First omit the suspected outlier (observation #70) and **scale** the data.
- (a) Perform the K-means clustering and plot the first two principal components by color of cluster membership.
- (b) Read about the `pam()` program in `cluster` library. The syntax is similar to that of `kmeans`, but `pam()` is more robust against outliers and has a useful display of the clusters. Describe the influence that the outlier (observation #70) has on this algorithm when it is reintroduced to the data.
- 11.7 (a) Show how we can assign statistical significance to the Jaccard Index. Suppose we have a finite sized population containing n items. One sampling method identifies m of these items, and a different, independent method identifies m' items. Let X denote the random variable counting the number of items that are common to both samples. Identify the distribution of X .
- (b) Suppose the set S is completely contained in the set T . What are the largest and smallest possible values of $J(S, T)$? Comment on the suitability of J as a measure of agreement.
- (c) Suppose the set Σ contains $2n$ items and the partitions $\mathbf{X} = \{\mathbf{x}_1, \mathbf{x}_2\}$ and $\mathbf{Y} = \{\mathbf{y}_1, \mathbf{y}_2\}$ are both composed of two sets of sets, each containing n items. When n is large, what are the largest and smallest values of $\text{Rand}(\mathbf{X}, \mathbf{Y})$?
- (d) Suppose \mathbf{x}_1 and \mathbf{y}_1 of the previous question both contain only one item, then what is range of $\text{Rand}(\mathbf{X}, \mathbf{Y})$?
- (e) Compare the Dunn Index with the F-ratio used to assess statistical significance in a one-way ANOVA.
- 11.8 Examine the `lung` data set in the `pvclust` library. This data has gene expression on 916 genes for 72 human lung tissues, including 67 lung tumors. See how much of the analysis of Sect. 11.3 you can repeat on this much larger data set. How many clusters of genes do you estimate? What evidence do you use to support this claim?
- 11.9 The Older Americans Act (OAA) is a federal program began in 1965 to provide social services and nutritional assistance to senior citizens. Table 11.6 lists the percent composition of people served in each state.

Table 11.6: Composition of seniors served by the OAA, Title III in 2011

State	Percentage			
	Poverty	Minority	Poverty and minority	Rural
AL	9	28	3	26
AK	39	34	21	80
AZ	26	42	16	48
:	:	:	:	:
WI	22	6	3	70
WY	18	3	1	73
US				
Total	30	25	11	37

Source: US Department of Health & Human Services, Administration on Aging

Examine this data using hierarchical clustering methods. Are there unusual groups of states? Do geographically similar states cluster together?

- 11.10 Simulate the Dunn Index in the `mouse` data under a model of no clustering.
- Specifically, generate bootstrap samples by separately generating random columns of genetic marker values. Calculate the Dunn Index on each sample, draw a histogram of these values, and compare these to the index on the original value. Comment on this figure. What evidence does the Dunn Index provide of the validity of $K = 3$ clusters in the original data?
 - Can you give a possible explanation for the bimodal distribution of the simulated Dunn Index appearing in Fig. 11.11?
- 11.11 The `car90` data frame in the `rpart` library cites an article from 1990 *Consumer Reports* on 34 measurements on 111 different car models. There are many *NAs* in this data, so you might want to use the `complete.cases` command to eliminate those cars with incomplete data.
- Use K-means clustering to identify groups of similar cars. What is an appropriate value of K ? What are the defining characteristics of these car groups?

- (b) Consider recursive partitioning methods to classify the reliability measurement. Reliability is coded using the ordered categories:

much worse < worse < average < better < much better .

Use a regression tree approach to identify those variables associated with the most and least reliable cars. Briefly, which types of cars appear to have the most and least problems?

- 11.12 The data frame `wpbc` in the `TH.data` library contains 34 measurements on the tumors of 198 women with breast cancer treated in a clinic in Wisconsin.

(a) Examine this data using K-means and estimate how many different tumor types there are in this data.

(b) The `help` file for this data frame contains a list of suggested regressions that can be fitted to model different response variables. Examine one of these models using a regression tree approach. How well does the regression tree coincide with the K-means approach that you found in part (a)?

- 11.13 Table 11.7 lists the largest oil companies and their production statistics for 2006 and change from 2005.

(a) Use hierarchical clustering to show that Gazprom, the world's largest producer of natural gas, is very different from the other companies in this table. Without Gazprom, the oil companies cluster into three distinct groups.

(b) Apply K-means or other methods to demonstrate the clustering pattern of these companies. Figure 11.13 is an example.

Table 11.7: Reserves and production of global oil companies

Company	Reserves	Current years	2006 Oil and gas production	
	(MM boe)	of production	Amount	% change
BP	17,368	10.4	3926	-1.9
ChevronTexaco	11,020	10.9	2667	6.1
ExxonMobil	21,518	11.3	4238	3.8
Royal Dutch shell	11,108	6.7	3474	-1.0
Hess	1243	7.9	358	7.0
BG group	2149	6.2	601	19.0
ConocoPhillips	6676	8.7	2359	29.7
ENI	6406	11.2	1770	5.8
Marathon	1262	7.1	377	9.0
Norsk-Hydro	1916	9.3	573	2.0
Petro-Canada	1301	8.4	345	-3.1
Repsol YPF	2600	5.2	1128	-3.0
Petrobras	11,458	14.2	2287	4.5
CNOOC	503	3.0	455	11.7
Gazprom	144,668	39.7	9965	6.0
LUKOIL	18,144	27.2	1838	4.5
PetroChina	16,260	15.6	2907	5.0

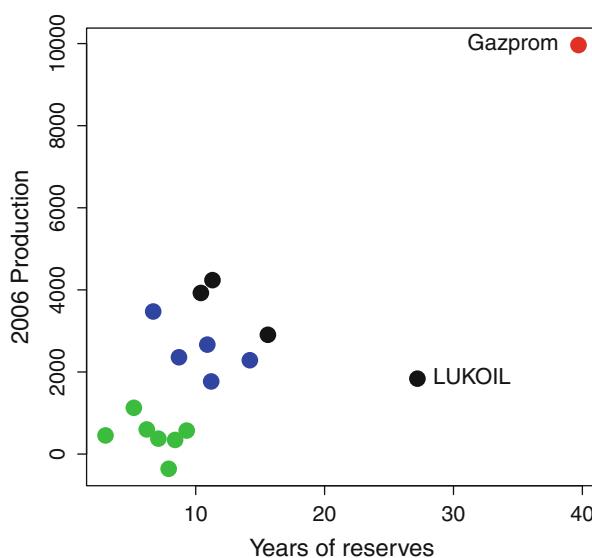


Figure 11.13: Clustering of oil producing companies

Chapter 12

Time Series Models

THE MODELS for data described so far have been concerned with independent observations on multivariate values. The data examined in this chapter is for settings where the successive observations are also correlated. This type of data appears frequently in environmental and economic studies where a sequence of observations are taken over an evenly spaced time period. Such *time series* take into account the serial correlations: Adjacent observations are positively correlated, and observations farther apart in time act more independently.

A full study of time series methods is beyond the scope of this book, but a number of elementary procedures for this type of data are introduced and computed in R. We will concentrate on two types of analysis. One of these, *autoregressive models*, is useful when the correlation between observations is related to the difference in time between their measurement. A different example of these models is described in Sect. 7.5. This second method, *spectral decomposition*, reexpresses the observed data in terms of cyclical patterns that repeat periodically within the observed data. Let us begin by introducing some examples of the type of data that we are likely to encounter and then go over a simple analysis that can be performed in R.

12.1 Introductory Examples and Simple Analyses

Table 12.1 presents the annual combined US cancer rates (per 100,000 persons) by race (black, white) and sex. This data was reported by the Surveillance, Epidemiology, and End Results (SEER) Program of the National Cancer Institute. The SEER program began in 1973 as part of the “War on Cancer” initiated under then President Nixon. Currently, in addition

Table 12.1: Annual combined cancer rates in the US by sex and race 1975–2007

Year	All races			Whites			Blacks		
	Both sexes	Male	Female	Both sexes	Male	Female	Both sexes	Male	Female
1975	400.39	466.78	365.84	402.12	468.58	369.56	426.23	525.13	356.46
1976	407.40	481.17	367.40	409.69	481.86	373.12	427.38	553.02	340.44
1977	407.74	486.49	363.71	409.26	487.08	367.86	442.62	577.65	352.01
⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮
2006	462.14	535.72	410.08	471.25	539.95	423.20	487.43	614.56	400.20
2007	461.08	536.61	407.18	468.47	539.49	418.31	482.04	609.17	394.46

Source: SEER

to national-level statistics, SEER collects detailed information on all cancer cases, by diagnosis, in eight states, several metropolitan and rural areas, as well as in selected Native American populations.

A portion of the data in Table 12.1 is plotted in Fig. 12.1 for the overall population as well as separately for white and black females. The cancer rates are somewhat higher at the end of this time period than at the beginning. There was a sharp peak for males in 1991 followed by a quick reversal, but this did not much affect the female populations. The generally increasing rates covered in this data are partly explained by the facts of longer life expectancy and advances in treating heart disease and stroke. People who would have died from other causes in an earlier time are now living long enough to develop cancer.

A simple examination of this data would be to fit a model of cancer rates as a linear or possibly quadratic function of the year. The problem with this approach is that the statistical significance of the regression coefficients would be distorted because of the lack of independence of the observations from one year to the next. A high rate in one year is more likely than not to be followed by another high rate the following year.

There are some other questions we may want to address in this data. Does the year-to-year correlation carry over 2 or more years later? That is, do each year's rates depend on the past few years? Perhaps there is a random noise component, as we saw in regression models in Chap. 9. Do these random errors in one year influence cancer rates several years later? How do we express the correlation between two different series? Do these also have temporal correlations? That is, does a high rate or model error in one series influence the other series a year later? We will describe models to answer these questions in Sect. 12.2.

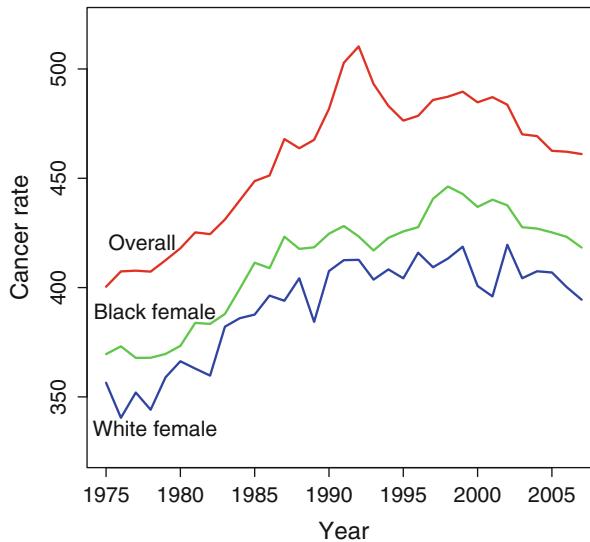


Figure 12.1: US cancer rates for selected populations, 1975–2007

Table 12.2: Monthly measures of the global environment

Year	Month	CO ₂	Sea ice		Snow in	
			% extent	in 10 ⁶ km	10 ⁶ km	El Niño
1978	11	333.76	12.02	8.95	31.49	21.99
1978	12	334.83	14.12	10.85	43.65	23.30
1979	1	336.21	15.54	12.33	49.12	24.77
⋮	⋮	⋮	⋮	⋮	⋮	⋮
2009	11	385.99	10.26	7.98	34.44	22.11
2009	12	387.27	12.48	10.17	45.86	23.16
2010	1	388.45	13.78	11.59	48.27	24.82

Source: *Climate Charts & Graphs*. Courtesy of Kelly O'Day

Let us introduce another set of data to illustrate the methods of this chapter. The data in Table 12.2 summarizes a set of global environmental measures reported monthly from November 1978 through January 2010 for the northern hemisphere. The CO₂ values are atmospheric carbon dioxide, measured in parts per million. Sea ice is reported as both percentage of extent and in millions of square km. Sea ice usually peaks in March/April and reaches its annual minimum in September or October. Snow cover is also reported in millions of square km. El Niño is a measure of the Pacific currents that bring rain and wind from the warm areas near the equator. A small number of missing values have been linearly interpolated.

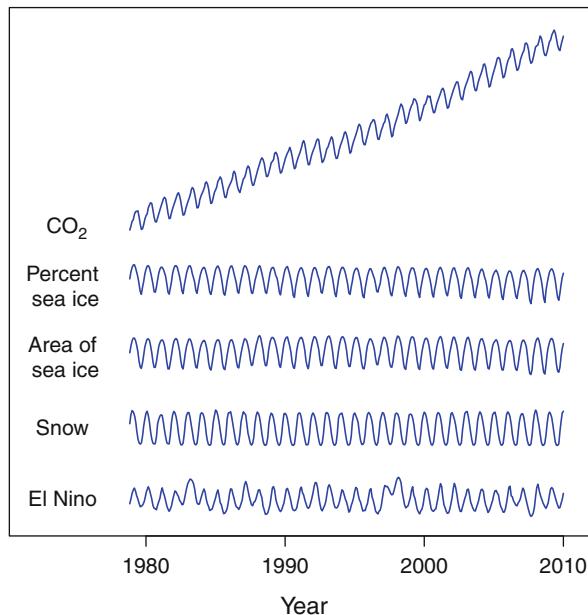


Figure 12.2: Plot of the five environmental time series appearing in Table 12.2

A plot of this data appears in Fig. 12.2. We see the annual, cyclical patterns that vary with the seasons in the northern hemisphere. There are trends, most clearly seen in CO₂ levels, but possibly in some of the other series, as well. The objective of the data analysis is to correct for the trends, if present, adjust for the annual cycle, and then examine the joint residuals in order to see if any additional information can be extracted from this data. As with the cancer rate data, we are looking for correlations of observations that are temporally closely spaced. This data will be modeled in Sect. 12.3.

Let us end this section with a third data set and an illustration of some simple analyses that we can perform in R. This data on the monthly birth rates in New York City can be read directly from the web, producing a `data.frame` as follows:

```
> NYCbirth <-
+   scan("http://robjhyndman.com/tsdldata/data/nybirths.dat")
Read 168 items

> print(NYCbirth, digits = 3)
[1] 26.7 23.6 26.9 24.7 25.8 24.4 24.5 23.9 23.2 23.2 21.7
[13] 21.9 21.4 21.1
[15] 23.7 21.7 21.8 20.8 23.5 23.8 23.1 23.1 21.8 22.1 21.9
[17] 20.0 23.6 21.7
```

```
[29] 22.2 22.1 23.9 23.5 22.2 23.1 21.1 21.6 21.5 20.0 22.4
     20.6 21.8 22.9
     . . . . . . . . . .
```

In R there is a special data structure called `ts` that acts as a `data.frame` but is better suited for some time series analyses. The `ts()` function creates a `ts` object, identifying the frequency period (months) and starting time. We create a `ts` object, adding these time coordinates:

```
> NYCts <- ts(NYCbirth, frequency = 12, start = c
  (1946, 1))
> print(NYCts, digits = 3)
  Jan  Feb  Mar  Apr  May  Jun  Jul  Aug  Sep  Oct
  Nov  Dec
1946 26.7 23.6 26.9 24.7 25.8 24.4 24.5 23.9 23.2 23.2
  21.7 21.9
1947 21.4 21.1 23.7 21.7 21.8 20.8 23.5 23.8 23.1 23.1
  21.8 22.1
1948 21.9 20.0 23.6 21.7 22.2 22.1 23.9 23.5 22.2 23.1
  21.1 21.6
  . . . . . . . . . .
```

A simple time series analysis decomposes the observed data into three component parts:

$$\text{observed data} = \text{trend} + \text{seasonal effect} + \text{residual}.$$

The observed data and these three component parts are separately plotted in the top panel of Fig. 12.3. This figure and the components can be obtained using the `decompose` function:

```
NYCd <- decompose(NYCts)
plot(NYCd, xlab = "Year", col = "red")
```

The `decompose` function takes a `ts` object and produces a `decomposed.ts` object with components: `$x` (original data), `$seasonal` (the periodic effect), `$trend` (the trend component of the model), and `$random` (the residual).

In the upper panel of Fig. 12.3, we can see the trend for a declining birth rate 1946–1948, followed by a sharp increase through 1956 and a leveling off after that. The `seasonal` effect shows a repeated pattern for each year: lowest in February (also the shortest month) and highest in July and August. There are no extreme residuals or outliers for us to report in the `random` plot.

Another useful display is to superimpose the observed values and the overall trend, as in the lower panel of Fig. 12.3. This figure was produced using

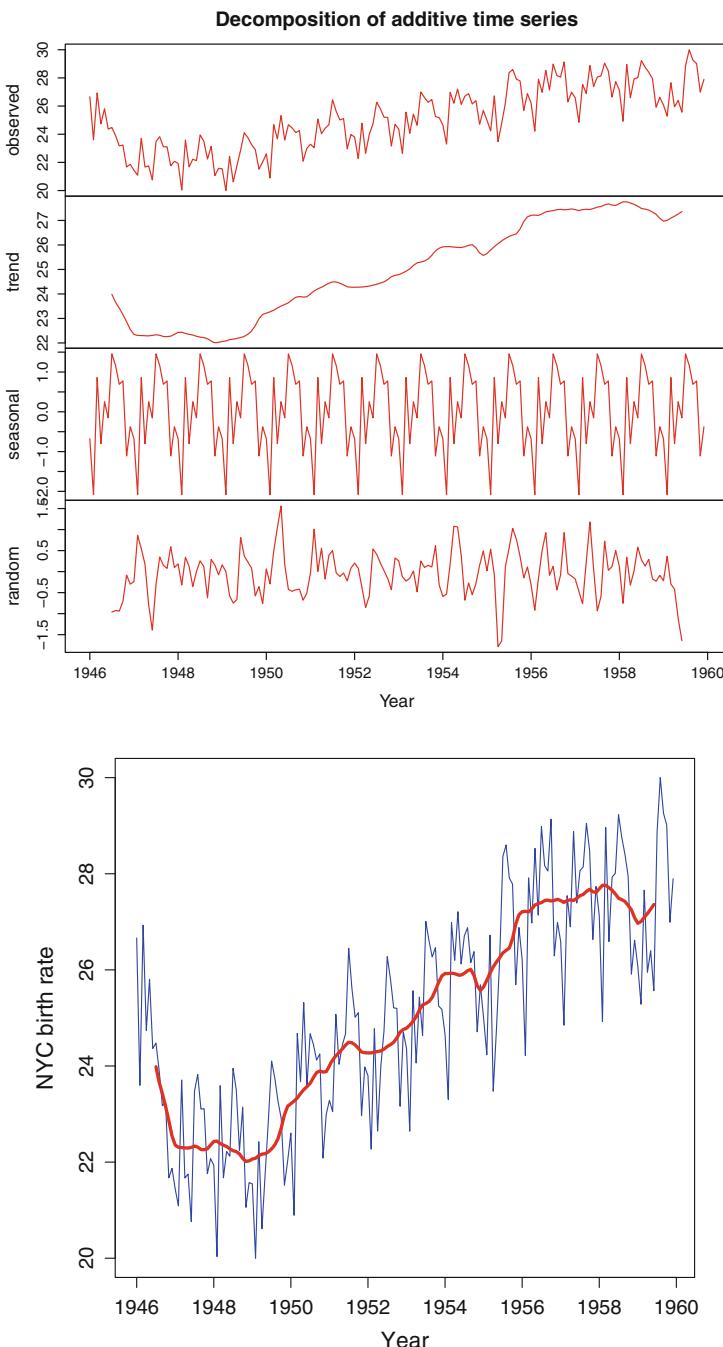


Figure 12.3: Observed New York City birth rates decomposed into trend, cyclical (or seasonal) component, and residual in the *top panel*, and displayed as superimposed observed and trend (*bottom*)

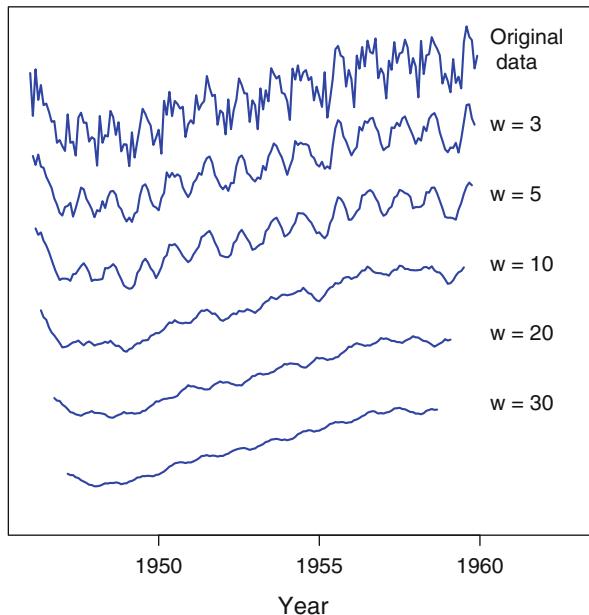


Figure 12.4: Birth rates smoothed with different moving averages of window widths w , as specified

```
plot(NYCd$x, xlab = "Year", ylab = "NYC birth rate",
     col = "blue")
lines(NYCd$trend, col = "red", lwd = 3, type = "l")
```

A more sophisticated decomposition of a time series can be performed using the `stl()` function in R. This program has more options available including the loess smoothing of the seasonal trend. This smoothing usually produces a better image of the seasonal trend. See Exercise 12.1 for an illustration of its use.

We can control the amount of smoothing in a time series using the `filter()` function which performs a *moving average*. A moving average, as the name implies, is the series of all sequential averages of a number of adjacent observations. The number of points in the moving average is called the *window* or sometimes the *window width*.

As a mathematical example, a moving average \mathbf{m} on a time series $\mathbf{x} = (x_1, \dots, x_n)$ with window $w = 5$ is calculated as

$$m_t = (x_{t+2} + x_{t+1} + x_t + x_{t-1} + x_{t-2}) / 5 \quad (12.1)$$

so that the five adjacent observations are averaged.

The moving average is illustrated for the birth rate data in Fig. 12.4 both for the original data and a range of different window widths. Small values of window w remove the short-term noise and emphasize the annual cycles. Values of w greater than 12 will remove much of the annual cycle and leave a smooth image of the overall trend.

In (12.1), we see the moving average m_t is centered around x_t and gives equal weights to all five observations. Some moving averages give greater weight to those observations closer to the center. Again, in (12.1) we see that the first and last two m_t s are undefined for $t = 1, 2, n - 1$, and n . Similarly, notice how the different moving averages in Fig. 12.4 become shorter at each end. In some settings where forecasting future trends is the objective, we may want to define moving averages only on the lagging or trailing observations.

In R, we calculate moving averages as

```
filter(x, filter = rep(1 / w, w))
```

The `filter=rep(1 / w, w)` parameter specifies that the weights in the average are all equal. In some cases, we might want to give more weight to those observation nearer the center of the window.

12.2 Autoregressive Models

We begin with an ordered collection of multivariate observations $\mathbf{x}(1), \mathbf{x}(2), \dots, \mathbf{x}(n)$ that were taken over a series of evenly spaced time intervals. These observations are correlated both within the components of $\mathbf{x}(t)$ as well as temporally correlated between $\mathbf{x}(t)$ and $\mathbf{x}(t - k)$. An important assumption we make is that the series is *stationary*. This means that the marginal distribution of $\mathbf{x}(t)$ does not change over time and is the same for every value of t . We will explain this point again below and also test its validity.

The models we build will demonstrate the intuitive property that observations that are made closer in time are more highly correlated than observations made farther apart. Our interest is to identify trends in the mean of this series of observations but also to describe regressions that model later observations on earlier ones. As an example, can we forecast one year's cancer rates using the data from all previous years?

We can describe the temporal, univariate correlations between other observations in the same series

$$\hat{\rho}_k = \text{corr}\{x(t), x(t - k)\}$$

for $t = 2, 3, \dots, n$ and $k = 1, 2, \dots$

This is referred to as the *autocorrelation* of *lag* k because it measures the correlation of the data with itself, offset by k observations. The x 's in this definition are scalar valued. If the x 's were vector valued, then the ρ 's would be correlation matrices.

The assumption that the data is stationary means that these correlations are the same for every value of t . Ideally, sufficiently long lags would indicate that observations far apart also behave independently. A plot of the autocorrelation $\hat{\rho}_k$ by the length of the lag k is called the *correlogram, periodogram*, or a *variogram*. Useful lag values k are generally much smaller than the sample size n and rarely larger than 15 or 20.

The `acf` function in R computes autocorrelations of a scalar-valued time series and plots the correlogram as function of the lag for a range of lags. Figures 12.5, 12.6, and 12.7 are examples of these. Figure 12.5 plots the correlogram for a set of randomly distributed standard normal variates. This figure can be obtained with

```
acf(rnorm(125))
```

in R.

The autocorrelation with a lag of $k = 0$ is equal to one, corresponding to the correlation of the data with itself. In this example, higher lags have negligible autocorrelations because the data is randomly generated.

Figure 12.6 is the estimated autocorrelation function for US total cancer rates, combined over all populations. These correlations are all very high for small lags indicating a high degree of autocorrelation between close years' values. High lags have negative correlations reflecting a regression to the mean for observations that are far apart.

There is also a cross-correlation function that allows us to measure the lagged correlation of one series with another. That is, we can measure the correlation

$$\text{corr}\{x(t), y(t - k)\}.$$

The lag, k , could be either positive or negative depending on which series we can interpret as leading or lagging the other.

The cross correlation is calculated in R using the `ccf(x= , y=)` function. An example of these appears in Fig. 12.7. In this figure we see the cross correlation of cancer rates for white females lagged by the overall US rates. This plot demonstrates that there is a high correlation between the two time series.

Figures 12.5, 12.6, and 12.7 include bounds (as dotted lines) for 95 % confidence intervals of autocorrelations under the null hypothesis that observations are generated independently. The autocorrelation function for the normal random observations are generally within these bounds and those of the cancer rates are well outside their bounds.

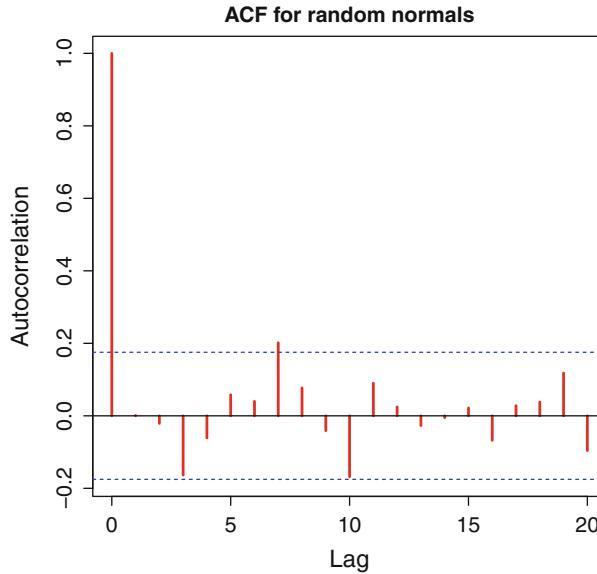


Figure 12.5: Autocorrelation function for random normally distributed data

The Ljung–Box test (Ljung and Box 1978) is a single test that several autocorrelations are all zero. In a sample of n observations with estimated autocorrelation $\hat{\rho}_k$ of order k , the statistic

$$Q = n(n + 2) \sum_{k=1}^h \frac{\hat{\rho}_k^2}{n - k} \quad (12.2)$$

behaves approximately as chi-squared with h df.

In R we compute this test using

```
Box.test(x, lag = 1, type = "Ljung-Box")
```

where x is the time series data and the `lag` specifies h , the number of autocorrelations to be tested. We won't illustrate the use of this statistic at this point: It is better suited to examine the autocorrelations of residuals from regression models that we describe next.

Given a series $\{\mathbf{x}(1), \dots, \mathbf{x}(n)\}$ of temporally ordered multivariate observations, the *autoregression model*

$$\mathbf{x}(t) = \boldsymbol{\theta} + \boldsymbol{\Theta}_1 \mathbf{x}(t-1) + \dots + \boldsymbol{\Theta}_p \mathbf{x}(t-p) + \mathbf{e}(t) \quad (12.3)$$

regresses each data point $\mathbf{x}(t)$ on the p previous observations plus multivariate normally distributed error $\mathbf{e}(t)$.

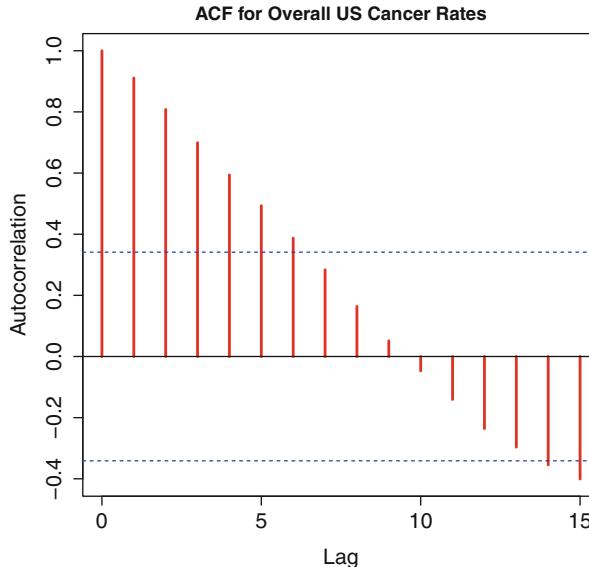


Figure 12.6: Autocorrelation for US cancer rates for all populations

In this model the parameters to be estimated are $\boldsymbol{\theta}$, a vector-valued intercept, and matrices $\boldsymbol{\Theta}_1, \dots, \boldsymbol{\Theta}_p$ of regression coefficients. The lag, p , is usually chosen as a small value because of the large number of estimated parameters involved. Model (12.3) is similar to multivariate linear regression described in Chap. 9, except the autoregression model includes earlier observations as the explanatory variables. Intuitively, this model forecasts the next observation as a linear function of the previous p observations.

The multivariate autoregressive model can be fitted using the **VAR** (vector autoregressive) routine. An example of this is

```
library(vars)
acan <- read.table(file = "AnnualCancer.txt", header = T)
ofc <- acan[, c("Overall", "Wfemale", "Bfemale")]
varofc <- VAR(ofc, p = 1, type = "both")
summary(varofc)
res <- residuals(varofc)
```

In this R code, we read the cancer data, then select the overall rate as well as those for black and white females. The **VAR** function fits model (12.3) with $p = 1$. There is a large amount of output from this program and a portion is reproduced in Output 12.1. This includes the estimated regression coefficients in (12.3), their standard errors, and tests of statistical significance. The correlation matrix of the residuals is also included.

In Output 12.1 see that the white female series is highly correlated with its own value from the previous year and also has a statistically significant

Output 12.1: A portion of the autoregression output for US cancer rates

```
Estimation results for equation Wfemale:
=====
Wfemale = Overall.l11 + Wfemale.l11 + Bfemale.l11 + const + trend

      Estimate Std. Error t value Pr(>|t|)

Overall.l11 -0.1081    0.1076 -1.004  0.3243
Wfemale.l11  0.8911    0.1635  5.450 9.12e-06 ***
Bfemale.l11  0.2898    0.1405  2.063  0.0489 *
const       -12.6488   35.6494 -0.355  0.7255
trend       -0.2743    0.2479 -1.107  0.2783
---
Residual standard error: 5.826 on 27 degrees of freedom
Multiple R-Squared: 0.9495,      Adjusted R-squared: 0.942
F-statistic: 127 on 4 and 27 DF,  p-value: < 2.2e-16

Estimation results for equation Bfemale:
=====
Bfemale = Overall.l11 + Wfemale.l11 + Bfemale.l11 + const + trend

      Estimate Std. Error t value Pr(>|t|)

Overall.l11  0.27915   0.16816  1.660  0.1085
Wfemale.l11  0.46300   0.25549  1.812  0.0811 .
Bfemale.l11  0.04281   0.21953  0.195  0.8468
const       57.65281  55.70207  1.035  0.3098
trend       -0.04098   0.38728 -0.106  0.9165
---
Residual standard error: 9.103 on 27 degrees of freedom
Multiple R-Squared: 0.8583,      Adjusted R-squared: 0.8373
F-statistic: 40.89 on 4 and 27 DF,  p-value: 4.394e-11

Correlation matrix of residuals:
      Overall Wfemale Bfemale
Overall  1.0000  0.6115  0.4475
Wfemale  0.6115  1.0000  0.4533
Bfemale  0.4475  0.4533  1.0000
```

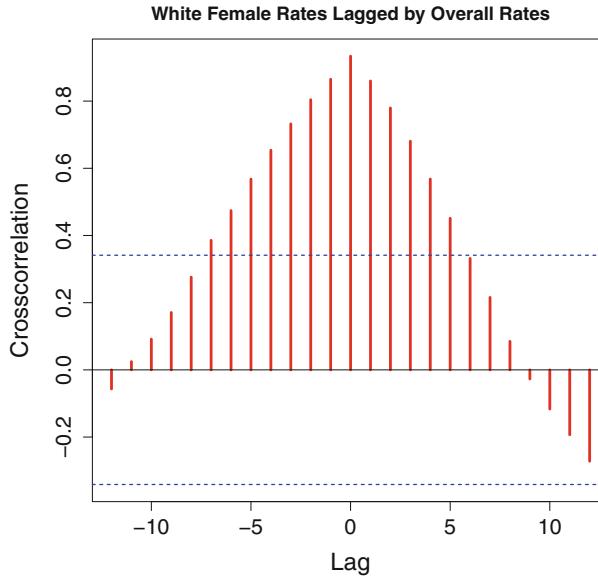


Figure 12.7: Cross correlation of cancer rates in US White women lagged by total US population

regression on black women's cancer rates of the previous year. The fitted regression model for black female cancer rates is statistically significant according to the overall F-test, but no single regression coefficient is significant. The estimated trends are not statistically significant for either of these two populations. The negative values of the estimated trends indicate that no overall trend remains after correcting for the regression coefficients.

The multivariate residuals from this regression are plotted in the upper panel of Fig. 12.8. These values have been scaled because the three series have different estimated variances. Scaling each column to zero mean and unit variance is performed using the `scale()` function. The rug plot on the right margin of this figure does not indicate any deviations from a marginal normal distribution. A test of normality on the residuals can be performed using

```
normality.test(varofc)
```

also in the `vars` library.

The `normality.test` computes the multivariate Jarque–Bera test on this data ($p = 0.80$) and separately for the multivariate skewness ($p = 0.45$) and kurtosis ($p = 0.94$). These p-values give us no empirical evidence of a departure from multivariate normal residuals. The details of the Jarque–Bera test are described in Sect. 5.4.

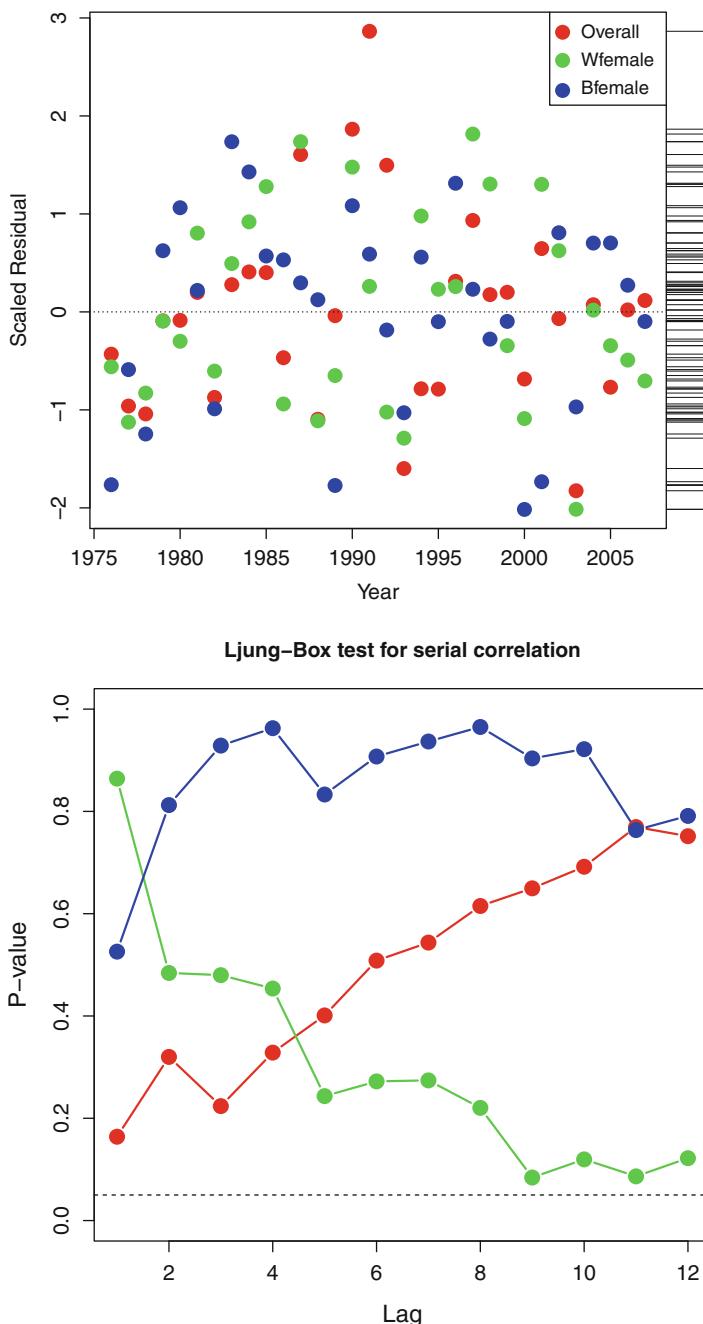


Figure 12.8: Residuals and p-values for the Ljung-Box test from autoregressive model of US cancer rates in selected populations

The Ljung–Box test statistic given in (12.2) can be used to detect any autocorrelation in the residuals of a fitted autoregression model, as well. Rejecting the null hypothesis of these residuals is indicative of autocorrelations that are not accounted for by the autoregression model. This would suggest that a larger number of parameters is needed in (12.3). The lower panel of Fig. 12.8 plots the p-values of these tests for each of the three time series in our model and these give no indication of any inadequacies in the model for only one regression variable.

Another assumption we need to examine is that of stationarity of the series. We assume that $\mathbf{x}(t)$ all have the same distribution, and this assumption can fail in a wide range of ways. There are many possible tests of these departures and several are available in R. See Exercise 12.7 for a list of these.

A graphical display of the stationarity assumption appears in Fig. 12.9. Instead of fitting a model with the whole data set, suppose we fit a series of models on a moving window subset $\{\mathbf{x}(t+1), \dots, \mathbf{x}(t+w)\}$ for window width $w > 0$. As the starting value, t , of the window varies, we should not expect to see much difference in the estimated model parameters if the series is truly stationary.

We used a window width of $w = 15$ years in Fig. 12.9 and examined the six estimated model variances, on a log scale, and the nine estimated regression coefficients Θ , in the bottom panel. The fitted model is the same as that in Output 12.1. The overall US cancer rate (in red on the bottom panel) has a higher estimated variance in the middle years than at either end of the data. A small number of estimated regressions have larger variability at the beginning of the series but otherwise are fairly stable throughout. In conclusion, we see no inadequacies in the autoregressive model for this data with $p = 1$ and the stationarity assumption seems reasonable.

Next, let us introduce a more general model for temporally correlated multivariate data. These models regress on both earlier observations as well as on their model errors. Autoregressive models in (12.3) contain multivariate normally distributed random errors $\mathbf{e}(1), \mathbf{e}(2), \dots$ associated with each observation. In autoregressive, integrated moving average (ARIMA) models, these errors are cumulative, and there are additional *moving average* regression coefficients associated with these as well.

Symbolically, the ARIMA model of order (p, q) is

$$\begin{aligned} \mathbf{x}(t) = & \boldsymbol{\theta} + \Theta_1 \mathbf{x}(t-1) + \Theta_2 \mathbf{x}(t-2) + \dots + \Theta_p \mathbf{x}(t-p) \\ & + \mathbf{e}(t) + \Delta_1 \mathbf{e}(t-1) + \Delta_2 \mathbf{e}(t-2) + \dots + \Delta_q \mathbf{e}(t-q). \end{aligned} \quad (12.4)$$

In the ARIMA model, each observed $\mathbf{x}(t)$ is regressed on each of the previous p observed $\mathbf{x}(t-1), \dots, \mathbf{x}(t-p)$ as well as on the errors $\mathbf{e}(t-1), \dots, \mathbf{e}(t-q)$ associated with the q previous observations.

The parameters to be estimated in the ARIMA model are the vector-

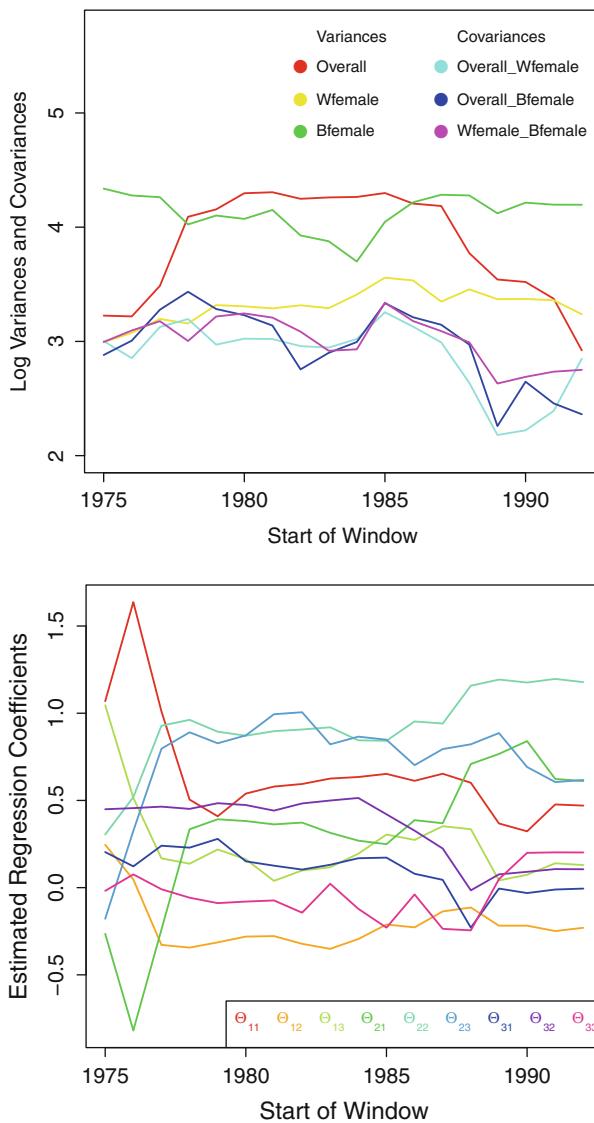


Figure 12.9: Moving window estimates of variances (log scale, at *top*) and regression coefficients Θ_1 (on *bottom*) in autoregression model of Output 12.1

valued intercept θ , matrices of autoregressive slopes $\Theta_1, \dots, \Theta_p$, and matrices of moving average slopes $\Delta_1, \dots, \Delta_q$. There are a very large number of parameters to be estimated in (12.4). As a consequence, only very long multivariate time series can be fitted. Below, we will illustrate the ARIMA models using only the univariate overall US cancer rate because of the large number of parameters associated with ARIMA models.

ARIMA models can be fitted using

```
arima(x, order = c(p, 0, q))
```

for univariate time series (x) and

```
VARMA(y, p = , q = )
```

for multivariate data (y). These functions are available in the TSA and MTS libraries, respectively.

The missing option (0) in the `order=` allows us to change the order of differencing, but it is best set to zero for most applications. When q is set to zero, these programs fit autoregressive models. The `arima` and `VARMA` programs have several other options including the ability to regress on other explanatory variables and a choice of whether or not to include an intercept θ .

The details from three fitted ARIMA models are given in Output 12.2. The output includes fitted regression parameters and measures of overall fit, relative to the other models. The three successive models are nested in the sense that each subsequent model adds additional parameters to the previous model. We can see the estimated variance of $e(t)$ (denoted by `sigma^2`) declines with more complicated models indicating a lower degree of uncertainty associated with each subsequent model. Similarly, the log-likelihood increases, also indicating a better fit according to this criterion.

In addition, there is an AIC measure that is minimized for the middle of these three models. We will explain this statistic next.

The object of model building is more than maximizing the log-likelihood. This could be accomplished in a complicated model with many parameters, not all of them useful. The AIC, then, charges a penalty to the model log-likelihood for every parameter included. The *AIC* is the Akaike¹ Information Criterion, and is defined as

$$\text{AIC} = -2 \times \text{Log-likelihood} + 2 \times \text{number of parameters}.$$

In words, every parameter in the model must make a meaningful contribution in order to be included. Maximizing the log-likelihood is one goal, but minimizing the AIC results in simpler models.

¹Hirotugu Akaike (1927–2009). Japanese statistician.

Output 12.2: Portions of three ARIMA models of overall cancer rates

```
> arima( acan[ , "Overall"] , order = c(1, 0, 0))
# autoregressive (1)
Coefficients:
      ar1  intercept
      0.9709   440.0603
  s.e.  0.0297   28.7600

sigma^2 estimated as 66.23:  log likelihood = -117.44,
  aic = 238.88
> arima( acan[ , "Overall"] , order = c(1, 0, 1)) # ARIMA
  (1,1)
Coefficients:
      ar1      ma1  intercept
      0.9555   0.3687   441.9634
  s.e.  0.0425   0.1480   27.3071

sigma^2 estimated as 56.2:  log likelihood = -114.9,
  aic = 235.79
> arima( acan[ , "Overall"] , order = c(2, 0, 2))
# ARIMA(2,2)
Coefficients:
      ar1      ar2      ma1      ma2  intercept
      0.7065   0.2170   0.7001   0.3771   444.2845
  s.e.  0.4227   0.4051   0.4108   0.3048   25.7473

sigma^2 estimated as 53.34:  log likelihood = -114.17,
  aic = 238.34
```

Specifically, the ARIMA(2,2) model in Output 12.2 has evidence of being *overfitted*, or having too many parameters. There is only a modest improvement in reduced `sigma^2` and slight increase in the log-likelihood ratio between the ARIMA(1,1) and ARIMA(2,2) models. Recall from Sect. 7.4 that twice the difference in the log-likelihood of two nested models should behave as chi-squared when the underlying parameters are zero. In the present case, the ARIMA(2,2) has two more parameters than the ARIMA(1,1) model. At the same time, the AIC has increased indicating that the improvement in fit is not enough to warrant the increase in parameters and model complexity.

The ARIMA(1,1) model for the year t of overall US cancer rates $x(t)$ has the smallest AIC of the three models in Output 12.2. The fitted parameters of this model are

$$x(t) = 441.96 + 0.96 x(t-1) + e(t) + 0.37 e(t-1),$$

where the e s are normally distributed with mean zero and their estimated variances are 56.2.

There are a number of diagnostics available for the `arima` program. The `tsdiag` program plots residuals, their periodogram, and tests of different lags in the Ljung–Box test. Exercise 12.7 explores different significance tests of the stationarity assumption. We next examine models that exploit cyclical patterns in the time series.

12.3 Spectral Decomposition

In the previous section, we saw that we can build regression models where the observed value in one time period is regressed or explained by observations made at earlier times. In the example of the US cancer rates, we saw that reasonable models can be constructed using the previous year's data. Such models are useful when the observed data is relatively smooth but also temporally correlated. The models we examine here are useful for data that exhibits marked cyclical patterns such as those seen in the seasonal variations of the climate data in Fig. 12.2 and, to a smaller degree, in the birth rate data of Fig. 12.3. The approach taken in this section is to decompose the data into its cyclical components of all possible frequencies. We will see that simple models can be obtained by omitting many terms in the model. In this case, we can delegate many of the high-frequency components to the residuals.

The background theory needed is the *Fourier*² transform. Suppose we have a set of numbers $\mathbf{x} = \{x_1, \dots, x_n\}$. Then there is a unique representa-

²Joseph Fourier (1768–1830). French mathematician and physicist.

tion of \mathbf{x}

$$x_i = \sum_{k=1}^{n/2} a_k \sin(2\pi i k/n) + b_k \cos(2\pi i k/n) \quad (12.5)$$

in terms of other numbers $\mathbf{a} = \{a_k\}$ and $\mathbf{b} = \{b_k\}$ for every $i = 1, \dots, n$.

The representation of \mathbf{x} in terms of its *frequency spectrum* \mathbf{a} and \mathbf{b} is called the Fourier transform. This is analogous to the way we can use a prism to decompose white light into its component colors.

The representation in (12.5) is unique, in part because there are n numbers on both sides of Eq. (12.5). Further, given \mathbf{a} and \mathbf{b} , it is possible to invert this relationship using the *inverse Fourier transformation* and obtain the original \mathbf{x} again. If n is an odd number then we set the last b_k to zero in (12.5).

There was a time when computing (12.5) took a lot of computing power. This changed with the publication of the *fast Fourier transformation* by Cooley and Tukey (1965), although earlier versions were known but not as well utilized. In today's applications, for example, a Fourier transformation can greatly simplify the transmission of a video image, omitting some of the noise or high-frequency spectrum, at the expense of losing some fine detail in the picture.

Mathematical models with periodic sines and cosines are most useful when the data \mathbf{x} exhibits strong cyclical patterns. Intuitively, when one a_k and/or b_k is large, then there is a large cyclical effect with period $2\pi k/n$ in \mathbf{x} . A useful display, as in Fig. 12.10, is to plot the magnitude of $\{a_k, b_k\}$ against k . The vertical axis in this figure plots values of $\sqrt{a_k^2 + b_k^2}$.

The complete set of magnitudes of all frequencies (expressed in terms of \mathbf{a} and \mathbf{b}) is referred to the *spectral decomposition* of the data. These are computed and plotted in Fig. 12.10 using

```
spec.pgram(climate, detrend = TRUE)
```

for the climate data.

The `spec.pgram` program computes and plots the spectral decomposition for each of the series. The `detrend` option removes linear trends such as the one that is so apparent in the CO₂ series. The program fits and plots the periodogram in the left panel of Fig. 12.10. The obvious problem is the large amount of noise in the raw periodogram making it difficult to see the underlying pattern in the data.

A *smoothed periodogram* is a much more useful diagnostic. To smooth the periodogram, we add the `span` option as in

```
spec.pgram(climate, detrend = TRUE, span = c(9, 9))
```

The arguments to the `span` option are a pair of odd integers, where larger values result in greater smoothing and smaller values result in greater fidelity

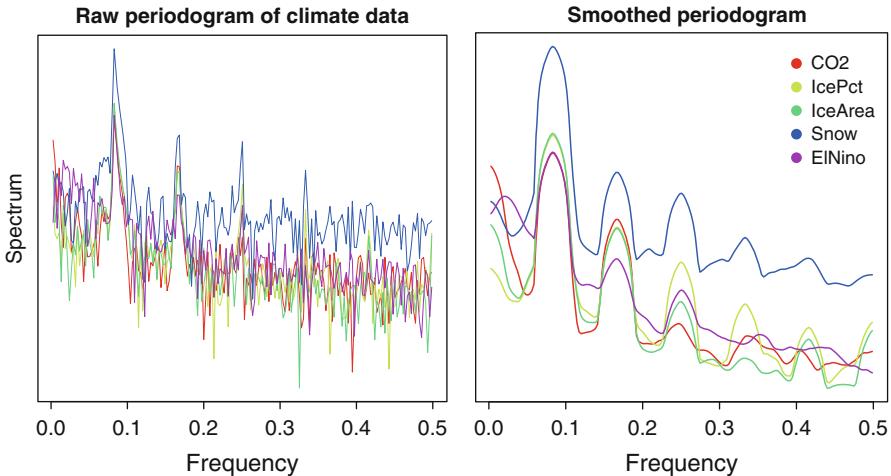


Figure 12.10: Raw and smoothed periodograms of the climate data

to the original values. This is similar to determining the window width when computing a moving average as seen in Fig. 12.4. The choice of parameter values usually takes some trial and error to produce just the right balance of smoothing and fidelity to the original data.

The vertical axis of the periodogram is called the *spectrum* and is a measure of the strength of each frequency within the series. In Fig. 12.10 the spectrum is given on a log scale. The *frequency* on the horizontal axis tells us how often the cyclical pattern occurs within the data. These patterns are clearer in the smoothed periodogram. The frequencies with largest values occur at $1/12 = 0.0833$ indicating the 12-month cyclical pattern in the data. There are also smaller echoes of the twelve-month cycle occurring at $2/12 = 0.1667$, $3/12 = 0.25$, and so on. We notice how these spectral patterns run parallel for each of the five climate time series.

Smoothing the periodogram cures other problems as well as those seen in Fig. 12.10. The estimate of the spectral density is affected by the abrupt truncation that occurs at the beginning and end of the time series. Collecting more data on a longer series does not improve the situation because a longer series means that there are more Fourier coefficients (\mathbf{a} and \mathbf{b}) to estimate.

We end this section with a simple, graphical diagnostic for examining the presence of periodicity in the data. This can be accomplished using the *cumulative periodogram*, computed using the `cpgram()` function in R. The individual spectral values are divided by the total, so the cumulative sum increases to one. Two examples are given in Fig. 12.11 for the New York City birth rate data.

The cumulative periodogram includes dotted lines that provide a range of values where the white noise should fall. The original birth rate data jumps outside these bounds for low frequencies corresponding to the strong

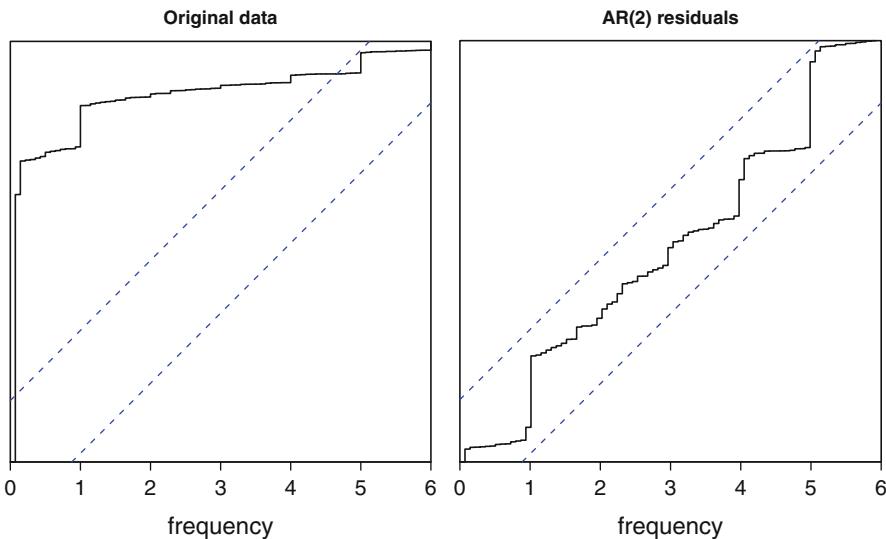


Figure 12.11: Cumulative periodogram of original NYC birth data and residuals from an AR(2) model

annual effects. If we fit an AR(2) model to this data and plot the residuals, then there is good evidence that there is no periodic effect remaining. These figures were produced using the R code:

```
cpgram(NYCTs, main = "Original data")
cpgram(ar(NYCTs, order.max=2)$resid, main = "AR(2)
residuals")
```

In summary, time series data can be analyzed either using autoregressive regression models or through their spectral decomposition. The choice of these two different approaches depends on the summary you want to make. Begin by understanding the process that gave rise to your data and then draw a few plots to motivate your models.

12.4 Exercises

12.1 Reexamine the New York City birth rate data using `stl`.

- (a) Is the loess smoothed seasonal trend more informative than the trend plotted in Fig. 12.3? Or does the loess fit look like one of the moving averages in Fig. 12.4?
- (b) Is there evidence that the periodic component in this series is not stationary? Does a multiplicative model offer a better fit?

- (c) A longer series of all US births is available as `birth` in the `astsa` library. Display the annual periodic component. Is there evidence of a nonstationary property? Can you demonstrate this?
- 12.2 The `prescrip` data in the `TSA` library lists the average US monthly prescription costs between August 1986 and March 1992. Decompose the series into a trend and a cyclical pattern. Can you explain the annual cycle in this data?
- 12.3 The `blood` data set in the `astsa` library is a time series of daily measurements made on one person for 91 days. There are three variables recorded: $\log(\text{white blood count})$, $\log(\text{platelet})$, and hematocrit . There are many missing values, recorded as `NA`, and these increase in frequency towards the end.
- (a) Is there evidence of periodicity in any of the three series?
 - (b) Is there evidence of cross correlation between the series? Does one measurement appear to lead another?
- 12.4 Exercise 9.3 uses linear regression methods to examine multiple time series of personal health care expenditures by Medicare recipients. The data appears in Table 9.3. Use autoregressive models to fit this data. Which method (linear regression or autoregressive) provides a more valid summary of this data? Which method is more consistent with the properties of the sampled data?
- 12.5 The data set `ambientNOxCH` in the `robustbase` library is another environmental time series, providing 366 daily measurements of air quality in 13 different locations in Switzerland. These locations are very different from each other: one is located along a highway, another in urban areas, and one is on an isolated wooded mountain. There are a number of missing values, and linear interpolation between adjacent non-missing values should be a suitable solution to fill these.
- (a) Apply some graphical techniques to this data. Which of these series exhibit seasonal effects? There is only a little more than a year's worth of data, so we will have to assume that seasonal patterns repeat every year. How many of these seasonal patterns appear due to a small number of outlying observations?
 - (b) How do the cross correlations compare with those in Fig. 12.7?
- 12.6 The `boardings` data set in the `TSA` library is a bivariate time series measuring use of public transportation (boardings of bus and light rail services) and gasoline price in the metropolitan Denver, Colorado, region.

- (a) Is there evidence for a seasonal, periodic effect in either of these two series?
- (b) Does the use of public transportation rise and fall with the price of gasoline?
- 12.7 Several of the statistical tests of stationarity available in R include the Phillips–Perron test (`PP.test`), the Kwiatkowski–Phillips–Schmidt–Shin (KPSS) test (`kpss.test`), and the Augmented Dickey–Fuller test (`adf.test`). Some of these embed the fitted model into a more general model, and others examine the spectral decomposition of the data. Apply these to the `boardings` data of the previous exercise and interpret your findings. Does the `boardings` data appear stationary? If not, how does it fail this assumption?

Chapter 13

Other Useful Methods

THIS FINAL CHAPTER provides a collection of useful multivariate methods that do not fit into any of the previous chapters. The Bradley–Terry model gives a way to rank a set of objects that are subjected to pairwise comparisons. Such examples include sports teams that play against each other. Canonical correlations generalize the definition of correlation of a pair of scalar-valued variates to two groups of several variables that are considered jointly. The study of extremes allows us to examine several of the largest values in a collection of data.

13.1 Ranking from Paired Comparisons

We are familiar with rankings. Headlines proclaim the best city to live in or the best university to attend. There is a lot of quantitative data behind such rankings, but, of course, the results depend highly on the relative weights we give to each measurement. Principal components may be helpful, but the interpretation of the weights and loadings may not correspond to any useful sense of ranking the observations.

We can easily rank one-dimensional data. For instance, there is a tallest and a shortest person in the room. We can easily make pairwise comparisons of the heights of any two persons, and the random variability of such a comparison is negligible. We are also familiar with pairwise comparisons between sports teams. At the end of the season we can rank the teams on the basis of their record of wins and losses. Taken to a light-hearted extreme, the website

Table 13.1: Cross citation rates among selected probability journals in 1987–1988

Cited journal	Citing journal					
	AnnPr	PrTh	StochPr	JAppPr	ThPrApp	AnnSt
AnnPr	468	255	33	46	72	74
PrTh	333	322	47	47	72	76
StochPr	208	155	93	76	40	41
JAppPr	121	31	37	283	26	35
ThPrApp	101	60	23	38	344	63
AnnSt	76	81	13	14	50	1009

Source: Stigler (1994). Used with permission

<http://william.hoza.us/rank/> attempts to rank *everything* by means of asking viewers to make pairwise comparisons between two seemingly unrelated things.¹

As a specific example, consider the problem of associating a level of prestige associated with academic journals. Academic faculties need to publish their results and want to have these appear in the highest-impact journals. At the same time, we need a way of performing a pairwise comparison. A solution, presented by Stigler (1994), was to count the number of times articles in one journal cite articles in the other journal. The premise is that a journal that tends to be cited more often is also viewed as the source of the newest and best ideas. There are flaws in this argument, of course, but perhaps we can think of information flowing between the journals. It would be useful to have a measure of the directions of these flows.

The data in Table 13.1 is part of Stigler’s article.² The names of the citing journals are listed as the columns and the names of the journals being cited are the rows. As an example, in 1987–1988, the *Annals of Probability* (AnnPr) was cited 74 times in the *Annals of Statistics* (AnnSt).

In our model of ranking, we will consider the event that journal i is cited by journal j at a greater rate than journal j is cited by journal i . As a shorthand, we will use the notation “ $i > j$ ” to signify that journal i has greater impact than journal j , consistent with our goal of ranking. See Exercise 13.9 for details of this notation.

¹A recent visit to this website asked to viewer to choose between the better of “pig” or “castanet.”

²A smaller subset of Stigler’s data is also available in R as the `citation` data in the `BradleyTerry2` library. The interested reader can build comparisons between other journals and years using *Journal Citation Reports*.

The pairwise comparisons do not allow for *ties*, so we make no provision for the event “ $i = j$ ” where the journals have equal rankings. Similarly, the probability that i beats j is complementary to the probability that j beats i and we have

$$\Pr[i > j] = 1 - \Pr[i < j].$$

A journal that cites itself provides no information in its ranking among others. Let n_i denote the number of citations in journal i to a journal other than itself. A journal with many citations, for example, is more likely to have many citations to other journals, and we need to adjust for this. Similarly, the rate of $i > j$ (versus $i < j$) should be in the ratio n_j/n_i if the citation rates are equal.

Written in another way, we expect

$$\text{logit } \Pr[i > j] = \log(n_j/n_i) \quad (13.1)$$

if the citation rates were the same between the journals i and j .

Recall from (10.1) that the logit is shorthand for “log-odds” so (13.1) models

$$\text{logit } \Pr[i > j] = \log \left\{ \frac{\Pr[i > j]}{1 - \Pr[i > j]} \right\} = \log \left\{ \frac{\Pr[i > j]}{\Pr[i < j]} \right\}.$$

One way to think about (13.1) is to consider a randomly chosen citation between journals i and j . We want to model the probability that this citation represents a citation of journal i by journal j . The number of citations n_i made by journal i counts against it in this competition for ranking and prestige.

Bradley and Terry (1952) proposed a method for modeling comparisons of this type that can also be used for ranking purposes. Suppose the i th journal has a prestige or influence score λ_i that we will estimate. The Bradley–Terry model comparing journals i and j is

$$\text{logit } \Pr[i > j] = \lambda_i - \lambda_j + \log(n_j/n_i), \quad (13.2)$$

after taking into account the marginal number of citations as in model (13.1).

Larger values of λ_i correspond to greater strength in the pairwise comparisons of journal i with all other competitors. Given the estimated values λ_i , we can rank but also assign a relative strength to each journal.

Before we fit the Bradley–Terry model (13.2) in R, let us point out two features of this model. First, notice how we can add a constant to all of the λ s and still obtain the same model. Such a model is said to be *non-identifiable*. A non-identifiable model is one in which different parameter values give rise to the same model.

A simple solution to make model (13.2) identifiable is to arbitrarily set λ_1 equal to zero. Then all λ s are interpreted as comparisons with this item. The item associated with λ_1 is then referred to as the *reference category*. This choice of reference category can be changed in the R program that fits the Bradley–Terry model, as described below.

A second feature of model (13.2) is the inclusion of the $\log(n_j/n_i)$ term. We see that this term is included in the model, but there is no associated parameter to estimate with it. Such a term in a model is called an *offset*. In the present example, the offset adjusts for the different underlying number of citations with no additional estimation necessary.

Output 13.1 shows how we can fit the Bradley–Terry model given in (13.2). This code includes some of the output from R. The `countsToBinomial` routine is a handy feature that converts a contingency table format as in Table 13.1 to a list of all pairwise comparisons. A portion of the output from this routine is given to illustrate this feature. The values `win1` and `win2` list how many times each pair of journals cites each other.

The `BTm` routine fits the model, and the output in Output 13.1 lists the different estimated λ s along with their standard errors and significance levels. The first listed journal, *Annals of Probability* (`AnnPr`), is the reference category and has an assigned $\lambda = 0$ for identifiability.

All of the estimated λ s are negative indicating that the *Annals of Probability* has the highest citation rate. Each successive journal has a lower rates of citation as we read down the list of estimated coefficients in Output 13.1. The third and fourth journals have the word “Applied” in their titles and the last, *Annals of Statistics* (`AnnSt`), is very mathematical but not primarily a journal of research in probability. This conclusion agrees with the finding of Stigler (1994) who reports that the citations of the newest ideas appears to flow from the theoretical journals to the more applied journals and not as much in the other direction.

Exercise 13.10 asks you to compare the citation rates of other statistics journals. Exercise 13.11 shows how we can assign relative strength to different sports teams.

13.2 Canonical Correlations

Correlations are defined between pairs of column vectors of data \mathbf{x} and \mathbf{y} . How can we generalize this concept to the correlation between sets of several columns $\mathbf{X} = \{\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n\}$ and $\mathbf{Y} = \{\mathbf{y}_1, \mathbf{y}_2, \dots, \mathbf{y}_m\}$? As an example, consider the BRFSS health survey data introduced in Sect. 9.3. We want to identify a relationship between several measures of behaviors with several measures of health outcomes. Is there anything we can say about the group of behaviors that have any relationship with the group of health outcomes?

Output 13.1: Program and selected output fitting Bradley–Terry model to journal data

```

> prcite <- read.table(file = "probcite.txt", header =
+   TRUE,
+   row.names = 1)
> prcite <- prcite[-7, -7]      # remove Totals in margins
>                               # number of non-self
  citations
> ns <- colSums(prcite) - diag(as.matrix(prcite))
> library(BradleyTerry2)        # necessary package
> # convert contingency table to list and remove self
  reference
> clist <- countsToBinomial(prcite)
> names(clist)[ 1 : 2] <- c("journal1", "journal2")
> clist

  journal1 journal2 win1 win2
1  AnnPr      PrTh  255  333
2  AnnPr     StochPr   33  208
3  AnnPr     JAppPr   46  121
. . .
14 JAppPr     AnnSt   35   14
15 ThPrApp   AnnSt   63   50

> ni <- ns[match(clist$journal1, names(ns))]
> nj <- ns[match(clist$journal2, names(ns))]
> os <- log(nj / ni)           # offset
> clist <- cbind(clist, os)
>
> fitBTo<- BTm(cbind(win1, win2), journal1, journal2,
+   offset = os, data = clist)
> summary(fitBTo)

.
.
.
Coefficients:
            Estimate Std. Error z value Pr(>|z|)
..PrTh     -0.01349   0.06878 -0.196   0.845
..StochPr  -0.19659   0.10159 -1.935   0.053 .
..JAppPr   -0.71494   0.10458 -6.836 8.13e-12 ***
..ThPrApp  -0.71571   0.09739 -7.349 1.99e-13 ***
..AnnSt    -0.87605   0.09925 -8.826 < 2e-16 ***
---
Signif. codes:  0 *** 0.001 ** 0.01 * 0.05 . 0.1  1

```

The idea of *canonical correlations* is attributed to Hotelling (1935). He proposed methodology to find a pair of weights \mathbf{a} and \mathbf{b} such that the correlation of the linear combinations $\mathbf{a}'\mathbf{X}$ and $\mathbf{b}'\mathbf{Y}$ is maximized.

The values of $\mathbf{a}'\mathbf{x}_i$ and $\mathbf{b}'\mathbf{y}_i$ are called *canonical scores* for the i th individual. These scores serve to reduce this individual's multivariate data $(\mathbf{x}_i, \mathbf{y}_i)$ to a pair of scalars that capture much of the information needed to compute the correlation. The weights \mathbf{a} and \mathbf{b} are the same for every individual and need to be estimated.

This approach is analogous to principal components in which a weighted average of every individual's complete data captures the maximum variability. By further analogy to principal components, there are first, second, and subsequent canonical scores

$$(\mathbf{a}'_1\mathbf{x}_i, \mathbf{b}'_1\mathbf{y}_i), (\mathbf{a}'_2\mathbf{x}_i, \mathbf{b}'_2\mathbf{y}_i), \dots$$

that are highly correlated and also mutually orthogonal with the other canonical scores.

How is this approach different from multivariate linear regression? Multivariate linear regression, described in Sect. 9.2, expresses the mean of each column of \mathbf{Y} as a separate linear combination of the columns in \mathbf{X} resulting in a set of separate regression coefficients. We then examine the set of multivariate residuals in a principal components analysis, looking for additional explanatory value among the \mathbf{Y} after having corrected for the \mathbf{X} .

In canonical correlation, we seek linear combinations of columns in \mathbf{X} and \mathbf{Y} resulting in separate, respective univariate measures that are highly correlated with each other. The idea is to distill all of the linear information in \mathbf{X} and \mathbf{Y} resulting in scalar-valued canonical scores that are highly correlated.

As an example of how we use this method, consider the car data examined in Sect. 9.2. Every car has 11 different attributes, each of which we described as either being a design feature built into the car by the engineers at the factory or else an empirical feature that was readily experienced by the driver.

How can we combine all of the design features and show that these are related to a combination of the driver features? Further, can we assess the relative importance of each of the design features equally important in creating the driver experience? Equivalently, which driver experiences dominate or summarize the others? Which cars appear on different ends of this scale?

The variables in the `mtcars` dataset that we consider as user features are cylinders, displacement, rear axle ratio (drat), forward gears, “v” or straight arrangement of the cylinders. Driver features are miles per gallon, horsepower, weight, 1/4 mile time, and automatic or manual transmission.

The program to compute the canonical correlations and plot loading of first coefficients is given in Output 13.2. The plot of first canonical correlation loadings appears in Fig. 13.1. Two of the extremes are identified. Large luxury cars appear in the lower left corner, and smaller economy cars are

Output 13.2: Program to compute canonical correlations and plot the loadings

```

require(datasets, CCA)
design <- mtcars[ , c(2, 3, 5, 8, 10, 11)]# cyl, disp, carb, drat, gear,vs
driver <- mtcars[ , c(1, 4, 6, 7, 9)]      # mpg, hp, wt, qsec, am

cancor(design, driver)
cc(design, driver)  # CCA package enhancement
ccs <- cc(design, driver)

desc1 <- ccs$scores$xscores[ , 1]
drivcc1 <- ccs$scores$yscores[ , 1]

sdr <- sort(drivcc1)
sdr <- sdr[c(1, length(sdr))]  # first and last
ext <- match(sdr, drivcc1)

plot( desc1, drivcc1,
      xlab = "Design canonical scores",
      ylab = "Driver canonical scores")
text(desc1[ext], drivcc1[ext], labels = rownames(mtcars)[ext],
     pos = c(4, 2), cex = .8)

```

in the upper right. Overall, there is a very high correlation between these scores. These correspond exactly to the first canonical correlation, which we can verify:

```

> cancor(design, driver)$cor
[1] 0.9850787 0.8471577 0.5796657 0.4137175 0.2548956

> cor(desc1, drivcc1)

[1] 0.9850787

```

The additional `$cor` values correspond to the second and subsequent canonical correlations.

We see the canonical correlation scores in Fig. 13.1 correspond, roughly, to the size and weight of the car, the compact Honda Civic in one corner and the Chrysler Imperial in the other. There is some evidence that there are groups of individual cars on this scale. There are four cars located near the Imperial. The other three are Cadillac Fleetwood, Lincoln Continental, and Maserati Bora.

In summary, the canonical correlations can be used similar to the way we used principal components analysis to identify and distinguish between groups of individuals. See Exercise 13.12 for more on this interpretation. In

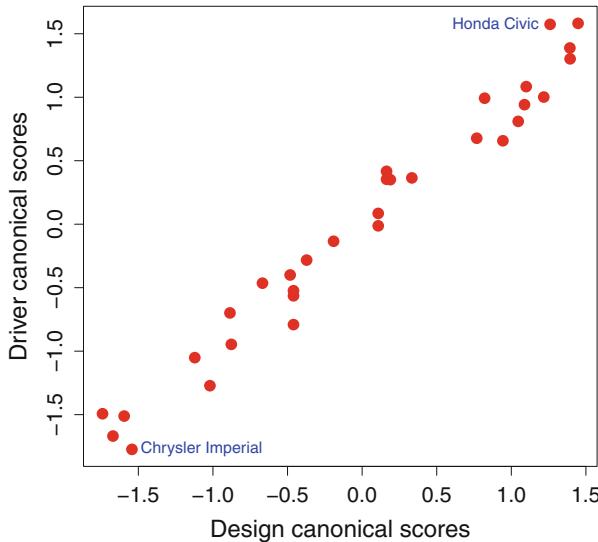


Figure 13.1: Loadings of canonical correlation analysis of car data

the following example, the canonical correlation does not separate individuals well but identifies groups of variables that work together or against each other.

The BRFSS data is introduced and explained in Sect. 9.3. We examined the health characteristics of these US cities in terms of behavioral measures and the corresponding health outcomes. In the present analysis, we will use canonical correlations to find linear combinations of behavior rates that have a high correlation with a linear combination of health outcomes.

The plot of canonical correlations for behaviors and health outcomes is given in Fig. 13.3. The most extreme cities identified in this plot are Provo, Utah, and Arcadia, Florida. These cities are not the same extremes that were identified using multivariate linear regression methods in Sect. 9.3. It is not obvious how these cities are remarkably different. This figure is not entirely useful in that regard. A better summary of this analysis is to examine the weights given to each of the survey questions, as we show next.

The CCA library contains a number of useful enhancements to the basic canonical correlation program offered in R. The `plt.cc` program provides a graphical display of the variable weights that go into each of the first two canonical correlations.

An example of the use of this program is

```
library(CCA)
out <- c(2, 3, 5, 6, 7, 8, 11, 14)  # health outcome variables
beh <- c(1, 4, 9, 10, 12, 13, 15, 16, 17, 18) # behavioral measures
ccs <- cc(BRFSS[,out], BRFSS[,beh])
```

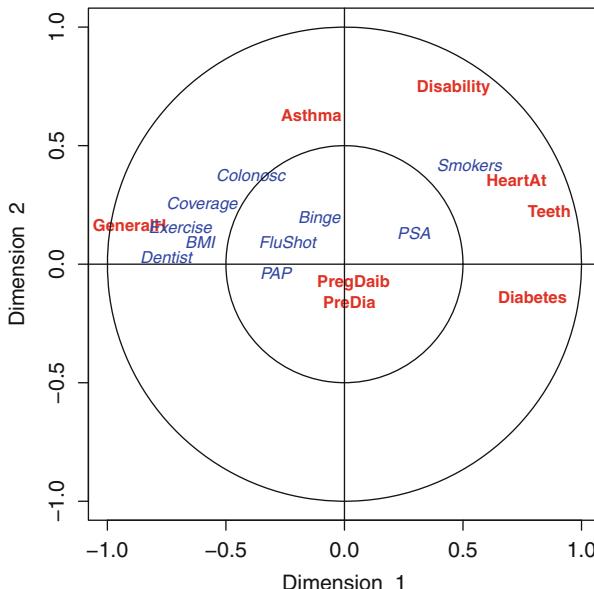


Figure 13.2: Variable weights for the first two canonical correlations in the BRFSS data

```
plt.cc(ccs, d1 = 1, d2 = 2, type = "v", var.label = TRUE)
```

and this code produces Fig. 13.2.

The weights for the first two canonical correlations are plotted in this figure: red for health outcomes and blue for behavioral variables. Variables listed within the inner target have low weight and are generally not useful in performing the canonical correlation. Specifically, the binge drinking, prostate test, flu shot, or PAP test are not useful in describing the canonical score for behaviors. Similarly, pregnancy diabetes or a prediabetic condition are not useful in summarizing health outcomes in a canonical correlation analysis. Health outcomes and behavioral variables appearing in the outer doughnut shape are more important to the canonical correlation summary of this data.

Important behavior measures include visiting a dentist, body mass index, exercise, health care coverage, and smoking. Important health outcomes are general health perception, asthma, and negative weights on each of disability, heart attack, and tooth loss. Notice also that asthma is an important health outcome in the second canonical correlation but not the first. In words, asthma is a separate or *orthogonal* outcome and is different from the others.

In summary, the canonical correlation analysis of multivariate data is useful when all variables can be classified into two groups: driver and design features for the car data, and the behavioral measures and health outcomes

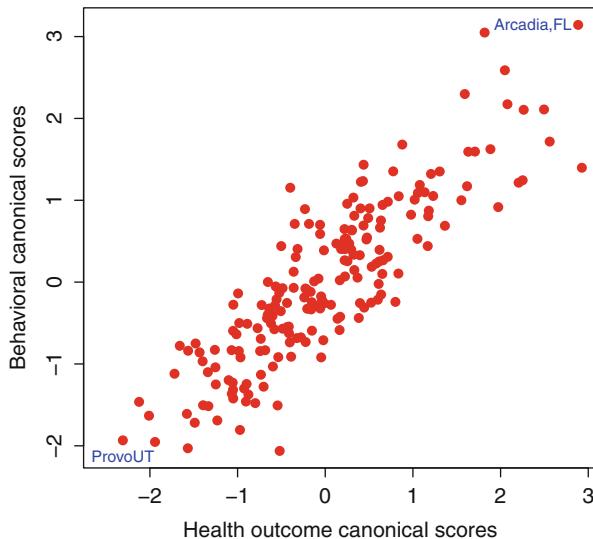


Figure 13.3: Loadings of canonical correlation analysis of BRFSS survey data

for the BRFSS data, for example. The canonical correlation approach creates a linear combination of variables in the separate groups having high correlation with each other. In the car data, we see how canonical correlations can help identify groups of individuals, as in a factor analysis or clustering. In the BRFSS we see canonical correlation can be used to identify variables more (and also less) important in reducing multivariate data into scalar-valued linear combinations or variables.

13.3 Methods for Extreme Order Statistics

Statisticians are prone to looking at measures of central tendency such as the mean or the median. But it is often the extremes in the data grabbing the attention of the public. We talk about the worst flood, instead of the typical rainfall. Headlines shout about the largest clusters of cancer cases, not the average morbidity rate. The extremes cause us to sit up and notice the best and worst of things.

Nobody much cares about the average marathoner's record, for example. In a race, somebody has to be fastest, and we usually only care about the winner. Are the first few finishers so much stronger than the rest of the pack or are they all about the same in their abilities? In athletic endeavors, to continue this example, we may point to one extraordinary individual achieve-

Table 13.2: Largest financial advisors in first half of 2012

Advisor	Number of deals	Value in \$B	Market share in %
Goldman Sachs	190	279	25
Morgan Stanley	170	249	22
JPMorgan Chase	138	221	20
Deutsche Bank	116	214	19
Barclays	146	195	18
Credit Suisse	117	184	17
Citigroup	100	152	14
Bank of America	95	140	13
Lazard	111	116	10
Nomura	89	105	9
Rothschild	116	89	8
BNP Paribas	35	75	7
UBS	82	68	6
RBC	91	53	5
M Klein	1	49	4

Source: NYTimes (July 3, 2012) and Thompson Reuters

ment but then ask whether this one person is much stronger than the second- and third-place finishers. Some runners will finish faster, but do their abilities outshine the others? Is it possible to identify a small number of outstanding athletes whose performance is completely beyond the rest of the pack?

The study of extremes is also tantamount to asking where the tail of the distribution begins. Sometimes we just want to know about the approximate distribution of the single, largest value, but there are situations where the joint, multivariate distribution of several of the largest values is also of interest.

For another example, consider the 15 largest financial advisors, ranked by the value of the deals they brokered in the first half of 2012. The data in Table 13.2 includes the number of merger and acquisition deals brokered and percentage of market share.

It is easy to identify the largest deal-makers, but are their numbers completely out of line relative to the other numbers in this table? After all, some advisory firms have to be the largest. One could argue a firm with familiarity in negotiating large transactions would be best suited for conducting more of the same.

In this section we want to describe a model for the tail behavior of several of the most extreme order statistics. Define $x_{(1)} \geq x_{(2)} \geq \dots$ as the ordered data values, in decreasing order. The usual notation for order statistics is to put the subscripts in parentheses. We do this to distinguish the ordered values from a random list of the data.

Let us introduce some theory for the behavior of extremes. The *stan-*

standardized extreme values z_i are defined as

$$z_i = (x_{(i)} - b)/a$$

for $i = 1, 2, \dots, k$.

These values are ordered $z_1 \geq z_2 \geq \dots \geq z_k$ and standardized by the location parameter b and scale parameter $a > 0$. We will show how to estimate a and b , below.

The literature on extreme order statistics talks about the extreme tail behavior of a distribution in terms of its *domain of attraction*. The domain of attraction is shorthand for how fast the upper tail of the distribution tapers off. Specifically, we will assume the population we are sampling from is in the domain of attraction of the Type I or Gumbel³ distribution. This means that, when properly normalized, z_1 behaves as an observation from the Gumbel distribution with cumulative distribution function

$$F(z) = \exp(-e^{-z}).$$

This assumption holds for a variety of commonly encountered distributions including the normal, gamma, log-gamma, Weibull, and logistic, as well as the Gumbel distribution itself, but not the uniform or Cauchy distributions.

Under the assumption of a Type I domain of attraction, the joint distribution of z_1, z_2, \dots, z_k has an approximate density function

$$f(z_1, z_2, \dots, z_k) = \exp\left(e^{-z_k} - \sum z_i\right) \quad (13.3)$$

for $z_1 \geq z_2 \geq \dots \geq z_k$.

In order for (13.3) to hold, we will also assume the sample size n is very large, but the number of observations in the tail k is modest. It is not necessary to know the value of the full sample, n . In the data of Table 13.2, for example, the full census of all financial advisors is likely to be very large, but we only observe the largest of these. Below, we will also demonstrate a method for estimating the values of k in the data where (13.3) appears to be valid.

When (13.3) holds, the marginal distribution of z_i has density function

$$f_i(z) = \exp\left(-e^{-z} - iz\right)/(i-1)!.$$

Figure 13.4 plots the first five extreme value marginal densities. The largest value z_1 has a skewed distribution. Order statistics, with larger

³Emil Julius Gumbel (1891–1966). German mathematician and political writer.

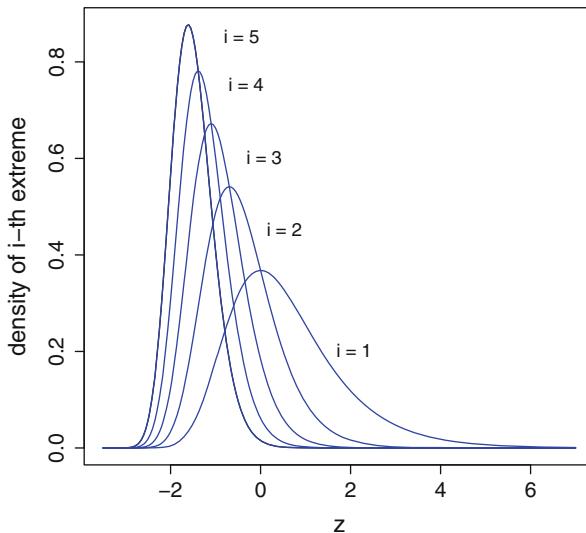


Figure 13.4: The density functions of the first five extremal value distributions

values of i , are nearer the center of the population. Those closer to the center will have less skewed and more nearly normal distributions.

The mean of the marginal distribution z_1 of the largest extremal distribution is γ where

$$\gamma = 0.577216\dots$$

is the *Euler constant*.⁴

The mean of z_i for $i = 2, 3, \dots$ is $\gamma - S_i$ where

$$S_k = 1 + 1/2 + \dots + 1/(k-1).$$

The variance of z_1 is $\pi^2/6$ and the variance of z_i is

$$\pi^2/6 - 1 - 1/2^2 - \dots - 1/(i-1)^2)$$

for $i = 2, 3, \dots$

In words, the mean and variance of extreme order statistics become smaller as we consider order statistics farther below the largest. The distributions farther from the largest are also more symmetric and look

⁴Leonhard Euler (1707–1783). Swiss physicist and mathematician.

more like a normal. We will use these expressions for the means and variances of z_i in the construction of Fig. 13.6, below.

The parameter values for scale a and location b are estimated as follows. Define

$$\bar{x}_k = k^{-1}(x_{(1)} + \cdots + x_{(k)})$$

as the average of the k largest observations.

Then we estimate a as

$$\hat{a}_k = \bar{x}_k - x_{(k)}$$

and

$$\hat{b}_k = \hat{a}_k + k(S_{k-1} - \gamma) + x_{(k)}.$$

The estimates of a and b depend on the choice of k so it is useful to write these estimates as \hat{a}_k and \hat{b}_k .

The discussion so far shows how we can fit models of extremes and describe their approximate density function. We still need a way to determine whether these models are appropriate for our data. A useful approach to studying goodness of fit is to examine the spacings or differences between adjacent ordered values. Spacings were introduced in Sect. 2.5.

Define the *normalized spacings* as

$$d_i = i(x_{(i)} - x_{(i+1)})$$

for $i = 1, 2, \dots, k$.

The theory of extremes (see Weissman 1978, or Zelterman 1993, for examples) is that these normalized spacings will all be approximately independent, and all have the same exponential distribution. The farther out in the tail we go, the farther apart the observations should be from each other. This helps explain the “ i ” multiplier in the definition for d_i .

Several assumptions go into this claim, of course. We need statements about the actual shape of the tail (domain of attraction) of the parent distribution giving rise to x_1, x_2, \dots, x_n . The conditions on the actual shape of the tail are harder to describe in mathematical terms, but usually appear in practice. Next we will show how to estimate the value of k where this approximation works.

Where does the tail of the distribution begin, and what is an appropriate value of k for the data? To answer this question, we will consider a test

for independent, exponentially distributed observations based on the Gini⁵ statistic. Gail and Gastwirth (1978) describe the Gini statistic in this context.

The Gini statistic is

$$G_k = \sum_{i=1}^{k-1} i(k-i) (d_{(i)} - d_{(i+1)}) \Bigg/ (k-1) \sum_i^k d_i . \quad (13.4)$$

This statistic behaves approximately as normal with mean $1/2$ and variance $12(k-1)$ when the spacings d_i are approximately distributed as exponential. Notice there is no need to estimate the mean parameter of these exponential variates. The test of the exponential character of the spacings of the original data is based on the spacings of those spacings. Let us show how to use this statistic to estimate where the tail of the distribution of the xs begins for the corporate asset data.

For each of the $k = 2, 3, \dots, 15$ financial advisors in this dataset, we calculated the Gini statistic G_k and plotted the p-value for each in Fig. 13.5. In this figure, we see the largest 10 values in this dataset jointly follow the model of extreme values but the largest 12 (or more) of these start to fail the assumptions. Even so, there is good evidence in Fig. 13.6 for using all of the extreme data.

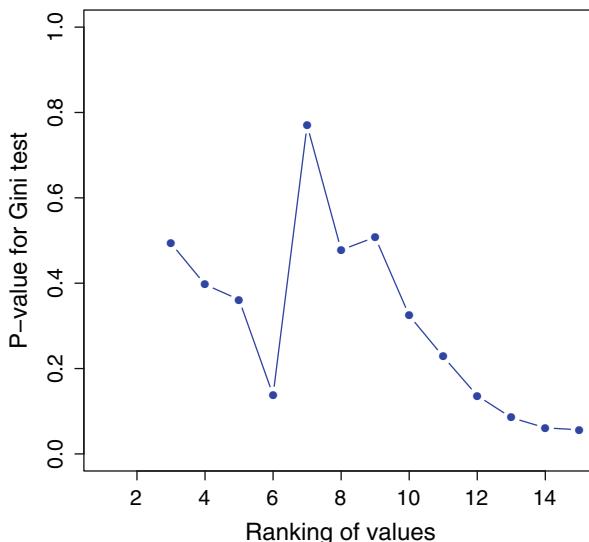


Figure 13.5: p-Values of Gini statistic (13.4) for the deal values in Table 13.2

⁵Corrado Gini (1884–1965). Italian statistician, demographer, and social theorist.

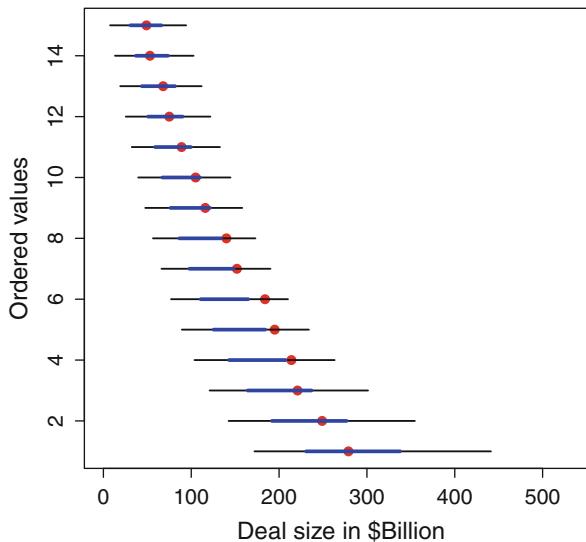


Figure 13.6: Largest financial deals brokered in the first half of 2012 (in *red*) and fitted extreme value distributions. The central 50 % of each distribution is in *blue* and 95 % in *black*

The observed and fitted density functions are displayed in Fig. 13.6. The observed values are given as large red dots in this figure, plotted against their ordered values on the vertical axis. The thin black lines are central 95 % of the marginal (individual) distributions f_i and the thick blue lines are the central 50 %. The ordered values $x_{(i)}$ appear to be where the extreme value distributions would expect them to occur. In summary, the extreme values in this dataset do not appear to be out of line. There are many other companies not listed in this data, and the present sample is within the expectation of the extreme value theory.

In Fig. 13.6 we used all of the data to estimate values of a and b . See Exercise 13.4 for a discussion of the choice of k in estimating these parameters. Other exercises examine extremes in salaries, oil spills, and votes for candidates in a primary election.

13.4 Big Data and Wide Data

As we come to the end of this book, we should ask: Where is all of this going next? The short answer is we are headed towards larger and more massive datasets than were considered in this volume. The advantage of the modest sized datasets considered here is they are useful for illustrating the statistical methods. However, the real application for the methods is to summarize the large datasets being collected today.

Computing power needs to keep up. We should look back at Table 1.7 comparing SAS and R. Perhaps we should have been discussing SAS all along, in order to make use of its data handling capacity. If the data doesn't fit into the software package then of what use is it? There are versions of R being developed to address this shortcoming, but they are arriving late to the party.

Many of the methods described in this book are easily scalable to larger sizes of data. We pointed out histograms and boxplots are scalable but scatterplots are not. Similarly, principal components analysis relies on only data being reduced to a matrix of covariances. If this matrix is not too large, then it doesn't matter how many observations there were in the original data. As another example, we can perform linear regressions because these also only require the covariance matrices. Looking for outliers in these models may be difficult.

Here is an example of the analysis big data has been successful. *Google Flu Trends* follows Internet searches to detect an epidemic. If many people are suddenly searching on the keyword *fever*, for example, then there must be something going around. But Google's search algorithm changes, so one year is not comparable to the searches conducted at the same time in previous years. Even so, commercial gains can be made by exploiting the search algorithm. Pharmaceutical manufacturers may abruptly increase their advertising budget to associate their product with treatment of the flu. Drug companies already have years of experiences with sales of their products so their Bayesian prior knowledge may be as good or better than the search data can tell us.

Big is not necessarily better. We may need to combine large datasets collected at different times, under different conditions. Suppose we had all of the weather data or baseball statistics in one place: Would we be able to make better predictions? Weather forecasting is useful to all of us, but of what purpose would baseball predictions serve, outside of the specialized groups of gamblers or coaches?

Wide data is another interesting development. Instead of a relatively small amount of data collected on each of many patients, medical studies in genetic markers and *micro-arrays* allow us to collect huge amounts of data on a relatively small number of subjects. For each marker, we need to identify the associated genetic pathway. These markers sometimes work in parallel with others, or as a single road block, shutting down the whole process. This suggests the measurements are associated with each other and a priori need to be considered collectively.

The reader who has worked out many of the exercises here has benefited by not being concerned with the huge data cleaning tasks preceding the statistical analysis. The data cleaning and concern for missing values is much more time consuming than setting up and running the computer program summarizing these. What's more, the proper planning for collecting the appropriate data can be quite involved as well.

There is much work yet to be done.

13.5 Exercises

- 13.1 In the housing data of Table 1.1, are the extreme housing prices and apartment rents completely out of line with the remainder of the data? Examine a plot, similar to Fig. 13.6, to make a case whether or not the extremes in Fig. 3.10 could be called outliers.
- 13.2 The dataset `planets` in the HSAUR2 library lists properties of known *exoplanets*. These are known planets which orbit stars other than our sun. The first column is the estimated mass, in multiples of Jupiter. Let us concentrate on the mass values, specifically the largest of these. Is there evidence of *size bias*, meaning only some of the largest exoplanets have been discovered? Or does our current knowledge look more like a representative random sample of what is lurking in outer space? What do we need to assume about the underlying distribution of exoplanet masses? Do the largest of these follow the distributions of extremes?
- 13.3 Table 13.3 lists the sizes of the largest oil spills, along with their dates and locations. The estimated amounts of oil spilled are given in thousands of tons, barrels, and US gallons. Many of these data values are rough estimates. The units may not be precisely convertible from one to another, but are close to being constant multiples of each other. If a range is provided, the midpoint of the interval is given here.
- (a) Use the extreme value methods of Sect. 13.3 to show the largest of these was a far greater environmental disaster than expected, relative to the others on this list.
- (b) If we exclude the single largest of all oil spills, use the Gini statistic (13.4) to show several of the remaining largest spills are not out of line with what we would expect to see. Estimate the number of largest observations following the extremal value distribution.
- 13.4 In Sect. 13.3, how much do the estimates of a_k and b_k depend on the value of k ? Specifically, take the corporate asset data in Table 13.2 and calculate estimates of these two parameters for a range of values of k providing reasonable p-values for the Gini statistic in Fig. 13.6. Describe how these estimates change when the value of k varies. How critical is the value of k when estimating these parameters?
- 13.5 The dataset `schizophrenia` in the HSAUR2 library lists the age at onset of schizophrenia, separately for male and female patients. Show that, overall, the age is skewed but there are no extreme outliers among the oldest and youngest patients. The 15 most extreme observed values in both tails are largely where we would expect them to appear. *Hint:*

Table 13.3: Largest oil spills

Name	Location	Year	Estimated size of spill in thousands		
			Tons	Barrels	Gallons
Kuwaiti oil fires	Kuwait	1991	170,500	1,250,000	32,500,000
Kuwaiti oil lakes	Kuwait	1991	5114	37,500	1,575,000
Lakeview Gusler	California	1910–1911	1200	9000	378,000
Gulf War oil spill	Persian Gulf	1991	955	7000	294,000
Deepwater Horizon	Gulf of Mexico	2010	573	4500	176,000
Ixtoc I	Gulf of Mexico	1979–1980	467	3425	143,829
Atlantic Empress/ Aegean Captain	Trinidad & Tobago	1979	287	2105	88,396
Fergana Valley	Uzbekistan	1992	285	2090	87,780
Nowruz Field	Persian Gulf	1983	260	1907	80,080
ABT Summer	Angola	1991	260	1907	80,080
Castillo de Bellver	South Africa	1983	252	1848	77,616
Amoco Cadiz	France	1978	223	1635	68,684
MT Haven	Italy	1991	144	1056	44,352
Odyssey	Canada	1988	132	968	40,656
Sea Star	Iran	1972	115	843	35,420
Irene's Serenade	Greece	1980	100	733	30,800
Urquiola	Spain	1976	100	733	30,800
Torrey Canyon	UK	1967	100	730	30,660
Greengpoint spill	New York City	1940s	76	555	23,500

Source: Wikipedia

Table 13.4: Highest paid CEOs of nonprofit organizations

Organization	Compensation	Total revenue in \$m	
		Total	Gov't
American Cancer Society	\$1,045,887	429	9
American Heart Association	995,424	645	0
Boys & Girls Clubs of American	988,591	107	41
March of Dimes	627,104	237	10
American Red Cross	455,690	3300	125
Big Brothers, Big Sisters	349,563	33	11
Mothers Against Drunk Driving	256,380	41	9

Source: NYTimes July 27, 2010, page A12

To examine the *lower tail*, we can reverse the tails by transforming the data with a minus sign, as in $70 - \text{age}$.

- 13.6 Table 13.4 lists the highest compensation for the chief executive officer (*CEO*) among all nonprofit groups. Is there evidence the highest paid among these executives is over-compensated? What use can you make of the additional data in this table on total revenue for the organization?
- 13.7 Repeat the analysis of the data in Table 13.2 for the *number* of deals and percent of market share. Do these extreme values seem out of line or consistent with what we would expect of the several most extreme observations?
- 13.8 The New York City mayoral primary was held on September 10, 2013. With 55 % of the precincts reporting, the results for the top candidates in the Democratic Party are given in Table 13.5.
- Fit an extremal distribution to these values. Is there evidence of a group of leaders who received votes far above those of the rest of the “also rans”?
 - The law requires a second, run-off election if no candidate receives 40 % of the vote. At this point in the vote tabulating, what probability can you assign to the need for a runoff?
- 13.9 Consider the notation of ranking academic journals where “ $i > j$ ” means journal i is cited at a greater rate by journal j than journal j is cited by journal i . We can also write $i = j$ if journals i and j cite each other at the same rate. Prove the following relationships, or provide counterexamples:

Table 13.5: Votes earned by the top candidates in a primary election

Candidate	Votes
Bill de Blasio	130,008
Wm C. Thompson Jr.	85,506
Christine C. Quinn	51,059
John C. Liu	27,349
Anthony D. Weiner	17,356
Erick J. Salgado	8470
Randy Credico	6289
Sal F. Albanese	3444
Neil Grimaldi	2757

Source: NY Times

Table 13.6: Cross citation of statistics journals 1987–1989

Citing journal	Cited journal								
	AnnSt	Biocs	Bioka	ComSt	JASA	JRSSB	JRSSC	Tech	Totals
AnnSt	1623	42	275	47	340	179	28	57	2591
Biocs	155	770	419	37	348	163	85	66	2043
Bioka	466	141	714	33	320	284	68	81	2107
ComSt	1025	273	730	425	813	276	94	418	4054
JASA	739	264	498	68	1072	325	104	117	3187
JRSSB	182	60	221	17	142	188	43	27	880
JRSSC	88	134	163	19	145	104	211	62	926
Tech	112	45	147	27	181	116	41	386	1055
Totals	4390	1729	3167	673	3361	1635	674	1214	16,843

Source: Stigler (1994). Used with permission

(a) If $i > j$ and $j > k$ then $i > k$.

(b) If $i = j$ and $j = k$ then $i = k$.

13.10 Table 13.6 summarizes cross citation of statistical journals for the years 1987–1989. Repeat the analysis from Sect. 13.1 for these journals and see if you reach the same conclusion, namely, ideas appear to flow from the theoretical journals to the applied ones. The four most theoretical journals are *Annals of Statistics* (AnnSt), *Biometrika* (Bioka), *Journal of the American Statistical Association* (JASA), and *Journal of the Royal Statistical Society, Series B* (JRSSB). The other four are generally considered to be more applied.

13.11 The `baseball` dataset in the `BradleyTerry2` library contains the win/loss records of seven baseball teams who played each other several

times throughout the 1987 season. Fit a Bradley–Terry model for the paired comparisons in this data and provide a ranking of the teams.

- (a) Is the offset necessary to account for the different number of games played by each team?
- (b) Do the fitted λ s in the Bradley–Terry model coincide with the win–loss records of these teams?
- (c) The data includes an indication of which games were played at home or away. How much of a home-field advantage is there?

13.12 Repeat the canonical correlation analysis of the car data.

- (a) Interpret the loadings for the driver features.
- (b) Perform a principal components analysis for the driver features. Are the loadings comparable to those of the canonical correlations in part a?
- (c) Repeat this comparison for the design features.

Appendix: Libraries Used

Name	First page cited
ape	289
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Selected Solutions and Hints

2.1 Some solutions are

```
c(0 : 10 / 10, 2 : 10)
c(seq(0, 1, .1), 2 : 10)
c(seq(0, 1, .1), seq(2, 10))
```

2.3 (a)

```
mad <- function(x)
{ mean( abs( x - mean(x) ) ) }
```

2.4 The R code

```
> pchisq(1.2, 1) - pchisq(.5, 1)
[1] 0.2061784
```

provides the result.

2.5 All the test scores are very highly correlated with each other. This suggests any one test score is representative of the whole data from each country. See also Exercise 8.7.

2.10 (c) Here are examples of operations resulting in `Inf` and `NaN`. Notice R only produces an error message in the second of these examples but not the third.

```
> 5 / 0
```

```
[1] Inf
```

```

> sqrt(-3)

[1] NaN
Warning message:
In sqrt(-3) : NaNs produced

> 0/0

[1] NaN

```

2.11 A simple solution is

```
spacing(x) <- function(x)  diff(sort(x))
```

Notice this code does not check for empty or a scalar x , situations where spacings are undefined. A somewhat more cryptic definition including the error checking is

```
spacing <- function(x) if(length(x) > 1) diff
  (sort(x)) else NA
```

3.7 This R program draws and peels away five convex hulls.

```

x <- housing$Apartment          # temporary copies of the data
y <- housing$House
plot(x, y, xlab = "Apartment", ylab = "House",
     pch = 19, col = 2, cex = 1.25)  # initial scatterplot
for (i in 1 : 5)                  # number of onion layers
{
  ch <- chull(x, y)            # indices of convex hull
  chl <- c(ch, ch[1])          # loop back to the first point
  lines(x[chl], y[chl], type = "l",
        col = 3)                # draw the layer
  x <- x[ -ch]                 # peel away the layer
  y <- y[ -ch]
}                                # ... and repeat

```

4.3 If \mathbf{y} is a vector of all 1s, then $\mathbf{y}'\mathbf{X}$ is a vector containing the column sums in \mathbf{X} and $\mathbf{X}\mathbf{y}$ (for \mathbf{y} of a possibly different length) are the row sums in \mathbf{X} .

4.6 The matrix inverse is

$$\begin{pmatrix} 1 & -1 \\ -1 & 2 \end{pmatrix}.$$

The eigenvalues are $(3 \pm \sqrt{5})/2$ or approximately 0.382 and 2.618.

5.2 Let U have a uniform distribution between 0 and 1. Then

$$\Pr[U \leq p] = p$$

for any number p , between zero and one. We also have

$$\Pr[U \leq \Phi(z)] = \Phi(z)$$

for any real number z and

$$\Pr[\Phi^{-1}(U) \leq z] = \Phi(z).$$

This shows the distribution of $X = \Phi^{-1}(U)$ has a standard normal distribution.

5.8 Denote the estimate of the mean by $\hat{\mu}$ and standard deviation by $\hat{\sigma}$. Use (5.7) to show the endpoints of the k categories with equal expectations are

$$\begin{aligned} & \{-\infty, \quad \hat{\mu} + \hat{\sigma} \Phi^{-1}(1/k)\} \\ & \{\hat{\mu} + \hat{\sigma} \Phi^{-1}(1/k), \quad \hat{\mu} + \hat{\sigma} \Phi^{-1}(2/k)\} \\ & \quad \vdots \\ & \{\hat{\mu} + \hat{\sigma} \Phi^{-1}((k-1)/(k)), \quad +\infty\}. \end{aligned}$$

6.2 (a) Figure 6.2 was produced using the following R code:

```
corcon <- function(x, y, correl)
{
  nx <- length(x)
  ny <- length(y)
  z <- matrix(rep(0, nx * ny), nx, ny)
  for (i in 1 : nx)
  {
    for (j in 1 : ny)
    {
      z[i,j] <- dmvnorm(c(x[i], y[j]),
      mean = c(0, 0), cov = diag(2))
    }
  }
  if (correl == "correlation")
  {
    z <- cor(z)
  }
  else if (correl == "covariance")
  {
    z <- cov(z)
  }
  else if (correl == "cov")
  {
    z <- cov(z)
  }
  else if (correl == "cor")
  {
    z <- cor(z)
  }
  else
  {
    z <- z
  }
  return(z)
}
```

```

c(0, 0),
  matrix(c(1, correl, correl, 1),
         2, 2)
}
}
return(z)
}

library(mvtnorm)
del <- .05      # how fine the grid
lim <- 3.25      # std normals plotted on +/- lim
par(mfrow = c(2, 4), mar = c(5, 0, 5, 0))  # Four plots across
contour(corcon(seq(-lim, lim, del), seq(-lim, lim, del), -.5),
         xlab = "Corr = -.5",
         drawlabels = FALSE, axes = FALSE, frame = TRUE)
contour(corcon(seq(-lim, lim, del), seq(-lim, lim, del), 0),
         xlab = "Corr = 0",
         drawlabels = FALSE, axes = FALSE, frame = TRUE)
contour(corcon(seq(-lim, lim, del), seq(-lim, lim, del), .5),
         xlab = "Corr = .5",
         drawlabels = FALSE, axes = FALSE, frame = TRUE)
contour(corcon(seq(-lim, lim, del), seq(-lim, lim, del), .9),
         xlab = "Corr = .9",
         drawlabels = FALSE, axes = FALSE, frame =
TRUE)

```

(b) Again, using the `corcon` function, defined above, Fig. 6.3 was drawn using

```

library(MASS,mvtnorm,graphics)
layout(t(matrix(c(1 : 2, rep(0, 2)), 2, 2)), widths = c(1, 1))
del < .025      # how fine the grid
lim <- 1.25      # std normals plotted on +/- lim image(corcon
  (seq( -lim, lim, del), seq( -lim, lim, del), 0.8), axes = FALSE)
del <- .3        # how fine the grid
lim <- 2.7        # std normals plotted on +/- lim
persp(corcon(seq( -lim, lim, del), seq( -lim, lim,
         del), 0.8),
      axes = FALSE, xlab = "", ylab = "", box = FALSE,
      col = "lightblue", shade = .05)

```

6.3 This program generates bivariate normals and transforms these to the shape of Fig. 6.7:

```

quad <- function(n)
{
  quad <- NULL
  for (i in 1 : n)
  {

```

```

x <- rnorm(1)
y <- rnorm(1)
dia <- sqrt(x ^ 2 + y ^ 2)
if(dia > rad)    # outside the circle
{
  if(x > 0) y <- abs(y)
  else y <- -abs(y)
  if(x < 0) y <- -abs(y)
  else y <- abs(y)
}
if(dia < rad)    # inside the circle
{
  if(x > 0) y <- -abs(y)
  else y <- abs(y)
  if(x < 0) y <- abs(y)
  else y <- -abs(y)
}
quad <- rbind(quad, c(x, y))
}
quad
}

```

Some trial and error suggests `rad` should be about 1.83.

6.5 Here is a useful reparameterization and objective function:

```

biv5r <- function(par)  # all five parameter,
  reparameterized
{
  sig1 <- exp(par[3])
  sig2 <- exp(par[4])
  rho <- par[5] / sqrt(1 + par[5] ^ 2)
  cov <- rho * sig1 * sig2
  biv5 <- sum(
    -dmvnorm(cancer, mean = c(par[1], par[2]),
      sigma = matrix(c(sig1 ^ 2, cov, cov, sig2
        ^ 2), 2, 2),
      log = TRUE) )
  print(c(par[1 : 2], sig1, sig2, rho, biv5))
  biv5
}

```

The code

```
nlm(biv5r, c(45, 45, 7.25, 7.25, 2))
```

then estimates the five parameters without warnings.

The estimated value of `par[5]` is 2.053445, so the estimate of ρ is

```
> 2.053445 / sqrt(1 + 2.053445 ^ 2)
[1] 0.8990582
```

- 7.5 Consider an election where citizens cast ballots for one of p different candidates. The data is the number of votes received by each candidate. Any vote for one candidate means fewer votes for all of the others.

- 7.7 (a) This program calculates energy residuals:

```
msqrt <- function(a)
# finds matrix square root of positive definite matrix
{
  a.eig <- eigen(a)           # eigenvalues and eigenvectors of x
  if ( min(a.eig$values) < 0 ) # check for positive definite
    warning("Matrix not positive definite")

  return(a.eig$vectors %*% diag(sqrt(a.eig$values)) %*% t(a.eig$vectors))
}

energy.resid <- function(dat, R=300)
{
  n <- dim(dat)[1]           # observations
  p <- dim(dat)[2]           # variables
  std <- dat - t(matrix(colMeans(dat), p, n))
  s <- var(dat)
  std <- as.matrix(std)  %*% solve(msqrt(s)) # standardized data
  rand <- matrix(rnorm(p * R), R, p) # independent normal data

  A <- rep(0, n)
  B <- rep(0, n)
  for (i in 1 : n)
  {
    a <- 0
    b <- 0
    for (j in 1 : R) a <- a + sqrt(sum((std[i, ] - rand[j, ]) ^ 2))
    A[i] <- a / R           # ave dist between data and random
    for (j in 1:n) b <- b + sqrt(sum((std[i, ] - std[j, ]) ^ 2))
    B[i] <- b / (n - 1)     # ave dist between data
  }
  cc <- 0
  for(i in 2 : R)  for (j in 1 : (i - 1))
    cc <- cc + sqrt(sum((rand[i, ] - rand[j, ]) ^ 2))
  C <- 2 * cc / (R * (R - 1))      # ave dist between
  random values

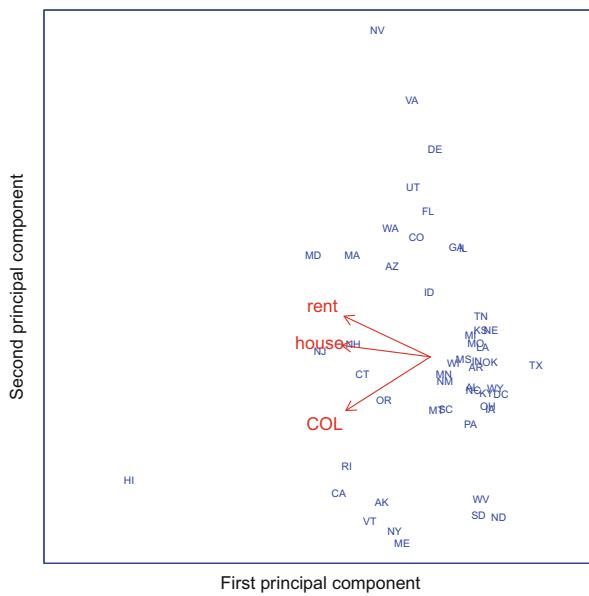
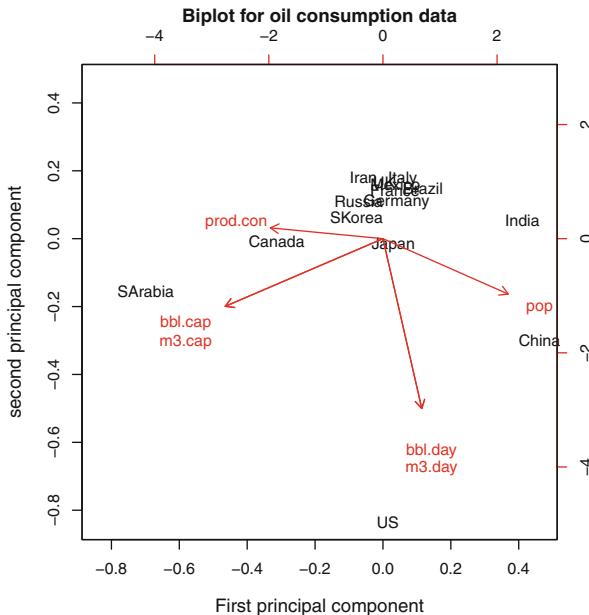
  2 * A - B - C
}
```

- 7.9 This program computes the autocorrelation when columns of the data represent sequential years:

```
autocov <- function(data)
    # Autocorrelation of annual columns in data
{
  nyears <- dim(data)[2] - 1
  autocov <- NULL
  for (lag in 1 : nyears)
  {
    lagcor <- 0
    for (year in 1 : (nyears - lag + 1))
      lagcor <- lagcor + cor(data[, year], data[, year + lag])
    lagcor <- lagcor / (nyears - lag + 1)
    autocov <- c(autocov, lagcor)
  }
  autocov
}

ac <- autocov(CS)
```

- 8.7 The academic scores are highly correlated with each other. Further, these have been standardized. (See Exercise 2.5.) The loadings of the principal components analysis are almost the same for each test score. This suggests any one score is representative for the whole set of values for each country.
- 8.12 The biplot for the correlation matrix of the oil consumption data given in Table 8.4 appears here:
- This figure separates low population, oil producing nations (Saudi Arabia and Canada) from high population, oil consuming nations (India and China).
- 9.1 The biplot of the three-dimensional residuals (given here) shows all dependent variables (cost of living, apartment rents, and house prices) remain highly correlated after correcting for the two explanatory variables (population and average state income). This first principal component explains over 90 % of the total variability. Standout outliers include Hawaii (high rents and house prices) and Nevada (high rents but moderate house prices), both states with low populations.



- 9.4 The mining technology has changed over this time span, as has the number of workers employed in mining and the amount of coal produced. We can't use this data alone as evidence of safer working conditions.

9.5 The R code

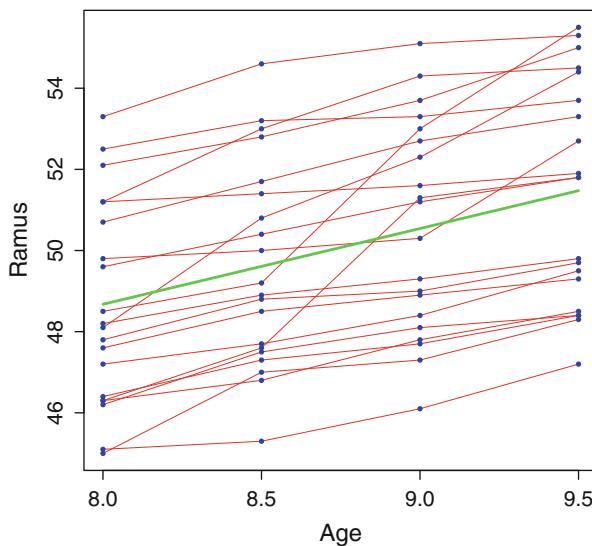
```

jaw <- read.table(file = "Ramus.txt", header = TRUE,
  row.names = 1)
n <- dim(jaw)[1]
plot(x = NA, type = "n", xlim = c(8, 9.5),
  ylim = c(min(jaw), max(jaw)),
  xlab = "Age", ylab = "Ramus")
age <- c(8., 8.5, 9, 9.5 )
longa <- NULL
longj <- NULL
for (i in 1:n)
{
  longa <- c(longa, age)
  ramus <- jaw[i,]
  longj <- c(longj, as.double(ramus))
  lines (age, ramus, col = "red")
}
lines(longa, longj, pch = 16, col = "blue",
  type = "p", cex = .8)
model <- lm(longj ~ longa)
fit <- model$coefficients[1] + model$coefficients[2]
  * age
lines ( age, fit, type = "l", col = "green", lwd = 3)
jres <- jaw - fit                         # residuals
sapply(jres, sd)

  age8    age8_5    age9    age9_5
2.805906 2.897436 2.808309 2.871713

```

produces the spaghetti plot of observed and fitted values:

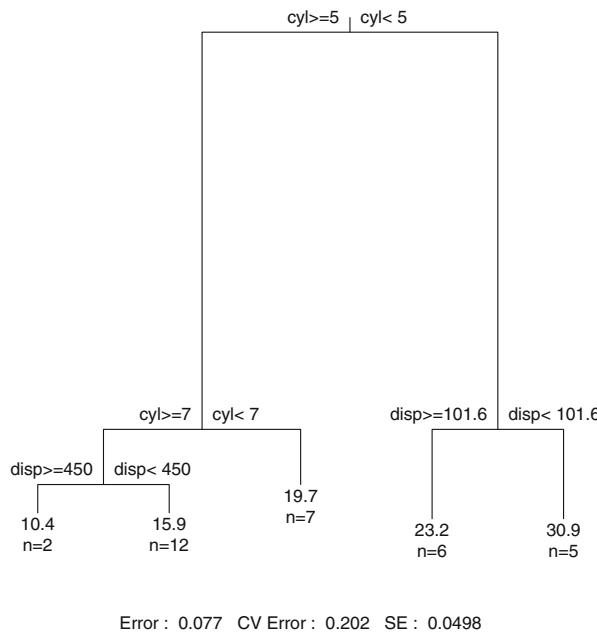


This plot provides good evidence the variances are constant across ages.

10.16 The R code

```
require(mvpart,datasets,graphics)
univ <- mvpart(mpg ~ cyl + disp + am + carb , data = mtcars)
```

produces a regression tree with four leaves:



11.6 (a) The code for clustering and principal components of the milk data

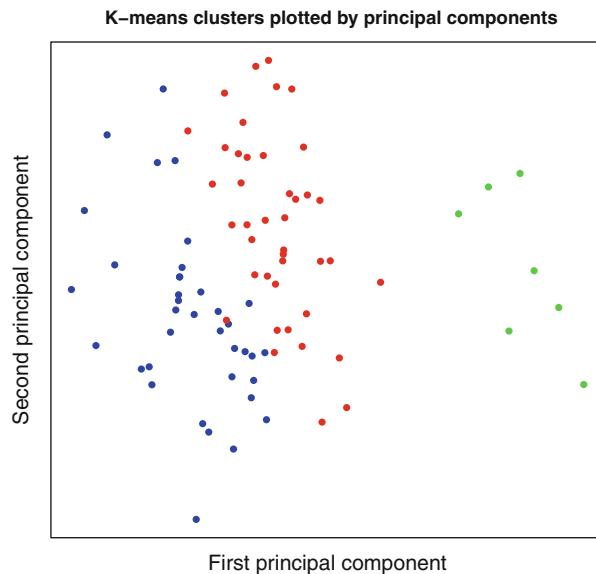
```
library(robustbase)           # library with the milk dataset
milk2 <- milk[ -70 , ]       # omit outlier
colnames(milk2) <- c("dens", "fat", "prot", "casein",
"Fdry",
"Ldry", "drysub", "cheese")# supply new names
# color schemes for K-means
color3 <- rainbow(3)[kmeans(scale(milk2), centers = 3)$cluster]
```

```

pcm <- princomp(milk2, scores = TRUE) # principal
  components
plot(pcm$scores[,1], pcm$scores[, 2], col = color3,
  pch = 16,
  xlab = "First principal component", xaxt = "n",
  yaxt = "n",
  ylab = "Second principal component",
  main = "K-means clusters plotted by principal
  components")

```

produces the figure:



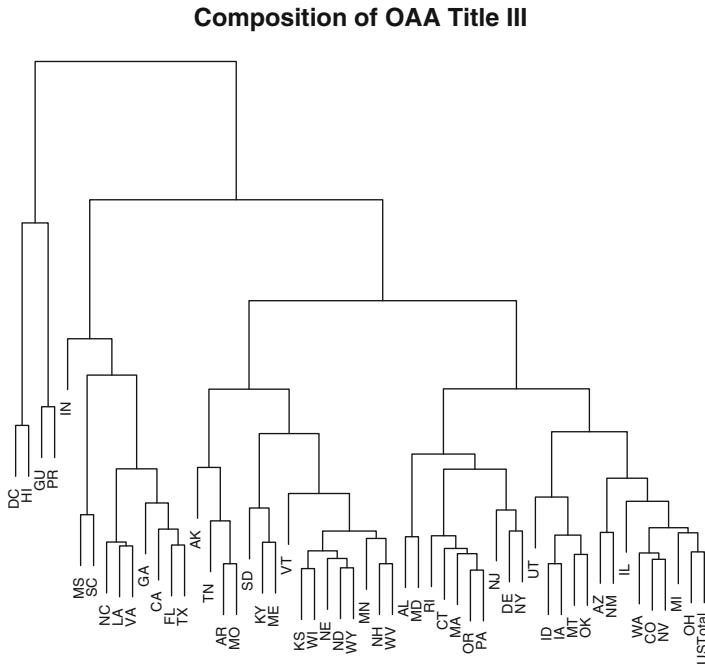
- 11.7 The distribution of X is hypergeometric with probability mass function

$$\Pr[X = x] = \binom{m}{x} \binom{N - m}{m' - x} / \binom{N}{m'}$$

defined for

$$\max(0, m + m' - N) \leq x \leq \min(m, m').$$

11.9 In the hierarchical cluster



we see DC, Puerto Rico, Guam, and Hawaii cluster together, as do New York, New Jersey, and Delaware. Indiana, Illinois, Alaska, Vermont, and Utah each appear different from all other states.

11.10 (b) There are $K = 3$ clusters and the simulation probably alternates between two different pairs of these identified as closest.

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