A HANDBOOK OF

Statistical Analyses using S-Plus

Second Edition

January 18, 2002

Dear Customer:

Thank you for your purchase of *A Handbook of Statistical Analyses using S-Plus* (Cat. #C2808) by Brian S. Everitt.

On the reverse are corrections for two figures. We sincerely regret any inconvenience this may have caused you. Please let us know if we can be of any assistance regarding this title or any other titles that CRC Press publishes.

Best regards,

CRC Press LLC

#C2808/1-58488-280-8

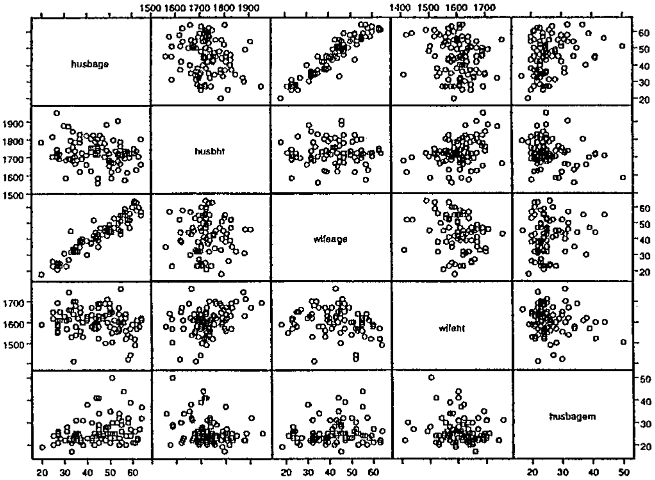


Figure 2.4 Scatterplot matrix for all five variables in the huswif data frame.

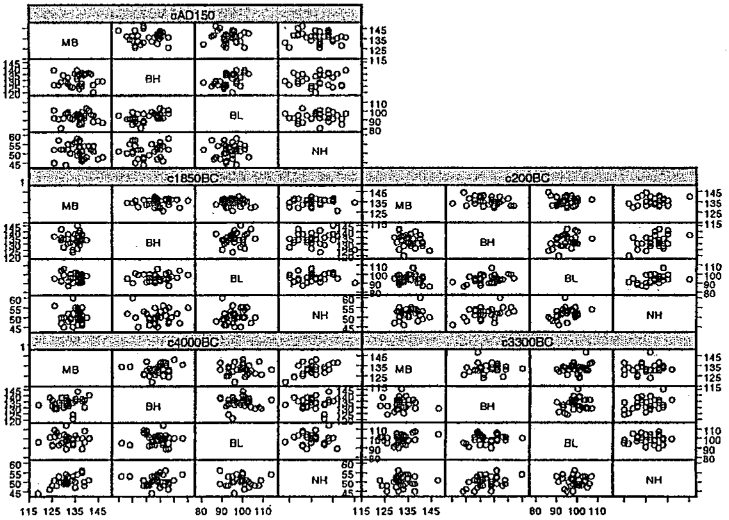


Figure 9.4 Scatterplot matrix of variables in the skulls data frame for each epoch.

A HANDBOOK OF

Statistical Analyses using S-Plus

Second Edition

Brian S. Everitt

CHAPMAN & HALL/CRC
A CRC Press Company
Boca Raton London New York Washington, D.C.

Library of Congress Cataloging-in-Publication Data

Everitt. Brian.
A handbook of statistical analyses using S-PLUS / by Brian S. Everitt.-- 2nd ed.
p. cm.
Includes bibliographical references and index.
ISBN 1-58488-280-8 (alk. paper)
1. Mathematical statistics--Data processing. 2. S-Plus. I. Title.

QA276.4 .E88 2001
519.5′0285--dc21 2001043682

This book contains information obtained from authentic and highly regarded sources. Reprinted material is quoted with permission, and sources are indicated. A wide variety of references are listed. Reasonable efforts have been made to publish reliable data and information, but the author and the publisher cannot assume responsibility for the validity of all materials or for the consequences of their use.

Direct all inquiries to CRC Press LLC, 2000 N.W. Corporate Blvd., Boca Raton, Florida 33431.

No claim to original U.S. Government works
International Standard Book Number 1-58488-280-8
Library of Congress Card Number 2001043682
Printed in the United States of America 1 2 3 4 5 6 7 8 9 0
Printed on acid-free paper

Contents

Preface

Since the first edition of this handbook was published in 1994 the development of S-PLUS has continued apace, and a flexible and convenient "point-and-click" facility has now been added to supplement the very powerful command language. In addition, many new methods of analysis and new graphical procedures have been implemented. The changes made in this second edition reflect these changes in the software. Most chapters have been completely rewritten and many new examples are included. And, some of the more embarassing code from the first edition are now excluded. A mixture of the S-PLUS command language and the S-PLUS Graphical User Interface (GUI) is used throughout the book so that readers can become familiar with using both. An appendix gives a relatively concise account of the command language.

It is hoped that this new edition will prove useful to applied statisticians, statistics students, and researchers in many disciplines who wish to learn about the many exciting possibilities for dealing with data presented by the latest versions of S-PLUS, S-PLUS 2000, and S-PLUS 6. All the data sets used in the text are available in the form of S-PLUS data frames from:

www.iop.kcl.ac.uk/IoP/Departments/BioComp/SPLUS.stm

Script files giving the command language used in each chapter are also available from the same address. (Comments given in the text versions are not included in these files.)

Thanks are due to Ms. Harriet Meteyard for her typing of the manuscript and general support during the writing of this book.

B.S. Everitt
June 2001

Distributors for S-PLUS

In the United Kingdom, S-PLUS is distributed by

Insightful
Knightway House
Park Street
Bagshot, Surrey
GUl9 5AQ
United Kingdom
Tel: +44 (0) 1276 450 111
Fax: +44 (0) 1276 451 224
sales@uk.insightful.com

In the United States. the distributors are

Insightful Corporation
1700 Westlake Avenue North
Suite 500
Seattle, WA 98109-3044
USA
Tel: (206) 283-8802
Fax: (206) 283-8691
infoQinsightful.com
Web address: www.insightful.com

Dedication

To my daughters, Joanna and Rachel and
my grandsons, Hywel and Dafydd

Chapter 1

An Introduction to S-PLUS

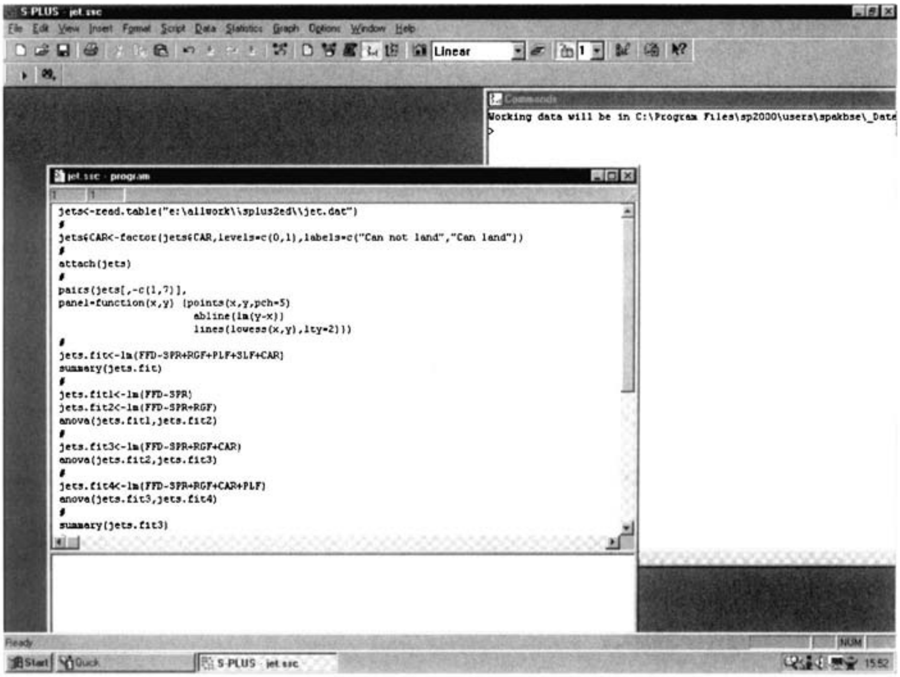
1.1 Introduction

S-PLUS is a language designed for data analysis and graphics developed at AT&T's Bell Laboratories. It is described in detail in Becker et al. (1988), Chambers and Hastie (1993), Venables and Ripley (1997), and Krause and Olson (2000). In addition to providing a powerful language, the most recent versions of the software, S-PLUS 2000 and S-PLUS 6, also include an extensive graphical user interface (GUI) on Windows platforms (this is not available in UNIX). The GUI allows routine (and some not so routine) analyses to be carried out by simply completing various "dialog boxes," and graphs to be produced and edited by a "point-and-click" approach.

In this chapter we introduce both the GUI and the command line language, although details of the former will be left for the remaining chapters of the book, and of the latter, for Appendix A.

1.2 Running S-PLUS

On a Windows platform S-PLUS is opened by double-clicking into the file (or shortcut for) S-PLUS.exe. The result is an S-PLUS window containing a Commands window and/or an Object Explorer window. During an S-PLUS session, Graphics windows may be opened and often output will



```
Working data will be in C:\Program Files\sp2000\users\spakbse\_Data
>
```

```
jets<-read.table("e:\allwork\\splus2ed\\jet.dat")
#
jets$CAR<-factor(jets$CAR,levels=c(0,1),labels=c("Can not land","Can land"))
#
attach(jets)
#
pairs(jets[,-c(1,7)],
panel=function(x,y) {points(x,y,pch=5)
                     abline(lm(y~x))
                     lines(lowess(x,y),lty=2)})
#
jets.fit<-lm(FFD~SPR+RGF+PLF+SLF+CAR)
summary(jets.fit)
#
jets.fit1<-lm(FFD~SPR)
jets.fit2<-lm(FFD~SPR+RGF)
anova(jets.fit1,jets.fit2)
#
jets.fit3<-lm(FFD~SPR+RGF+CAR)
anova(jets.fit2,jets.fit3)
#
jets.fit4<-lm(FFD~SPR+RGF+CAR+PLF)
anova(jets.fit3,jets.fit4)
#
summary(jets.fit3)
```

Figure 1.1 Windows seen during a typical S-PLUS session: Command window and script file are shown.

be sent to a Report window, this being opened by changing the default for text output routing in the Options list. The windows seen in a typical S-PLUS session are shown in Figure 1.1. At the top, below the S-PLUS title bar, is the menu bar. On the line below that is the tool bar.

S-PLUS provides a language for the manipulation of ‘objects’ such as vectors and matrices; commands can be typed into the Commands window next to the > prompt, and any resulting output will appear below, also in the Commands window, unless the Report window option has been selected. If a single command extends over one line of input, the > prompt changes to the plus sign, +. The contents of S-PLUS objects may be viewed by simply typing the name of the object.

The Object Explorer window displays objects of the current session by object category. This window can be opened by clicking into

At the end of a session, the user can select which objects created within the session should be saved within the 'current directory' or database. By default, this is the _data subdirectory of the directory where the S-PLUS files are located, for example, in C:\Program Files\sp6_data. The command search lists the current directory under [1].

Since it is usually preferable to keep the data for different projects in different directories, it is a good idea to start an S-PLUS session by setting the directory in which any objects are to be saved and which may contain relevant objects from a previous session. This is done by 'attaching' the directory at the first position of the search path using the command:

```
>attach("c:/project/_data",pos=1)
```

Note that forward slashes are used in the directory path rather than the usual backward slashes. Alternatively, two backward slashes may also be used.

1.3 The S-PLUS GUI: An Introduction

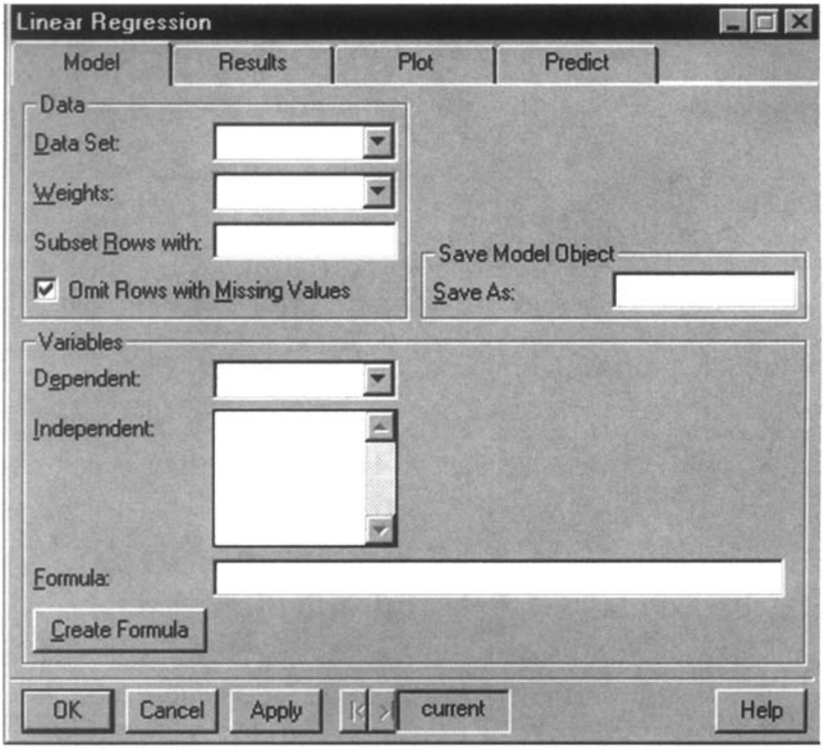
Use of the GUI involves menus, dialog boxes, and point-and-click graphics. For example, many statistical techniques can be applied in S-PLUS by using the **Statistics Menu** and then filling in the relevant dialog box. These boxes have many features in common as we shall see throughout the text. As an example we can look at the **Linear Regression** dialog. This is made available as follows;

- Click on **Statistics**.
- Select **Regression**.
- Select **Linear**.

The resulting dialog is shown in Figure 1.2.

To use the box to carry out a regression analysis would involve filling in the various sections of the box and requesting various options under the **Results**, **Plot**, or **Predict** tabs, as we shall illustrate in detail in Chapter 4.

The GUI approach to producing S-PLUS graphics is extensive and flexible, and can involve either the use of dialog boxes from the **Graphics Menu**, or the **Graphics palettes**. For example, to access the **Scatter Plot** dialog, click on **Graph** in the tools bar, select **2D** and **Scatter Plot** is highlighted by default. Click **OK** and the dialog box shown in Figure 1.3 appears.



☑ Omit Rows with Missing Values

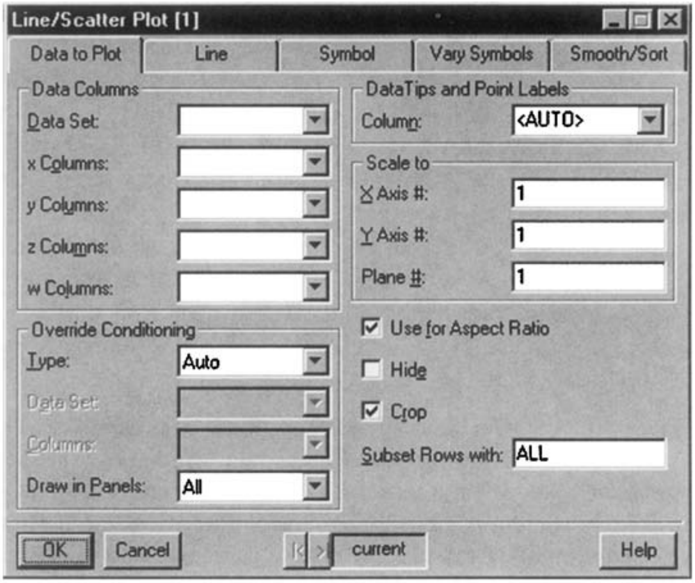
Figure 1.2 Linear Regression dialog.

Again, to use the box to produce a scatterplot would involve filling out the box appropriately; examples will be given in later chapters.

The 2D and 3D palettes are accessed by clicking on

or

respectively, and are shown in Figure 1.4. These can be used after selecting the required data set, to give a wide variety of graphics as we shall illustrate later.



Line/Scatter Plot [1]

Data to Plot | Line | Symbol | Vary Symbols | Smooth/Sort

Data Columns

Data Set:

x Columns:

y Columns:

z Columns:

w Columns:

DataTips and Point Labels

Column: <AUTO>

Scale to

X Axis #: 1

Y Axis #: 1

Plane #: 1

Override Conditioning

Type: Auto

Data Set:

Columns:

Draw in Panels: All

☑ Use for Aspect Ratio

□ Hide

☑ Crop

Subset Rows with: ALL

Figure 1.3 Line/Scatter Plot dialog.

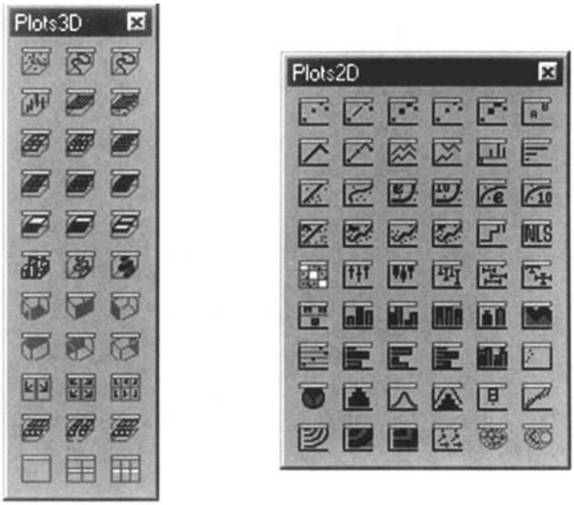


Figure 1.4 2D and 3D graphical palettes.

1.4 The S-PLUS Command Language: An Introduction

Although many users of S-PLUS will find its relatively recent GUI both convenient and sufficient for the analyses they require, it is the command language that remains the main reason that the software is so powerful and flexible. Familiarity with this aspect of S-PLUS enables customised analyses to be carried out relatively simply as we shall illustrate in later chapters. The differences between the GUI and the command language approaches and the advantages of the latter are nicely summarized in the following remarks made by a statistician who has been involved with computers for over 40 years, John Nelder:

> I am very much aware that for the modern student the menu mode is the one preferred, and indeed the only one known. I am, however, not convinced that the menu mode is optimum for all users or for all usages. The freedom of being able to say what you want, instead of responding to given lists, is to me worth having. Imagine how restrictive conversation would be, if instead of making your own points for yourself, you were restricted to pointing at sets of alternatives defined by the person you were talking to. The frustrations would soon become apparent.

In this section we shall simply introduce a few of the most important features of the S-PLUS command language, leaving a more detailed account to be given in Appendix A.

1.4.1 Elementary Commands

Elementary commands consist of either expressions or assignments. For example, typing the expression

```
>42+8
```

in the commands window and pressing return will produce the following output

```
[1] 50
```

Instead of evaluating just an expression, we can assign the value to a scalar, for example,

```
>x<-42+8
>x
[1] 50
```

1.4.2 Vectors and Matrices

Vectors may be created in several ways, the most common is via the concatenate function, c, which combines all values given as arguments to the function as a vector

```
>x<-c(1,2,3,4)
>x
[1] 1 2 3 4
```

(Note that S-PLUS is case sensitive, *x* and X, for example, are regarded as different objects.)

Arithmetic operations between two vectors return a vector whose elements are the results of applying the operation to the corresponding elements of the original vectors. We can also apply mathematical functions to vectors; the functions are simply applied to each element of the vector

```
>x<-c(1,2,3)
>y<-c(4,9,16)
>x*y
[1] 4 18 48
>sqrt(y)
[1] 2 3 4
```

Matrix objects are frequently needed in S-PLUS and can be created by use of the matrix function. For details of this function see Appendix A or use help(matrix) in S-PLUS. (Similar help files are available for all S-PLUS functions.)

```
>x<-c(1,2,3)
>y<-c(4,5,6)
>xy<-matrix(c(x,y),nrow=2)
>xy

        [,1]   [,2]   [,3]
[1,]     1      3      5
[2,]     2      4      6
```

1.4.3 Subsetting Matrices and Vectors

S-PLUS has two logical values, T (true) and F (false), and a number of logical operations that are extremely useful in choosing particular elements from vectors and matrices. (The logical operations are listed in Appendix A.) We can use a logical operator to assign logical values:

```
>x<-3==4
>x
[1] F

>x<-3<4
>x
[1] T

>x<-c(1,2,3,4,5)
>x<4
[1] T T T F F
```

A logical vector can be used to extract a subset of elements from another vector as follows:

```
>x[x<4]
[1] 1 2 3
```

Here the elements of the vector less than 4 are selected as the values corresponding to T in the vector *x*.

We can also select elements in *x* depending on the values in another vector *y*

```
>x<-c(1,2,3,4,5,6,7,8,9,10)
>y<-c(0,0,6,4,3,1,0,0,1,0)
>x[y==0]

[1] 1 2 7 8 10
```

1.4.4 Other S-PLUS Objects

A number of other important S-PLUS objects are mentioned briefly here and in detail in Appendix A. First list objects that allow other S-PLUS objects to be linked together, for example,

```
>x<-c(1,2,3)
>y<-matrix(c(1,2,3,4),nrow=2)
>xylist<-list(x,y)
>xylist
```

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

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

>xylist$x
[1] 1 2 3
```

Note the two alternatives for referring to elements in a list; either the 'double bracket' nomenclature or the **$name** nomenclature can be used.

Secondly, data frames that allow numerical and character vectors to be bound together are the most useful way of storing sets of data. Creating a data frame is described in detail in Appendix A, but as a simple example:

```
>height<-c(50,60,70)
>weight<-c(100,120,140)
>age<-c(20,40,60)
>names<-c("Bob","Ted","Alice")
>data<-data.frame(names,age,height,weight)
>data

     names   age   height   weight
1     Bob     20     50      100
2     Ted     40     60      120
3     Alice   60     70      140
```

A data frame can be used in S-PLUS by first 'attaching' it, using

```
>attach(data)
```

In this way, variables in the data frame can now be conveniently referred to by name.

```
>age
[1] 20 40 60
```

The S-PLUS language also provides the facility for creating functions for specific analyses of interest. Details are given in Appendix A and examples will be given in subsequent chapters.

Although commands can be typed into the commands window, it is far more convenient to use a **script file** (*.ssc), which is an ASCII text file that may be opened within S-PLUS to build up and keep a sequence of commands being used to analyse a particular data set, or indeed several data sets. In this way an entire analysis can be repeated at the press of a button if necessary, for example, if a data entry error is detected. The whole script file may be executed by selecting **Script** and **Run** from the menu bar or by pressing **F10**. Alternatively, one or more commands may be selected and run by highlighting the relevant text within the Script file and pressing the triangle insert button,

Script files can be commented by using the hash symbol, #, at the beginning of a line of text; S-PLUS ignores such lines. (In all but this chapter and Appendix A, we shall assume that commands are being run from a script file and, therefore, will dispense with the > before each command seen when using the commands window.) To open a script file, click on **File** in the menu bar, select **New**, and then highlight **Script File** in the list that appears.

1.5 An Example of an S-PLUS Session

As with any software, the easiest way to learn about S-PLUS is to use it, and this section attempts to give readers a preview of how S-PLUS is used in practice, which they can follow before reaching the more demanding material in subsequent chapters. Here we shall use both the GUI and the command language approaches to carry out some relatively straightforward analyses of the data shown in Table 1.1, which were originally given in Stanley and Miller (1979) and are also reproduced in Hand et al. (1994). (A more-detailed analysis of these data will be made in Chapter 4.)

We shall assume that the data in Table 1.1 are already available as an S-PLUS data frame object, `jets`. Details of data frames and how they are created from the raw data are given in Appendix A. By typing `jets` in the command window and hitting return its contents will be displayed — see Table 1.2. Initially it is sensible to attach the data frame using

```
>attach(jets)
```

To begin learning about the data we might want to look at some suitable summary statistics for each variable; for this we can use the S-PLUS `summary` function.

```
>summary(jets)
```

Table 1.1 Data on Jet Fighters

	Type	FFD	SPR	RGF	PLF	SLF	CAR
1	FH-1	82	1.468	3.30	0.166	0.10	0
2	FJ-1	89	1.605	3.64	0.154	0.10	0
3	F-86A	101	2.168	4.87	0.177	2.90	1
4	F9F-2	107	2.054	4.72	0.275	1.10	0
5	F-94A	115	2.467	4.11	0.298	1.00	1
6	F3D-1	122	1.294	3.75	0.150	0.90	0
7	F-89A	127	2.183	3.97	0.000	2.40	1
8	XF10F-1	137	2.426	4.65	0.117	1.80	0
9	F9F-6	147	2.607	3.84	0.155	2.30	0
10	F-100A	166	4.567	4.92	0.138	3.20	1
11	F4D-1	174	4.588	3.82	0.249	3.50	0
12	F1F-1	175	3.618	4.32	0.143	2.80	0
13	F-101A	177	5.855	4.53	0.172	2.50	1
14	F3H-2	184	2.898	4.48	0.178	3.00	0
15	F-102A	187	3.880	5.39	0.101	3.00	1
16	F-8A	189	0.455	4.99	0.008	2.64	0
17	F-104B	194	8.088	4.50	0.251	2.70	1
18	F-105B	197	6.502	5.20	0.366	2.90	1
19	YF-107A	201	6.081	5.65	0.106	2.90	1
20	F-106A	204	7.105	5.40	0.089	3.20	1
21	F-4B	255	8.548	4.20	0.222	2.90	0
22	F-111A	328	6.321	6.45	0.187	2.00	1

FFD first flight date, in month after January 1940
SPR specific power, proportional to power per unit weight
RGF flight range factor
PLF payload as a fraction of gross weight of aircraft
SLF sustained load factor
CAR a binary variable that takes the value 1 if the aircraft can land on a carrier, and 0 otherwise.

The output resulting from these commands is shown in Table 1.3. (Like many S-PLUS functions, summary is generic, meaning that it can be used to process many different classes of data and give results appropriate to each particular class. Further examples will be given in subsequent chapters.)

Summary statistics for the data in jets can also be found by using the GUI as follows:

- Click **Statistics**.
- Select **Data Summaries**.
- Select **Summary Statistics**.

Table 1.2 The Jets Data Frame

```
> jets
       Type  FFD    SPR   RGF    PLF   SLF         CAR
 1     FH-1   82  1.468  3.30  0.166  0.10 Cannot land
 2     FJ-1   89  1.605  3.64  0.154  0.10 Cannot land
 3    F-86A  101  2.168  4.87  0.177  2.90    Can land
 4    F9F-2  107  2.054  4.72  0.275  1.10 Cannot land
 5    F-94A  115  2.467  4.11  0.298  1.00    Can land
 6    F3D-1  122  1.294  3.75  0.150  0.90 Cannot land
 7    F-89A  127  2.183  3.97  0.000  2.40    Can land
 8  XF10F-1  137  2.426  4.65  0.117  1.80 Cannot land
 9    F9F-6  147  2.607  3.84  0.155  2.30 Cannot land
10   F-100A  166  4.567  4.92  0.138  3.20    Can land
11    F4D-1  174  4.588  3.82  0.249  3.50 Cannot land
12    F1F-1  175  3.618  4.32  0.143  2.80 Cannot land
13   F-101A  177  5.855  4.53  0.172  2.50    Can land
14    F3H-2  184  2.898  4.48  0.178  3.00 Cannot land
15   F-102A  187  3.880  5.39  0.101  3.00    Can land
16     F-8A  189  0.455  4.99  0.008  2.64 Cannot land
17   F-104B  194  8.088  4.50  0.251  2.70    Can land
18   F-105B  197  6.502  5.20  0.366  2.90    Can land
19  YF-107A  201  6.081  5.65  0.106  2.90    Can land
20   F-106A  204  7.105  5.40  0.089  3.20    Can land
21     F-4B  255  8.548  4.20  0.222  2.90 Cannot land
22   F-111A  328  6.321  6.45  0.187  2.00    Can land
```

The dialog box shown in Figure 1.5 appears. In the **Data Set** window choose **jets,** highlight all but **Type** in the **Variables** window and click **OK**; the results shown in Table 1.4 appear in a Report file which might be printed or copied and pasted into another application.

Perhaps separate summary statistics are required for the class of fighters that can land on a carrier and those that cannot. If so, they can be obtained by highlighting all but CAR in the **Variables** section of the **Summary Statistics** dialog and then highlighting **CAR** and **Type** in the **Group Variables** section. This leads to the results shown in Table 1.5. (Other summary statistics, for example, measures of *skewness* and *kurtosis*, can be requested simply by clicking on the **Statistics** tab of the **Summary Statistics** dialog.)

A t-test for the difference in the population mean values of, say, the variable FFD for planes that can land and cannot land on a carrier can be calculated using the **Two-sample t-test dialog** which is accessed as follows:

Table 1.3 Summary Statistics for the Jet Fighter Data

Type	*FFD*	*SPR*	*RGF*
YF-107A: 1	Min.: 82.0	Min.:0.455	Min.:3.300
XF10F-1: 1	1st Qu.:123.2	1st Qu.:2.172	1st Qu.:4.005
FJ-1: 1	Median:174.5	Median:3.258	Median:4.515
FH-1: 1	Mean:166.3	Mean:3.944	Mean:4.577
F9F-6: 1	3rd Qu.:192.8	3rd Qu.:6.025	3rd Qu.:4.972
F9F-2: 1	Max.:328.0	Max.:8.548	Max.:6.450
(Other):16			

PLF	*SLF*	*CAR*
Min.:0.0000	Min.:0.100	Cannot land:11
1st Qu.:0.1223	1st Qu.:1.850	Can land:11
Median:0.1605	Median:2.670	
Mean:0.1683	Mean:2.265	
3rd Qu.:0.2132	3rd Qu.:2.900	
Max.:0.3660	Max.:3.500	

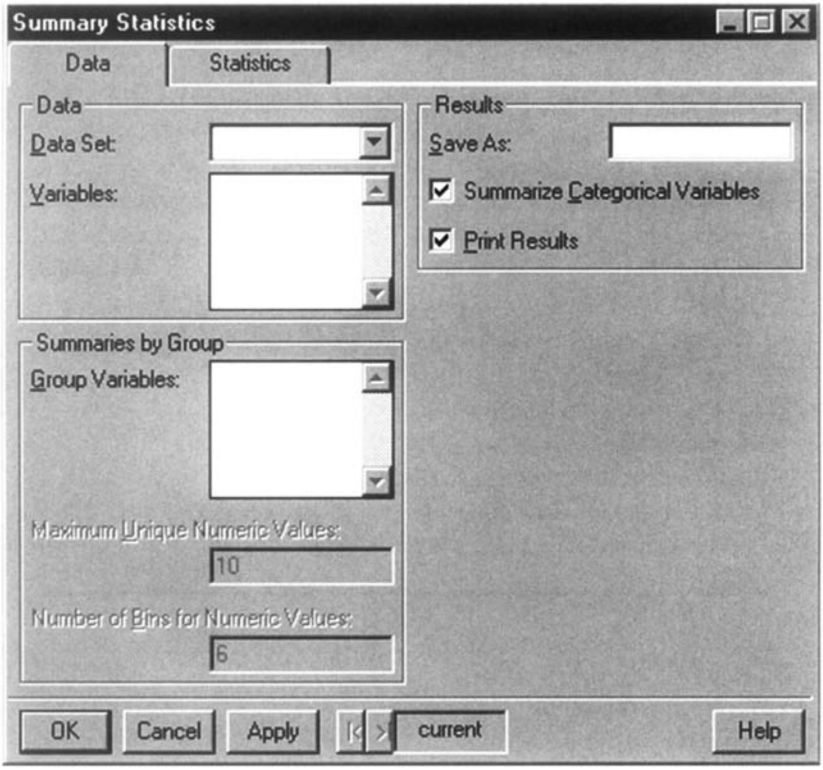
- Click on **Statistics**.
- Select **Compare Samples**.
- Select **Two Samples, t test**.

Again select the **jets** data set, highlight **FFD** as Variable 1 and **CAR** as Variable 2, then tick the button that shows Variable 2 as a **Grouping variable**. The results shown in Table 1.6 appear in a Report file. (With such a small sample it may be more appropriate to use the Wilcoxon rank sum test rather than the t-test; we leave this as an exercise for the reader since the steps are essentially identical to those described above.) With the command language, the same results can be found using

```
>t.test(FFD[CAR==“Can Land”],FFD[CAR==“Cannot land”]
```

Graphics are an essential component in the analysis of any data set, and a vast range of graphics are available when using S-PLUS, as we shall see in subsequent chapters. Here, however, we consider only the construction of a simple scatterplot. Using the GUI, we proceed as follows:

- Click on **Graph**.
- Select **2D Plot**.



☑ Summarize Categorical Variables

☑ Print Results

Maximum Unique Numeric Values: 10

Number of Bins for Numeric Values: 6

Figure 1.5 Summary Statistics dialog.

The **Insert Graph** menu appears. Since **Scatter Plot** is highlighted by default, simply click **OK** to arrive at the **Line/Scatter Plot** dialog. Select the **jets** data set and, say, **SPR** as the *x* column (the '*x* variable') and **FFD** as the *y* column (the '*y* variable'). Click **OK** to see the scatterplot of these two variables shown here in Figure 1.6. A more interesting scatterplot would be one with the points labelled by type of aircraft. This can again be constructed from the **Line/Scatter Plot dialog.**

We first repeat the steps used to obtain Figure 1.7, but now also select **Type** in the *z* Columns box, and then click the **Symbol** tab of the dialog. Tick **Use Text As Symbol** and in the **Text to Use** box select *z* column. The height of the plotting symbol might also be increased to, say, 0.15. Clicking **OK** now produces the scatterplot shown in Figure 1.7.

Finally, it might be useful to have Figure 1.8 alongside the corresponding scatterplot in which the points are labelled by whether the aircraft can or cannot land on a carrier. This diagram is obtained as follows:

Table 1.4 Summary Statistics for Jet Fighter Data

```
        *** Summary Statistics for data in: jets ***

       $$$"Factor Summaries":
              CAR
 Cannot land:11
    Can land:11

       $$$"Numeric Summaries":
                  FFD        SPR         RGF          PLF        SLF
      Min:   82.00000   0.455000   3.3000000   0.00000000   0.100000
  1st Qu.:  123.25000   2.171750   4.0050000   0.12225000   1.850000
     Mean:  166.27273   3.944455   4.5772727   0.16827273   2.265455
   Median:  174.50000   3.258000   4.5150000   0.16050000   2.670000
  3rd Qu.:  192.75000   6.024500   4.9725000   0.21325000   2.900000
      Max:  328.00000   8.548000   6.4500000   0.36600000   3.500000
  Total N:   22.00000  22.000000  22.0000000  22.00000000  22.000000
     NA's:    0.00000   0.000000   0.0000000   0.00000000   0.000000
 Std Dev.:   56.94122   2.367226   0.7529888   0.08665541   1.003312
```

- With Figure 1.7 constructed and visible, click on **Insert** in the tool bar and select **Graph**.
- Click **OK** on the **Insert Graph** menu that appears.
- Select the **jets** data set and **SPR** as x and **FFD** as y.
- Here, however, select **CAR** as z.
- Click the **Symbol** tab and repeat the appropriate steps described above.
- Click on **OK**.

The resulting diagram is shown in Figure 1.8. (It may have been sensible here to have kept the height of the plotting symbol at its default value for the second diagram; we leave this as an exercise for the reader.)

With the command language the scatterplot in Figure 1.7 is obtained from

```
>plot(SPR,FFD)
```

and the plot in Figure 1.8 from

```
> plot(SPR,FFD,type="n")
> text(SPR,FFD,labels=as.character(Type))
```

Many other examples of the use of the plot function will be presented in later chapters.

Table 1.5 Summary Statistics for Jet Fighter Data by Whether or Not Plane Can Land on Carrier

```
                 *** Summary Statistics for data in: jets ***

CAR: Cannot land
                  FFD          SPR          RGF           PLF          SLF
     Min:    82.00000     0.455000    3.3000000    0.00800000     0.100000
  1st Qu.:  114.50000     1.536500    3.7850000    0.14650000     1.000000
    Mean:   151.00000     2.869182    4.1554545    0.16518182     1.921818
  Median:   147.00000     2.426000    4.2000000    0.15500000     2.300000
  3rd Qu.:  179.50000     3.258000    4.5650000    0.20000000     2.850000
     Max:   255.00000     8.548000    4.9900000    0.27500000     3.500000
 Total N:    11.00000    11.000000   11.0000000   11.00000000    11.000000
    NA's:     0.00000     0.000000    0.0000000    0.00000000     0.000000
 Std Dev.:   51.03724     2.203758    0.5261248    0.07103354     1.200515
------------------------------------------------------------------
CAR: Can land
                  FFD          SPR          RGF           PLF          SLF
     Min:   101.00000     2.168000    3.9700000     0.0000000     1.000000
  1st Qu.:  146.50000     3.173500    4.5150000     0.1035000     2.450000
    Mean:   181.54545     5.019727    4.9990909     0.1713636     2.609091
  Median:   187.00000     5.855000    4.9200000     0.1720000     2.900000
  3rd Qu.:  199.00000     6.411500    5.3950000     0.2190000     2.950000
     Max:   328.00000     8.088000    6.4500000     0.3660000     3.200000
 Total N:    11.00000    11.000000   11.0000000    11.0000000    11.000000
    NA's:     0.00000     0.000000    0.0000000     0.0000000     0.000000
 Std Dev.:   60.75255     2.089900    0.7227926     0.1034527     0.642580
```

Table 1.6 Results of t-Test for Difference in FFD for Planes that Can and Cannot Land on a Carrier

```
Standard Two-Sample t-Test
data: x: FFD with CAR = Cannot land, and y: FFD with CAR = Can land
t = –1.2768, df = 20, p-value = 0.2163
alternative hypothesis: true difference in means is not equal to 0
95 percent confidence interval:
 –80.44900  19.35809
sample estimates:
 mean of x   mean of y
       151    19.35809
```

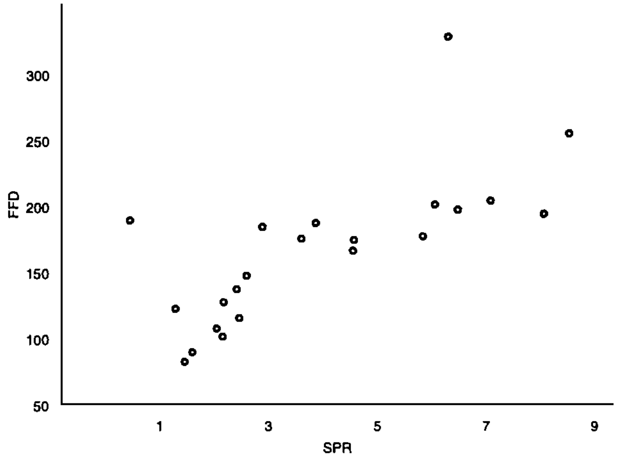


Figure 1.6 Scatterplot of SPR and FFD variables in jets data frame.

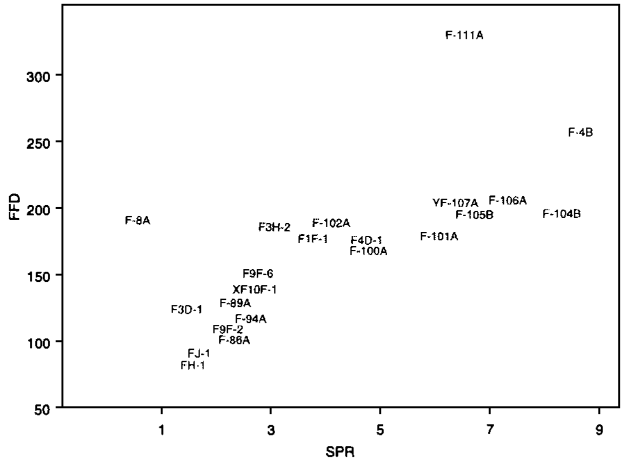


Figure 1.7 Scatterplot of SPR and FFD variables in jets data frame with points labelled by type of aircraft.

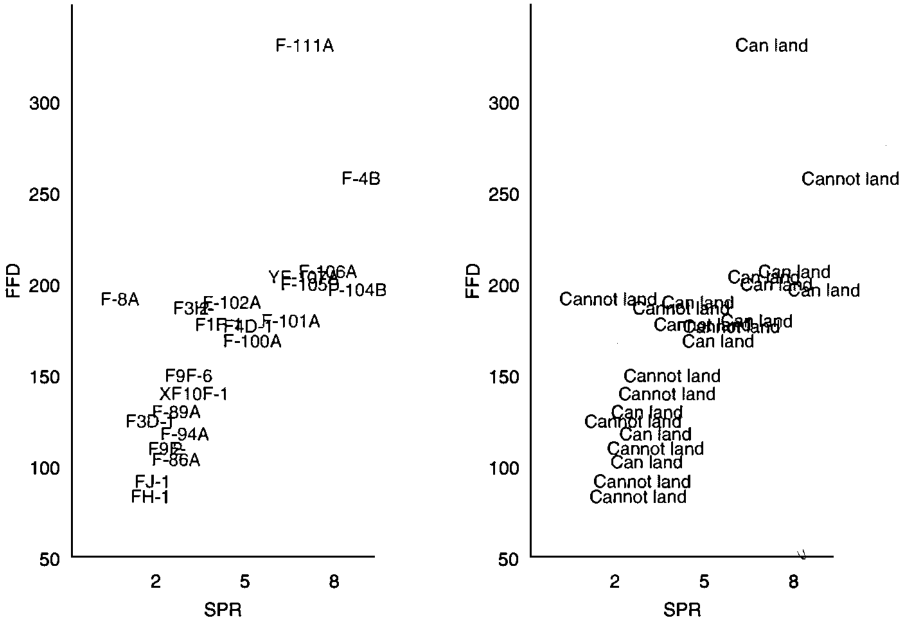


Figure 1.8 Side-by-side scatterplots for the SPR and FFD variables in the jets data frame.

Exercises

1.1. Investigate the use of the apply function to find the means of the numerical values in the jets data frame.

1.2. Use the rep function to help produce a new two-column data frame for the jet fighter data in which the numerical variable values for all planes are arranged in a single vector with the type of plane rearranged accordingly.

1.3. Use the boxplot function to construct box plots of the values of each numerical variable in the jets dataframe.

1.4. Explore the use of the hist and density functions for plotting histograms and calculating probability density estimates for some of the variables in the jets data frame.

1.5. Use the help function to find out about the pairs function and then apply this function to the variables in the jets data frame in ways that you think might be useful.

Chapter 2

Describing Data and Assessing Distributions: Husbands and Wives

2.1 Introduction

The data to be used in this chapter consist of five variables recorded on a random sample of 100 married men and their wives. The five variables are

- **husbage**: husband's age in years
- **husbht**: husband's height in mm
- **wifeage**: wife's age in years
- **wifeht**: wife's height in mm
- **husbagem**: husband's age at the time of the marriage

The data are given in Table 2.1. The label NA is used in S-PLUS to denote a missing value, here generally the result of the wife declining to give her age!

We shall use these data to illustrate some the features of S-PLUS for describing data and for assessing distributions.

Table 2.1 Data on Husbands and Wives

husbage	husbht	wifeage	wifeht	husbagem
40	1659	30	1620	38
58	1616	52	1420	30
32	1695	27	1660	23
42	1753	NA	1635	30
31	1685	23	1610	26
40	1713	39	1610	23
35	1736	32	1700	31
45	1715	NA	1522	41
35	1785	33	1680	24
47	1758	43	1630	24
38	1725	40	1600	31
45	1764	NA	1689	24
50	1674	45	1640	25
27	1700	25	1580	21
28	1721	25	1650	23
37	1829	35	1670	22
56	1710	55	1600	44
27	1745	23	1610	25
47	1809	43	1620	25
31	1585	23	1570	28
35	1705	35	1580	25
27	1721	NA	1560	26
45	1739	39	1610	25
59	1699	52	1440	27
43	1825	52	1570	25
48	1704	NA	1635	27
54	1679	53	1560	NA
43	1755	42	1590	20
54	1713	50	1600	23
61	1723	64	1490	26
51	1585	NA	1504	50
54	1724	53	1640	20
37	1620	39	1650	21
55	1764	45	1620	29
57	1738	55	1560	24
34	1700	32	1640	22
45	1804	41	1670	27
55	1664	43	1760	31
55	1788	51	1600	26
44	1715	41	1570	24

Table 2.1 (Continued) Data on Husbands and Wives

husbage	husbht	wifeage	wifeht	husbagem
42	1731	37	1580	23
34	1760	34	1700	23
45	1559	35	1580	34
48	1705	45	1500	28
44	1723	44	1600	41
59	1700	47	1570	39
64	1660	57	1620	32
34	1681	33	1410	22
37	1803	38	1560	23
49	1884	46	1710	25
63	1705	60	1580	27
48	1780	47	1690	22
64	1801	55	1610	37
33	1795	45	1660	17
52	1669	47	1610	23
27	1708	24	1590	26
33	1691	32	1530	21
46	1825	47	1690	23
27	1949	NA	1693	25
50	1685	NA	1580	21
42	1806	NA	1636	22
54	1905	46	1670	32
49	1739	42	1600	28
62	1736	63	1570	22
34	1845	32	1700	24
53	1736	NA	1555	30
32	1741	NA	1614	22
59	1720	56	1530	24
55	1720	55	1590	21
62	1629	58	1610	23
42	1624	38	1670	22
50	1653	44	1690	35
51	1620	44	1650	30
58	1736	50	1540	32
28	1691	23	1610	23
45	1753	43	1630	21
57	1724	59	1520	24
27	1725	21	1550	24
54	1630	NA	1570	34
25	1815	26	1650	20

Table 2.1 (Continued) Data on Husbands and Wives

husbage	husbht	wifeage	wifeht	husbagem
57	1575	57	1640	20
61	1749	63	1520	21
25	1705	23	1620	24
32	1875	NA	1744	22
37	1784	NA	1647	22
45	1584	NA	1615	29
44	1790	40	1620	24
52	1798	53	1570	25
60	1725	60	1590	21
36	1685	32	1620	25
35	1664	NA	1539	22
50	1725	49	1670	23
57	1694	55	1620	24
38	1691	38	1530	20
30	1880	31	1630	22
50	1723	47	1650	25
20	1786	18	1590	19
51	1675	45	1550	25
40	1823	39	1630	23
59	1720	56	1530	24

2.2 Some Basic Summaries

The analysis of most data sets begins with the calculation of suitable numerical summary statistics such as variable means and standard deviations, and relatively simple graphics such as *histograms* and *boxplots* describing variable distributions. In the case of multivariate data such as those in Table 2.1, correlations between variables may also be computed and *scatterplots* of pairs of variables constructed.

It may also be necessary to assess whether the individual variables are normally distributed prior to any analysis that makes this assumption. In addition it may be required to check whether the complete set of variables jointly have a multivariate normal distribution. In both cases one approach is to use *probability plots*, as we shall see later in the chapter.

2.3 Analysis Using S-PLUS

We assume that the data in Table 2.1 are available as the S-PLUS data frame huswif, with the variables labelled as shown in the previous section. To obtain the basic summary statistics of the data we can again use the **Summary Statistics** dialog as illustrated in Chapter 1; here, however, we will also request measures of skewness and kurtosis. The results are shown in Table 2.2. We see that 16 of the 17 missing values in the data occur for the age of wife variable. Husband's age at marriage has a relatively high degree of skewness.

Table 2.2 Summary Statistics for Husbands and Wives Data

```
         *** Summary Statistics for data in: huswif ***

               husbage         husbht        wifeage          wifeht
      Min:  20.0000000   1559.0000000     18.0000000    1410.0000000
  1st Qu.:  35.0000000   1691.0000000     33.7500000    1570.0000000
     Mean:  44.6400000   1727.5500000     42.3690476    1605.0800000
   Median:  45.0000000   1723.0000000     43.0000000    1610.0000000
  3rd Qu.:  54.0000000   1764.0000000     52.0000000    1641.7500000
      Max:  64.0000000   1949.0000000     64.0000000    1760.0000000
  Total N: 100.0000000    100.0000000    100.0000000     100.0000000
     NA's:   0.0000000      0.0000000     16.0000000       0.0000000
 Std Dev.:  11.1169358     71.8870291     11.4258002      62.8889803
 Skewness:   0.1539845      0.2938824      0.1732601       0.4584884
 Kurtosis:  -1.0105144      0.6896657     -0.7573466       0.9466165

              husbagem
      Min:   17.000000
  1st Qu.:   22.000000
     Mean:   25.868687
   Median:   24.000000
  3rd Qu.:   27.500000
      Max:   50.000000
  Total N:  100.000000
     NA's:    1.000000
 Std Dev.:    5.674228
 Skewness:    1.803211
 Kurtosis:    3.862735
```

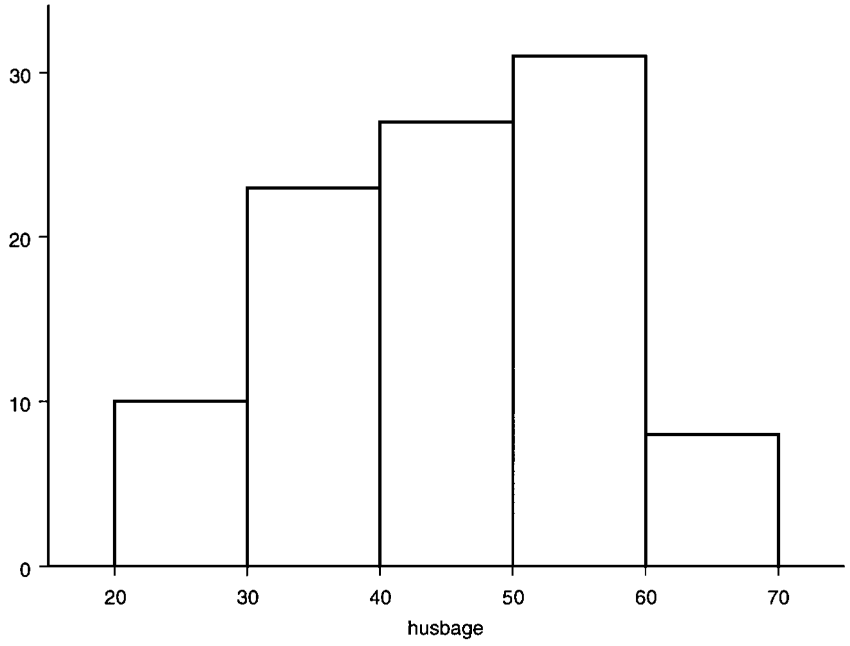


Figure 2.1 Histogram of husband's age.

In addition to the basic numerical summaries given in Table 2.2, graphics are an essential part of the initial examination of data. Here we shall begin by constructing histograms for each of the five variables first by using the **Graphics menu**.

- Click on **Graph**.
- Select **2D** and then highlight **Histogram (*x*)**.
- Click **OK** and the **Histogram/Density** dialog appears.
- Select **huswif** as the data set and say **husbage** as the *x* column.
- Click **OK** to give Figure 2.1, a histogram of husband's age.

A similar sequence of instructions can be used to produce histograms of each of the other variables, and by repeated use of **Insert, Graph**, they can all be arranged on the same sheet as shown in Figure 2.2. (On the screen the diagram will be colour; to print on a black and white printer use **Format, Apply Style, Black and White** before **File, Print Graph Sheet**.)

More useful than Figure 2.2 would be diagrams that contain a number of alternative graphical displays of the same variable, for example, a histogram, a box plot, and a normal probability plot. We now examine how this can be constructed for the husbage variable using the command language.

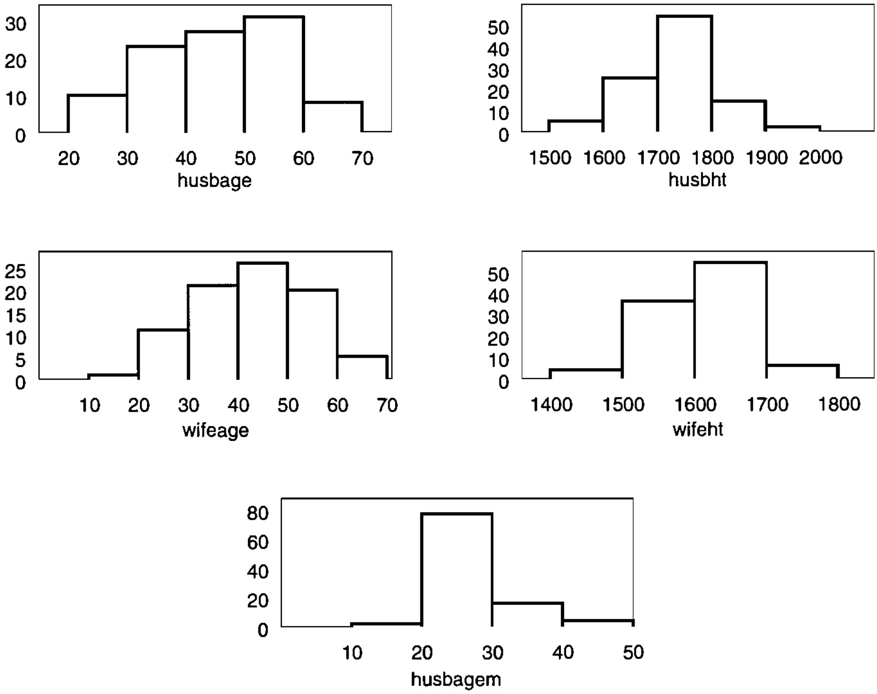


Figure 2.2 Histograms of all five variables in the huswif data frame.

```
attach(huswif)
#set up plotting area to take three graphs
par(mfrow=c(1,3))
#use hist function to plot histogram and label x and y
#axis appropriately
hist(husbage,xlab=“Age of husband”,ylab=“Frequency”)
#
#use boxplot function and label with variable information
boxplot(husbage,ylab=“Age of husband”)
#use qqnorm function to construct a normal probability
#plot
qqnorm(husbage)
qqline(husbage)
```

The resulting diagram is shown in Figure 2.3. The box plot shows that there are no obvious outliers on this variable, and the histogram suggests some degree of non-normality, also indicated in the probability plot. Similar diagrams could be drawn for the other four variables. We leave

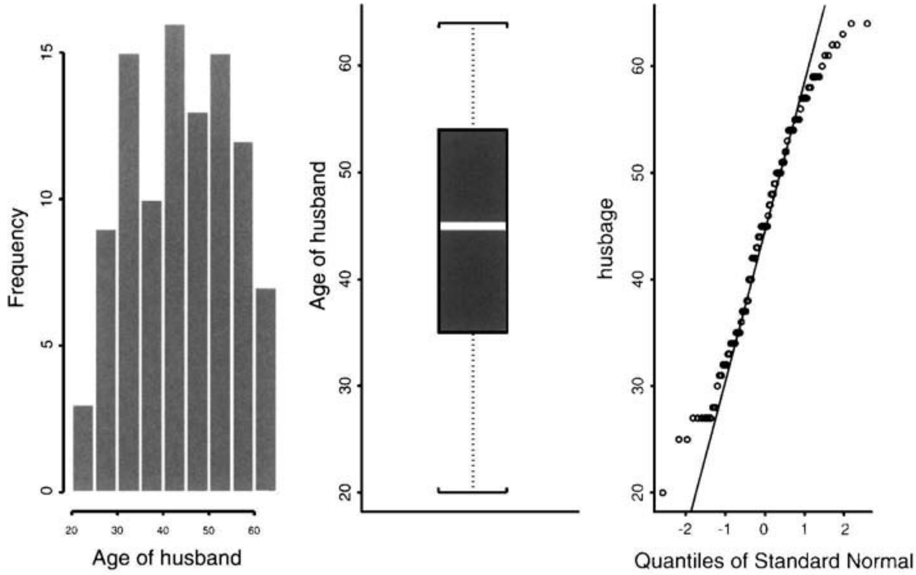


Figure 2.3 Histogram, box plot, and probability plot of husband's age.

this and the construction of Figure 2.3 using the GUI as exercises for the reader.

Having obtained both numerical and graphical information about individual variables in the data, we might now want to look at the relationships between variables. The most generally used numerical summary of these relationships is the *correlation matrix* of the variables. This can be obtained via the S-PLUS GUI as follows:

- Click on **Statistics**.
- Select **Data Summaries**.
- Select **Correlations**.

In the **Correlations and Covariance** dialog first select the huswif data set; **<ALL>** is highlighted by default in the variables section of the dialog, meaning that all variables in the chosen data frame will be included in the calculation of the correlation matrix. We now need to consider what to select in the **Method to Handle Missing Values** box. The default of **Fail** needs to be changed for the huswif data set. So select **Available** and then click **OK** to give the correlation matrix shown in Table 2.3. The correlations in this matrix are calculated on the basis of all observations available for each pair of variables.

Table 2.3 Correlation Matrix for Husbands and Wives Data

```
        *** Correlations for data in: huswif ***

           husbage      husbht      wifeage     wifeht   husbagem
 husbage  1.0000000  -0.20018660  0.96749749  -0.2358639  0.3002488
  husbht -0.2001866   1.00000000 -0.01332892   0.3594675 -0.2575508
 wifeage  0.9674975  -0.01332892  1.00000000  -0.2259641  0.1118882
  wifeht -0.2358639   0.35946747 -0.22596407   1.0000000 -0.1402032
husbagem  0.3002488  -0.25755083  0.11188819  -0.1402032  1.0000000
```

The values in the correlation matrix show that the ages of husbands and their wives are highly correlated (0.95); other pairs of variables, however, have only moderate correlations.

With the command language, the same correlation matrix can be found using the cor function:

```
cor(huswif,na.method="available")
#the na.method argument is used to select a procedure for
#dealing with missing values
```

Assessing the relationships between variables simply on the basis of the numerical values of their correlations is not, in general, to be recommended. Correlations can be badly distorted, for example, by outliers in the data, and can give misleading values if the relationships between the variables are anything but linear. Consequently, it is important to look at the numerical correlations alongside scatterplots of the variables. Scatterplots of each pair of variables are obtained either via the **Graphics menu** or the plot command, both of which were illustrated in Chapter 1. Here there are ten possible scatterplots for the five variables, and it is convenient to view them displayed in the form of what is usually called a *scatterplot matrix*. Formally, a scatterplot matrix is defined as a square symmetric grid of bivariate scatterplots (Cleveland, 1993). The grid has p rows and p columns, each one corresponding to a different one of the p observed variables. Each of the cells of the grid shows a scatterplot of two variables. Because the scatterplot is symmetric about its diagonal, variable i is plotted against variable j in the ijth cell, and the same variables also appear in cell ji with the x and y axes of the scatterplot interchanged. The reason for including both the upper and lower triangles in the matrix, despite the seeming redundancy, is that it enables a row or column to be visually scanned to see one variable against all others, with the scale for one variable lined up along the horizontal or the vertical.

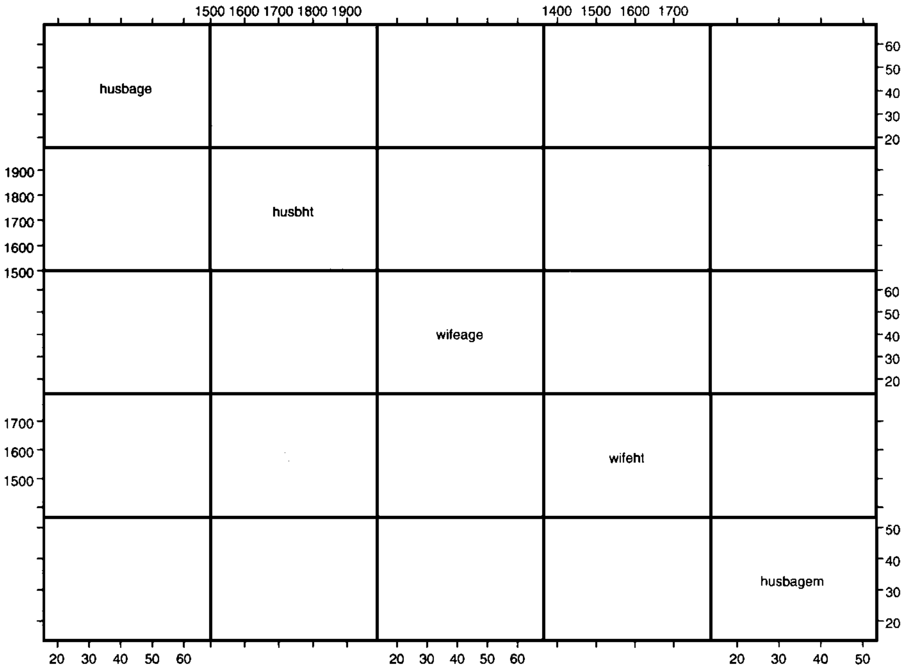


Figure 2.4 Scatterplot matrix for all five variables in the huswif data frame.

To obtain the scatterplot matrix of the five variables in the huswif data frame we can use the **Graphics menu** as follows:

- Click **Graph**.
- Choose **2D** and under **Axes Type** highlight **Matrix**.
- Click on **OK** and the **Scatter Plot Matrix** dialog appears.
- Select the **huswif** data frame and highlight all variables in the *x* columns box.
- Click **OK**.

This leads to the scatterplot matrix seen in Figure 2.4

The pattern of the relationships between the pairs of variables is made very clear in this diagram and it is also reassuring to see that there are no very obvious outliers or nonlinear relations with which to be concerned. Consequently, the correlation matrix in Table 2.3 does represent a reasonable numerical summary of the relationships between the five variables in the data.

With the command language, the scatterplot matrix can be obtained with the pairs function as follows:

```
pairs(huswif)
```

In some cases it may be informative to label the points in a scatterplot (and in a scatterplot matrix) in some way. Suppose for the huswif data we would like to label points according to whether the husband or wife is tallest, say “hw” if the husband is taller and “WH” if the wife is taller. The following commands label the points in this way in a scatterplot matrix of the data using the panel=function argument to do something other than simply the default, which is to plot the points in each panel of the grid of scatterplots.

```
difht<-husbht-wifeht
#find difference in heights of the couples
labs<-rep(“hw”,100)
#use the rep function to create a vector
#of length 100, each element of which is the label hw
labs[difht<=0]<-”WH”
#change elements of labs to WH for those
#couples where the wife is taller or equal
#in height to her husband
pairs(huswif,panel=function(x,y)text(x,y,labels=labs,cex=0.5))
#use the text function to plot the contents
#of labs in the appropriate positions in each
#scatterplot; cex is a parameter controlling
#the size of the plotted character.
```

The resulting plot is shown in Figure 2.5. As might be expected, most points are labelled ‘hw’, since husbands are, in general, taller than their wives. (Many other examples of using the panel=function argument of the pairs function will be given in later chapters.)

Earlier in this chapter probability plots were used to assess individual variables in the huswif data frame for normality. But it may be as important to assess the five variables jointly for multivariate normality. One possible method that can be used is a *chi-squared probability plot* of the *generalized distances* (*Mahalanobis distance*) of each observation from the mean vector of the data, i.e., for observation i with vector of values $\mathbf{x}_i$ the distance d_i given by

$$d_i = (\mathbf{x}_i - \bar{\mathbf{x}})' \mathbf{S}^{-1} (\mathbf{x}_i - \bar{\mathbf{x}}) \tag{2.1}$$

where $\bar{\mathbf{x}}$ is the sample mean vector and $\mathbf{S}$ the sample covariance matrix. If the observations do arise from a multivariate normal distribution, these distances have, approximately, a chi-squared distribution with degrees of

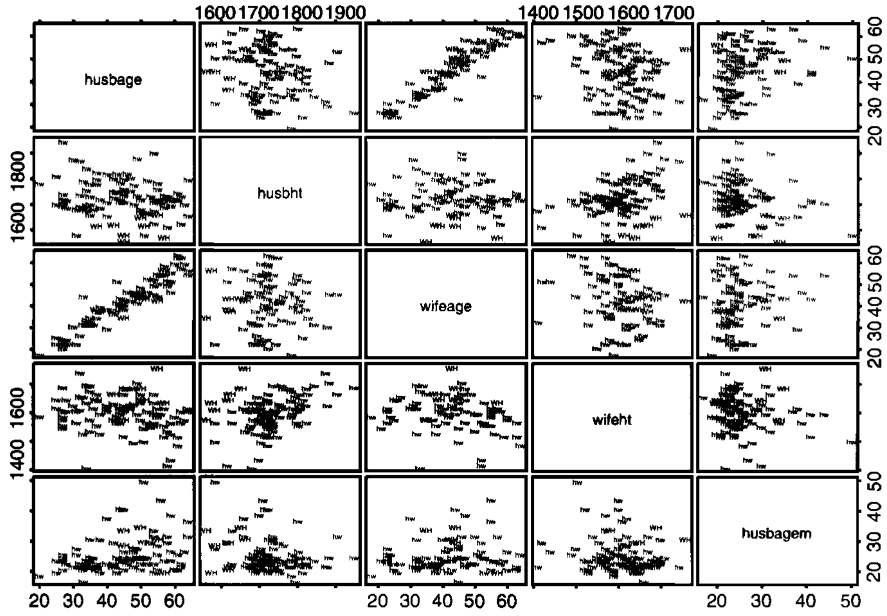


Figure 2.5 Scatterplot matrix for all five variables in the huswif data frame with points labelled according to whether husband (hw) or wife (WH) is taller.

freedom equal to the number of variables. So plotting the ordered distances against the corresponding quantiles of the appropriate chi-squared distribution should lead to a straight line through the origin. Such a plot is easily constructed using the S-PLUS command language and in particular the Mahalanobis function; suitable code is as follows;

```
#first use the na.exclude function to remove observations
#with missing values on any variable
huswif1<-na.exclude(huswif)
#use the apply function to find the mean vector of the
#data
meanv<-apply(huswif1,2,mean)
#use var function to find covariance matrix
S<-var(huswif1)
#use length function to find number of
#observations in huswif1
n<-length(huswif1[,1])
#Get sample quantiles
index <-(1:n)/(n+1)
```

```
#1:n produces the vector of values 1,2,...,n
#get corresponding chi-squared quantiles
quant <-qchisq(index,5)
#get generalized distances using Mahalanobis
#function
dist<-mahal(huswif1,mean,S)
#dist will contain the Mahalanobis distances of each
#observation from the mean vector of the data.
#plot ordered distances obtained using the
#sort function
plot(quant,sort(dist),ylab="Ordered distances",
xlab="Chi-square quantiles",pch= 1)
abline(0,1)
#use the abline function to add a line with intercept 0
#and slope 1, i.e., the line y=x
```

The resulting plot is shown in Figure 2.6. There is considerable deviation from a straight line in the plotted points. This gives relatively clear evidence that the data do not have a multivariate normal distribution, which may have implications for particular types of analysis that may be considered for the data.

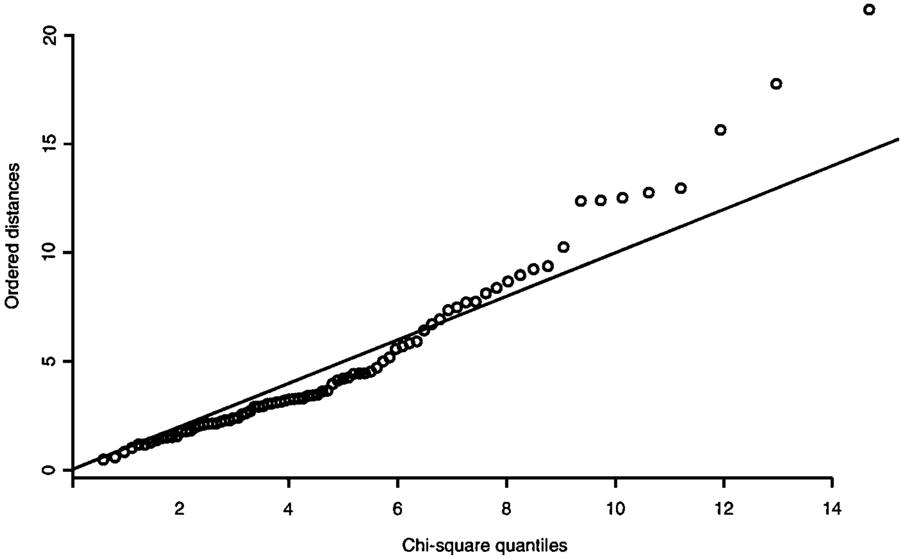


Figure 2.6 Chi-squared probability plot of all five variables in the huswif data frame.

Exercises

2.1. It is often important to include information about the marginal distributions of each variable on a scatterplot of a pair of variables. A simple procedure for this is the use of the rug function in S-PLUS (with perhaps the jitter function as well). Investigate by producing a scatterplot of husband's age against wife's age showing the marginal distributions of each variable.

2.2. Investigate the use of the density function in S-PLUS for enhancing histograms with a nonparametric estimate of the distribution of the variables. Additionally, examine the use of both the **Graph menu** and the **2D graphical palette** for the same thing.

2.3. Produce a scatterplot matrix of the variables in the husbands/wives data, with each panel the value of the correlation coefficient of the two variables shown.

2.4. Use the chi-squared plotting technique for assessing multivariate normality described in the text to assess only the first four variables in the huswif data frame. Do you think these four variables do have a multivariate normal distribution?

2.5. Explore the use of the hist2d function to get two-dimensional histograms for husband's age and wife's age. Use the persp function to view the histogram.

2.6. Use the **Scatter Plot Matrix** dialog to get the scatterplot matrix of the five variables in the huswif data frame, enhanced with a histogram of each variable on the main diagonal.

Chapter 3

Analysis of Variance: Poisoning Rats and Losing Weight

3.1 Description of Data

In this chapter we shall consider the analysis of two sets of data. The first, shown in Table 3.1, involves the survival times (in 10-hour units) of rats subjected to three different poisons and four different treatments. This is an example of a 3 × 4 factorial design with four replications in each cell.

The second data set we shall be concerned with here is shown in Table 3.2. These data arise from a study into the effectiveness of slimming clinics. Of particular interest is the question of whether adding a technical manual giving advice based on psychological behaviourist theory to the support offered would help clients to control their diet. So the first factor is Condition with two levels: 'Experimental' (those given the manual) and 'Control' (those without the manual). It was also thought important to distinguish between clients who had already been trying to slim and those who had not, giving rise to the second factor, Status, again with two levels: 'Experienced' (those who had been trying to slim for more than 1 year) and 'Inexperienced' (those who had been trying to slim for not more than 3 weeks). The response variable recorded for each participant in the study was

$$\frac{\text{weight at 3 months} - \text{ideal weight}}{\text{Initial weight} - \text{ideal weight}} \qquad (3.1)$$

Table 3.1 Survival Times of Rats

Poison	Treatment	Time
1	1	0.31
1	1	0.45
1	1	0.46
1	1	0.43
1	2	0.82
1	2	1.10
1	2	0.88
1	2	0.72
1	3	0.43
1	3	0.45
1	3	0.63
1	3	0.76
1	4	0.45
1	4	0.71
1	4	0.66
1	4	0.62
2	1	0.36
2	1	0.29
2	1	0.40
2	1	0.23
2	2	0.92
2	2	0.61
2	2	0.49
2	2	1.24
2	3	0.44
2	3	0.35
2	3	0.31
2	3	0.40
2	4	0.56
2	4	1.02
2	4	0.71
2	4	0.38
3	1	0.22
3	1	0.21
3	1	0.18
3	1	0.23
3	2	0.30
3	2	0.37
3	2	0.38
3	2	0.29

Table 3.1 (Continued) Survival Times of Rats

Poison	Treatment	Time
3	3	0.23
3	3	0.25
3	3	0.24
3	3	0.22
3	4	0.30
3	4	0.36
3	4	0.31
3	4	0.33

In this case the design is a 2 × 2 factorial, but the number of observations in each of the four cells is not the same; the data are *unbalanced*, rather than *balanced* as in the first example.

3.2 Analysis of Variance

Analysis of variance (ANOVA) encompasses a set of methods for testing hypotheses about differences between means. Underlying ANOVA is a linear model, which for both data sets introduced in the previous section would have the following form:

$$y_{ijk} = \mu + \alpha_i + \beta_j + \gamma_{ij} + \epsilon_{ijk} \qquad (3.2)$$

where y_{ijk} represents the k observation in the jth level of one factor and the ith level of the other. The parameters μ, α_i, β_j, and γ_{ij} represent, respectively, overall mean, main effects of each factor, and the interaction between the two factors. The ϵ_{ijk} are error terms assumed to have a normal distribution with zero mean and variance σ^2. (To make the model in Equation 3.2 identifiable, the parameters need to be constrained in some way, for example, by requiring that their sum over any subscript is zero.)

For the balanced survival time data, the variability in the observations can be portioned into sums of squares representing poisons, treatments, and the poisons × treatments interaction, *orthogonally*; i.e., they would be nonoverlapping. But for the unbalanced slimming data, this is not the case, because, for example, there is a proportion of the variability in the response variable that can be attributed to (explained by) either of the two factors in the study. A consequence is that Condition and Status

Table 3.2 Slimming Data

Condition	Status	Response
1	1	–14.67
1	1	–1.85
1	1	–8.55
1	1	–23.03
1	1	11.61
1	2	0.81
1	2	2.38
1	2	2.74
1	2	3.36
1	2	2.10
1	2	–0.83
1	2	–3.05
1	2	–5.98
1	2	–3.64
1	2	–7.38
1	2	–3.60
1	2	–0.94
2	1	–3.39
2	1	–4.00
2	1	–2.31
2	1	–3.60
2	1	–7.69
2	1	–13.92
2	1	–7.64
2	1	–7.59
2	1	–1.62
2	1	–12.21
2	1	–8.85
2	2	5.84
2	2	1.71
2	2	–4.10
2	2	–5.19
2	2	0.00
2	2	–2.80

together explain less of the variation in the response variable than the sum of which each explains alone. The result is that the sum of squares that can be attributed to a factor depends on which other factors have already been allocated a sum of squares; in other words, the sums of squares of the factors now depend on the order in which they are considered. There is a lack of uniqueness in partitioning the variation in the response variable. This is not so for balanced data. (For a more detailed discussion of the problems with unbalanced designs, see Nelder, 1977, and Aitkin, 1978).

3.3 Analysis Using S-PLUS

The data sets in Tables 3.1 and 3.2 are available as S-PLUS data frames called rats and slim, respectively, with the factors appropriately defined as S-PLUS factor variables and their levels suitably labelled.

In this chapter we shall be applying the analysis of variance model specified in Equation 3.2 and so this is a convenient point to say a little about the model formulae used in S-PLUS which are common to all its modelling procedures. A formula in S-PLUS is a symbolic expression that defines the structural form of the model and is interpreted by modelling functions. A simple example of an S-PLUS model formula is

```
y~x1+x2+x3
```

y is the response variable and *x*1 to *x*3 explanatory variables. The corresponding regression coefficients and the constant are implied in the formula. The term on the left-hand side can be an expression representing, say, a transformation of the response variable, for example,

```
log(y)~x1+x2+x3
```

A model formula such as

```
y~x1*x2
```

means that *y* is modelled using the main effects *and* the interaction of *x*1 and *x*3. Written out in full the model is

```
y~x1+x2+x1:x2
```

with the colon used to indicate the interaction term.

Variables on the right-hand side of a model formula can also be transformed, but since arithmetic operators have a different meaning in formulae (as we have seen above), the expressions must be enclosed in the I function; for example,

```
y~I(x1*x2)
```

means that *y* is modelled in terms of a single explanatory variable given by the product of *x*1 and *x*2, in addition to the constant.

More aspects of model formulae will be introduced in later chapters.

3.3.1 Analysis of Variance of Survival Times of Rats

The contents of the rats data frame are shown in Table 3.3. To begin, let us simply obtain the analysis of variance table for these data using the appropriate dialog box:

- Click on **Statistics**.
- Select **ANOVA**.
- Select **Fixed Effects**.

The **ANOVA** dialog now becomes visible, and we proceed as follows:

- Select the **rats** data frame.
- Click on the **Create Formula** tab to access the **Formula** dialog.
- Highlight **Time** in the **Choose Variables Section**.
- Click on the **Response** tab.

The following now appears in the **Formula** section.

```
Time~1
```

- Highlight both **Poison** and **Treatment** and check the **Main + Interact** tab to give the following formula:

```
Time~Poison*Treatment
```

This corresponds to the required main effects plus interaction model.

- Click on **OK** to return to the **ANOVA** dialog.
- Click **OK**.

This leads to the results shown in Table 3.4. The analysis of variance table indicates that the Poison × Treatment interaction is nonsignificant, but that both Poison and Treatment main effects are significant. (Note that the S-PLUS commands equivalent to the analysis carried out using the dialog approach appear in the Report file.)

So it appears that a simple main effects model is suitable for these data. We might now move on to consider the following:

Table 3.3 Contents of the rats Data Frame

```
> rats
     Poison  Treatment  Time
  1    P1        A      0.31
  2    P1        A      0.45
  3    P1        A      0.46
  4    P1        A      0.43
  5    P1        B      0.82
  6    P1        B      1.10
  7    P1        B      0.88
  8    P1        B      0.72
  9    P1        C      0.43
 10    P1        C      0.45
 11    P1        C      0.63
 12    P1        C      0.76
 13    P1        D      0.45
 14    P1        D      0.71
 15    P1        D      0.66
 16    P1        D      0.62
 17    P2        A      0.36
 18    P2        A      0.29
 19    P2        A      0.40
 20    P2        A      0.23
 21    P2        B      0.92
 22    P2        B      0.61
 23    P2        B      0.49
 24    P2        B      1.24
 25    P2        C      0.44
 26    P2        C      0.35
 27    P2        C      0.31
 28    P2        C      0.40
 29    P2        D      0.56
 30    P2        D      1.02
 31    P2        D      0.71
 32    P2        D      0.38
 33    P3        A      0.22
 34    P3        A      0.21
 35    P3        A      0.18
 36    P3        A      0.23
 37    P3        B      0.30
 38    P3        B      0.37
```

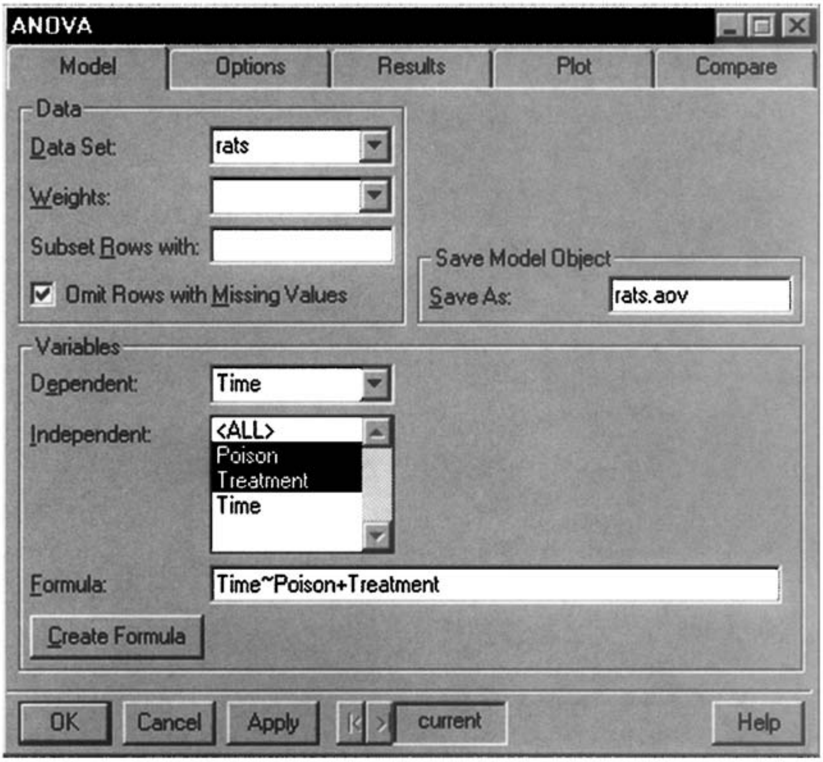
Table 3.3 (Continued) Contents of the rats Data Frame

```
> rats
       Poison    Treatment    Time
 39      P3          B        0.38
 40      P3          B        0.29
 41      P3          C        0.23
 42      P3          C        0.25
 43      P3          C        0.24
 44      P3          C        0.22
 45      P3          D        0.30
 46      P3          D        0.36
 47      P3          D        0.31
 48      P3          D        0.33
```

Table 3.4 Analysis of Variance of Survival Times of Rats

```
*** Analysis of Variance Model ***

Short Output:
Call:
   aov(formula = Time ~ Poison * Treatment, data = rats,
     na.action = na.exclude)

          Terms:
                    Poison  Treatment  Poison:Treatment  Residuals
  Sum of Squares     1.033      0.921             0.250      0.801
 Deg. of Freedom         2          3                 6         36

Residual standard error: 0.1491
Estimated effects are balanced

                    Df  Sum of Sq  Mean Sq  F Value   Pr(F)
          Poison     2      1.033   0.5165    23.22  0.0000
       Treatment     3      0.921   0.3071    13.81  0.0000
Poison:Treatment     6      0.250   0.0417     1.87  0.1123
       Residuals    36      0.801   0.0222
```

1. Whether the normality assumption made by the analysis of variance model is justified for these data;
2. Whether the constant variance assumption is justified;
3. Use of *multiple comparison tests* to examine in more detail which Poison means and which Treatment means differ.



Data Set: rats

Weights:

Subset Rows with:

☑ Omit Rows with Missing Values

Save As: rats.aov

Dependent: Time

Independent: <ALL> Poison Treatment Time

Formula: Time~Poison+Treatment

Figure 3.1 ANOVA dialog showing main effects model for the data on survival times of rats.

To check both the normality and constant variance assumptions, we shall examine the *residuals* from the fitted model, i.e., the differences between the observed values and those predicted by the model. A normal probability plot of the residuals will be used to assess assumption (1), and a plot of residuals against fitted values can be used to evaluate assumption (2). Departures from a 'horizontal band' shape give cause for concern. (More will be said about the use of residuals for diagnosing models in later chapters.)

So we return to the **ANOVA** dialog, set up the main effects model for the rats data frame, and request that the resulting model object be saved as, say, rats.aov (this is needed for the multiple comparison tests to be described later). The **ANOVA** dialog now appears as shown in Figure 3.1.

Now click on the **Plot** tab and tick the **Residuals v Fit** and **Residuals Normal QQ** options. Finally click on **OK** to give the results shown in Table 3.5 and the plots shown in Figures 3.2 and 3.3.

Table 3.5 Analysis of Variance of Survival Times of Rats: Main Effects Model

```
*** Analysis of Variance Model ***

Short Output:
Call:
   aov(formula = Time ~ Poison + Treatment, data = rats,
      na.action = na.exclude)

              Terms
                       Poison   Treatment   Residuals
  Sum of Squares        1.033       0.921       1.051
Deg. of Freedom             2           3          42

Residual standard error: 0.1582
Estimated effects are balanced

               Df    Sum of Sq    Mean Sq    F Value        Pr(F)
    Poison      2        1.033     0.5165      20.64    5.700e-007
 Treatment      3        0.921     0.3071      12.27    6.697e-006
  Residuals    42        1.051     0.0250
```

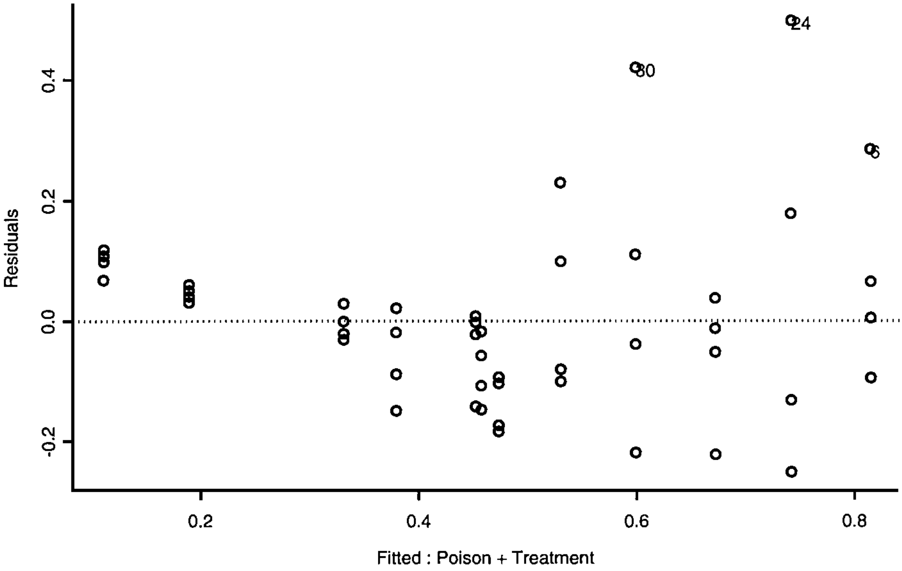


Figure 3.2 Residuals from main effects model for survival times of rats plotted against fitted values.

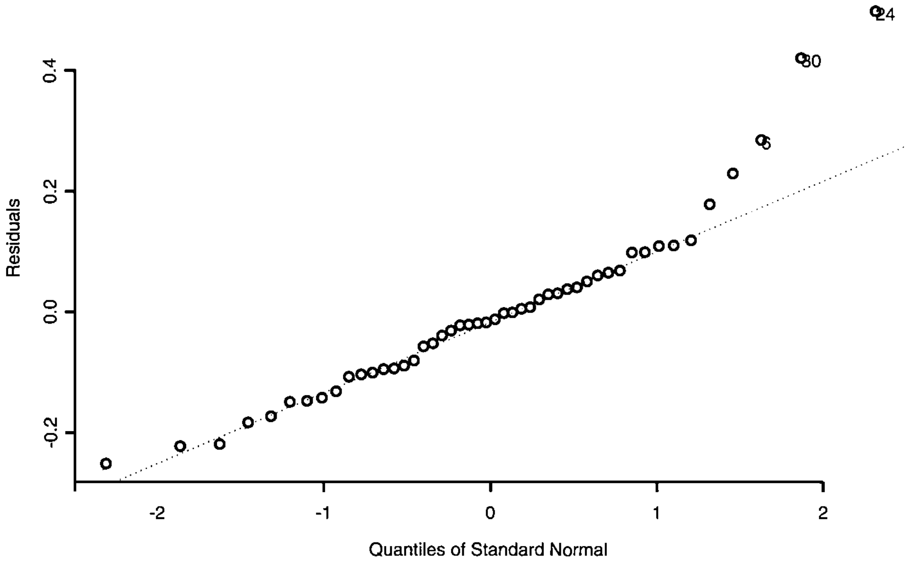


Figure 3.3 Normal probability plot of residuals from main effects model fitted to rat survival data.

The analysis of variance table in Table 3.5 confirms the highly significant main effects of both Poison and Treatment. The normal plot of the residuals suggests some departure from normality and the residuals vs. fitted values plot has a 'wedge shape' consistent with a departure from the constant variance assumption. Both findings suggest that analysing the survival times after a suitable transformation might be more appropriate than analysing the raw data. We leave this possibility to be investigated by the reader (see Exercise 3.1), and move on here to consider the use of multiple comparison tests to assess just which poison means and which treatment means differ. We shall use a test due to Scheffé. (This test in particular and multiple comparison tests in general are described in Everitt, 2001.)

- Click on **Statistics**.
- Select **ANOVA**.
- Select **Multiple Comparisons**.

In the **Multiple Comparisons** dialog, select the rats.aov created by previous use of the **ANOVA** dialog, select **Poison** in the **Levels of** section, and in the Method section select **Scheffé**. Click **OK** to see the numerical results in Table 3.6 and the graphical display of these results as seen in Figure 3.4. The results indicate that the mean survival time for P3 is

Table 3.6 Results of Scheffé's Multiple Comparison Test for Poisons

95% simultaneous confidence intervals for specified
linear combinations, by the Scheffé method

critical point: 2.5377
response variable: Time
rank used for Scheffé method: 2

intervals excluding 0 are flagged by '****'

	Estimate	Std.Error	Lower Bound	Upper Bound	
P1-P2	0.0731	0.0559	–0.0688	0.215	
P1-P3	0.3410	0.0559	0.1990	0.483	****
P2-P3	0.2680	0.0559	0.1260	0.410	****

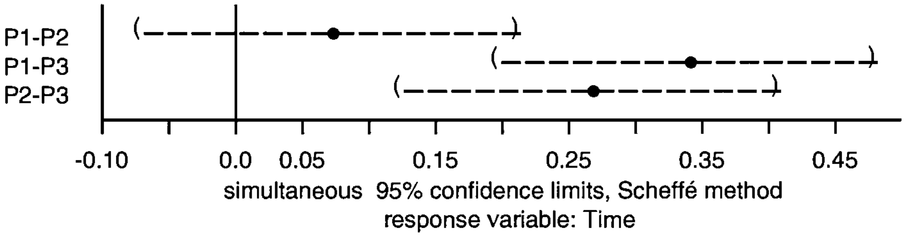


Figure 3.4 Scheffé multiple comparison results for levels of Poison in rat survival data.

significantly less than for P1 and P2, which themselves do not differ in mean survival time.

Repeating the process but now selecting **Treatment** leads to the results in Table 3.7 and Figure 3.5. It appears that the mean survival times for treatments A and B, A and D, and B and C differ.

3.3.2 Analysis of Variance of Slimming Data

The contents of the slim data frame are shown in Table 3.8. To analyse this data set we shall use the command language approach. The unbalanced nature of the data can be seen by examining the cell counts in the design. These are obtained using the tapply function and the length function

```
tapply(Response,list(Status,Condition),length)
```

Table 3.7 Results of Scheffé's Test for Treatments

95% simultaneous confidence intervals for specified
linear combinations, by the Scheffé method

critical point: 2.9122
response variable: Time
rank used for Scheffé method: 3

intervals excluding 0 are flagged by '****'

	Estimate	Std.Error	Lower Bound	Upper Bound	
A-B	–0.3620	0.0646	–0.5510	–0.1740	****
A-C	–0.0783	0.0646	–0.2660	0.1100	
A-D	–0.2200	0.0646	–0.4080	–0.0319	****
B-C	0.2840	0.0646	0.0961	0.4720	****
B-D	0.1420	0.0646	–0.0456	0.3310	
C-D	–0.1420	0.0646	–0.3300	0.0464	

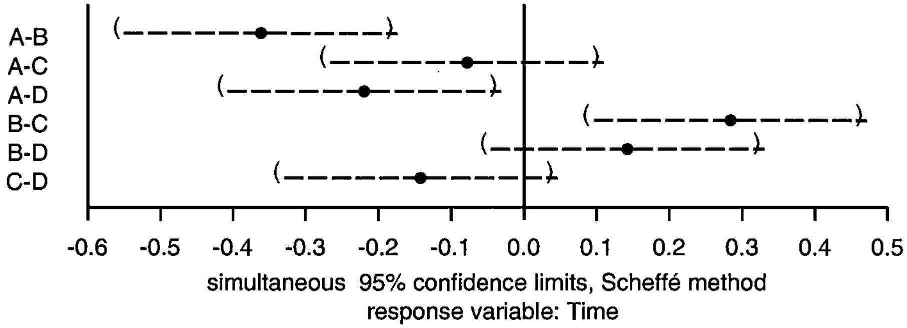


Figure 3.5 Scheffé multiple comparison results for Treatment levels in rat survival data.

to give the following:

	Experimental	Control
Experienced	5	11
Inexperienced	12	6

To begin, it may be helpful to examine some simple plots of the data. A plot of mean values for each level of each factor compared to a corresponding

Table 3.8 Contents of the slim Data Frame

	Condition	Status	Response
1	Experimental	Experienced	–14.67
2	Experimental	Experienced	–1.85
3	Experimental	Experienced	–8.55
4	Experimental	Experienced	–23.03
5	Experimental	Experienced	11.61
6	Experimental	Inexperienced	0.81
7	Experimental	Inexperienced	2.38
8	Experimental	Inexperienced	2.74
9	Experimental	Inexperienced	3.36
10	Experimental	Inexperienced	2.10
11	Experimental	Inexperienced	–0.83
12	Experimental	Inexperienced	–3.05
13	Experimental	Inexperienced	–5.98
14	Experimental	Inexperienced	–3.64
15	Experimental	Inexperienced	–7.38
16	Experimental	Inexperienced	–3.60
17	Experimental	Inexperienced	–0.94
18	Control	Experienced	–3.39
19	Control	Experienced	–4.00
20	Control	Experienced	–2.31
21	Control	Experienced	–3.60
22	Control	Experienced	–7.69
23	Control	Experienced	–13.92
24	Control	Experienced	–7.64
25	Control	Experienced	–7.59
26	Control	Experienced	–1.62
27	Control	Experienced	–12.21
28	Control	Experienced	–8.85
29	Control	Inexperienced	5.84
30	Control	Inexperienced	1.71
31	Control	Inexperienced	–4.10
32	Control	Inexperienced	–5.19
33	Control	Inexperienced	0.00
34	Control	Inexperienced	–2.80

plot of medians is sometimes a good place to start because it may highlight possible distribution problems with the data. The required plots may be constructed using the plot.design function.

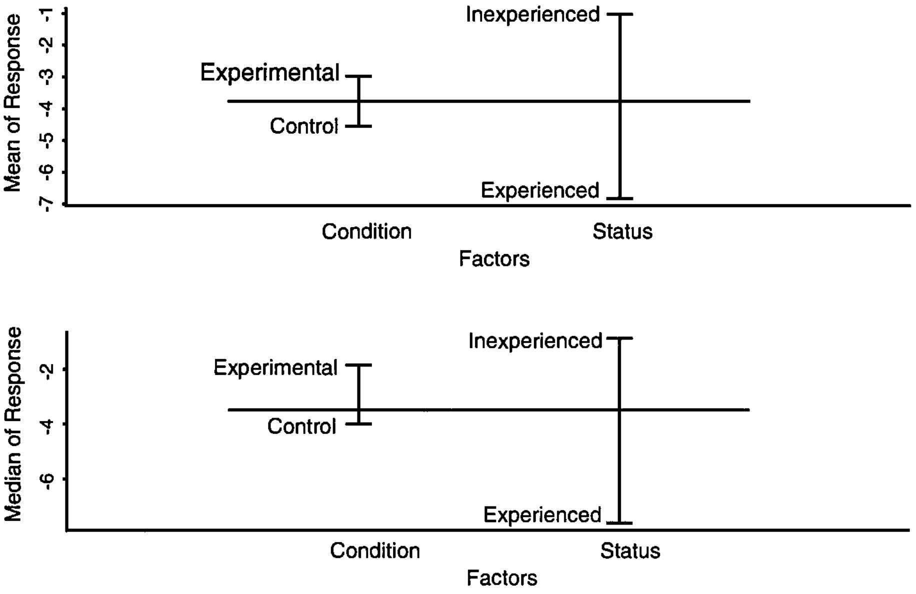


Figure 3.6 Plots of means and medians for slimming data.

```
par(mfrow=c(2,1))
#sets up plotting area to take both mean and
#median plots
plot.design(slim)
plot.design(slim,fun=median)
#fun=median specifies that the medians are to
#be plotted; the default is the mean
```

The resulting diagram is shown in Figure 3.6. There is some difference between treatment means and medians, particularly for the Conditions factor. This may result from one or two outliers and we can examine this possibility with a further simple diagram, namely, a box plot of the observations at each level of each factor; this is constructed using the plot.factor function.

```
par(mfrow=c(2,1))
plot.factor(slim)
```

The resulting diagram appears in Figure 3.7. A number of outliers are revealed in this diagram. There is, for example, one participant in the experimental group with a very large decrease in weight (–22.03) and in

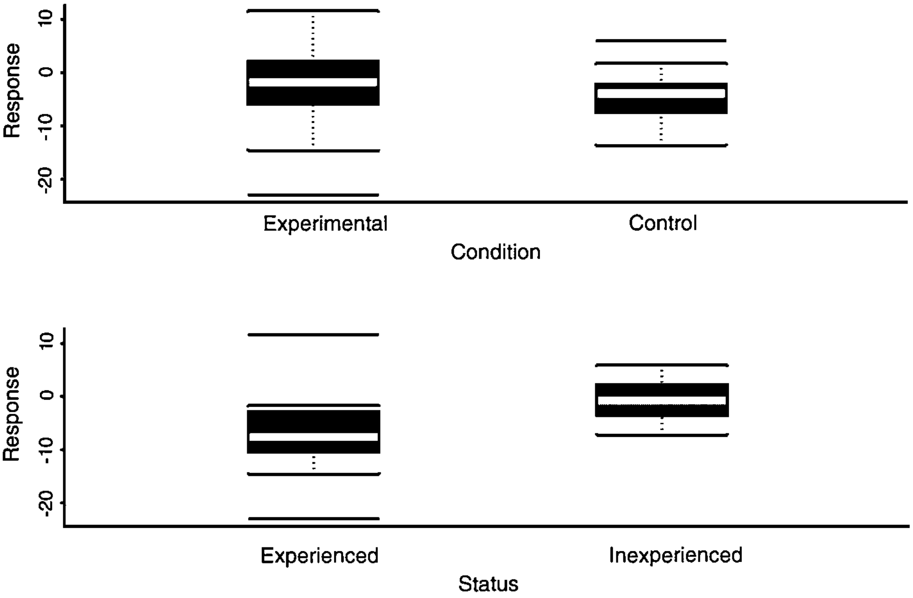


Figure 3.7 Box plots for slimming data.

the 'experienced' slimmers group there is one person with a large increase in weight (11.61). Consideration might be given to removing these observations but here we shall continue to include them in our analyses, and leave the reader to investigate the former possibility (see Exercise 3.2).

Now we will use the aov function to fit various analysis of variance models to the data, beginning with models including only the main effect of Condition and then the main effects of both Condition and Status.

```
summary(aov(Response~Condition,data=slim))
# the aov function requires a valid S-PLUS
# formula and, if not already attached,
# the name of a data frame.
# aov returns an analysis of variance object
# which when given to the summary function
# produces an analysis of variance table etc
summary(aov(Response~Condition+Status,data=slim))
```

The results are shown in Table 3.9. Now rerun, taking Status first followed by Condition (we now assume that the slim data frame is attached).

Table 3.9 Analyses of Variance of the Slimming Data with Status Added after Condition

```
> summary(aov(Response ~ Condition))
           Df  Sum of Sq  Mean Sq  F Value    Pr(F)
Condition   1         21    21.19   0.5041   0.4828
Residuals  32       1345    42.03
> summary(aov(Response ~ Condition + Status))
           Df  Sum of Sq  Mean Sq  F Value    Pr(F)
Condition   1         21     21.2    0.609   0.4412
   Status   1        266    265.9    7.640   0.0095
Residuals  31       1079     34.8
```

Table 3.10 Analyses of Variance of the Slimming Data with Condition Added after Status

```
> summary(aov(Response ~ Status))
           Df  Sum of Sq  Mean Sq  F Value     Pr(F)
   Status   1        285    285.0    8.435  0.006621
Residuals  32       1081     33.8

> summary(aov(Response ~ Status + Condition))
           Df  Sum of Sq  Mean Sq  F Value     Pr(F)
   Status   1        285    285.0    8.187    0.0075
Condition   1          2      2.1    0.061    0.8062
Residuals  31       1079     34.8
```

```
summary(aov(Response~Status))
summary(aov(Response~Status+Condition))
```

The results of these two commands are shown in Table 3.10. Notice how the sums of squares for each factor differ depending on whether they appear first or second in the model. This would not be the case if the design were balanced (readers can confirm this by using the series of commands above, suitably amended, to analyse the data in the rats data frame).

Finally, we can fit a model containing both main effects and the interaction,

```
summary(aov(Response~Status*Condition))
```

to give the results shown in Table 3.11. Clearly, the interaction is not significant, and the earlier results show that the levels of the Condition

Table 3.11 Analysis of Variance of Slimming Data

```
> summary(aov(Response ~ Status + Condition + Status:
          Condition))
                   Df   Sum of Sq   Mean Sq   F Value    Pr(F)
           Status   1         285     285.0     7.924   0.0085
        Condition   1           2       2.1     0.059   0.8094
 Status:Condition   1           0       0.1     0.004   0.9524
        Residuals  30        1079      36.0
```

factor do not have different means, but that there is a significant difference in the means of Experienced and Inexperienced slimmers. The two means can be found by again using the **tapply** function.

```
tapply(Response,list(Status),mean)
```

giving

```
Experienced    Inexperienced

   -6.832          -1.032
```

Experienced slimmers show, on average, a greater weight decrease than inexperienced slimmers.

Exercises

3.1. Reanalyse the survival times of rats data after taking a log transformation. Examine the residuals from whatever model you now find is appropriate to assess whether the normality and constant variance assumptions are met more satisfactorily than when modelling the raw data.

3.2. Reanalyse the slimming data after removing the two possible outliers identified in the text. Are the conclusions from the analysis the same as those discussed in the text?

3.3. Use the **predict** function on the results of a main effects analysis of variance model for the survival time data to find the fitted values. What do these fitted values correspond to in terms of Poison and Treatment means?

3.4. Investigate what happens if the **aov** function is applied to the slimming data with the Status × Condition interaction listed before the main effects of the two factors.

Chapter 4

Multiple Regression: Technological Change in Jet Fighters

4.1 Description of Data

The data to be used in this chapter were introduced previously in Chapter 1; see Table 1.1. The data give the values of six variables for 22 U.S. fighter aircraft. The variables are as follows:

FFD: First flight date, in months after January 1940
SPR: Specific power, proportional to power per unit weight
RGF: Flight range factor
PLF: Payload as a fraction of gross weight of aircraft
SLF: Sustained load factor
CAR: A binary variable specifying whether the aircraft can or cannot land on a carrier

Interest lies in modelling FFD as a function of the other variables. Here we shall concentrate on using *multiple regression*.

4.2 Multiple Regression Model

The multiple regression model has the general form

$$y_i = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \beta_p x_{ip} + \epsilon_i \tag{4.1}$$

where y_i and x_{i1}, x_{i2} … x_{ip} are, respectively, the values of a response variable and p explanatory variables for the ith observation in a sample of size n. The *regression coefficients,* β_0, β_1 … β_p are generally estimated by least squares — they represent the expected change in the response variable predicted by a unit change in the corresponding explanatory variables conditional on the values of the remaining explanatory variables. Significance tests for the regression coefficient can be derived by assuming that the residual terms ϵ_i, $i = 1$ … n, are from a normal distribution with zero mean and constant variance σ^2.

For n observations of the response and explanatory variables, the regression model may be written concisely as

$$\boldsymbol{y} = \boldsymbol{X}\beta + \epsilon \tag{4.2}$$

where $\boldsymbol{y}$ is the $n \times 1$ vector of responses, $\boldsymbol{X}$ is an $n \times (p + 1)$ matrix of known constants, the first column containing a series of ones corresponding to the term β_0 in Equation 4.1 and the remaining columns values of the explanatory variables. The elements of the vector β are the regression coefficients β_0 … β_p and those of the vector ϵ, the residual terms ϵ_1 … ϵ_n.

Full details of multiple regression are given in Rawlings (1988).

4.3 Analysis Using S-PLUS

The data are stored in the data frame **jets**, the contents of which are shown in Table 4.1.

Before proceeding with the regression modelling of the data it may be helpful to examine a scatterplot matrix of the variables, particularly if we label the points by aircraft type. By using the GUI, this involves the following:

- Click **Graph**.
- Select **2D**.
- Highlight **Matrix** under **Axes Type**, and click **OK**.
- Select the **jets** data set.
- In the x columns box highlight all variables but **Type** and **CAR**.
- In the y columns box highlight **Type**.

Table 4.1 The jets Data Frame

	Type	FFD	SPR	RGF	PLF	SLF	CAR
1	FH-1	82	1.468	3.30	0.166	0.10	Cannot land
2	FJ-1	89	1.605	3.64	0.154	0.10	Cannot land
3	F-86A	101	2.168	4.87	0.177	2.90	Can land
4	F9F-2	107	2.054	4.72	0.275	1.10	Cannot land
5	F-94A	115	2.467	4.11	0.298	1.00	Can land
6	F3D-1	122	1.294	3.75	0.150	0.90	Cannot land
7	F-89A	127	2.183	3.97	0.000	2.40	Can land
8	XF10F-1	137	2.426	4.65	0.117	1.80	Cannot land
9	F9F-6	147	2.607	3.84	0.155	2.30	Cannot land
10	F-100A	166	4.567	4.92	0.138	3.20	Can land
11	F4D-1	174	4.588	3.82	0.249	3.50	Cannot land
12	F1F-1	175	3.618	4.32	0.143	2.80	Cannot land
13	F-101A	177	5.855	4.53	0.172	2.50	Can land
14	F3H-2	184	2.898	4.48	0.178	3.00	Cannot land
15	F-102A	187	3.880	5.39	0.101	3.00	Can land
16	F-8A	189	0.455	4.99	0.008	2.64	Cannot land
17	F-104B	194	8.088	4.50	0.251	2.70	Can land
18	F-105B	197	6.502	5.20	0.366	2.90	Can land
19	YF-107A	201	6.081	5.65	0.106	2.90	Can land
20	F-106A	204	7.105	5.40	0.089	3.20	Can land
21	F-4B	255	8.548	4.20	0.222	2.90	Cannot land
22	F-111A	328	6.321	6.45	0.187	2.00	Can land

- Click on the **Symbol** tab and tick the **Use Text As Symbol** box.
- Specify *y* column as **Text to Use**.
- Click **OK**.

This leads to the labelled scatterplot matrix seen in Figure 4.1. In some panels fighter F-111A seems to be a possible outlier, as, to a lesser extent, does the F-105B. But at this stage it seems unwise to remove them, particularly given the small sample size.

Some of the panels in Figure 4.1 suggest perhaps that the relationship between some pairs of variables, at least, are nonlinear, for example, SPR and SLF. To investigate this possibility further before undertaking formal modelling of the data, we can plot the simple regression line linking each pair of variables onto the appropriate panel and a *locally weighted regression fit* (see Chambers and Hastie, 1992, for comparison). To avoid cluttering each scatterplot in the diagram we shall in this case not label

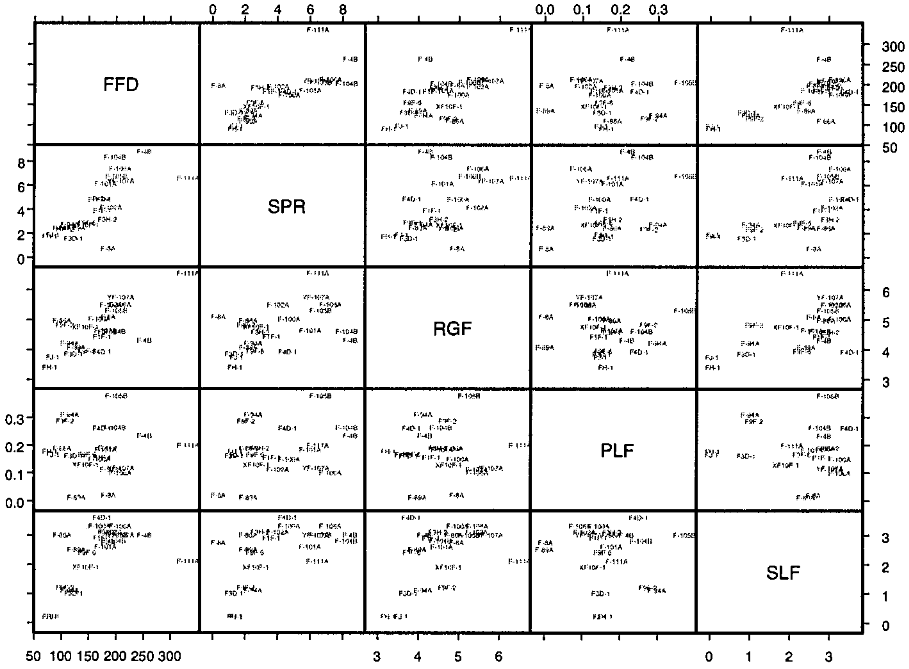


Figure 4.1 Scatterplot matrix of the variables in the jets data frame with points labelled by type of aircraft.

the plot with type of aircraft. With the command language, the required diagram can be found as follows:

```
attach(jets)
pairs(jets[,-c(1,7)],panel=function(x, y){
    points(x,y,pch=5)
    abline(lm(y~x))
    lines(lowess(x,y),lty=2)})
#
#first the Type and CAR variables are removed
#from the data frame prior to plotting
#In the panel function the points function is
#used to plot the data on each panel using
#plotting character number 5, the linear
#modelling function lm is used to regress the
#y variable on the x variable, and the result
#used by abline to plot the fitted regressions
```

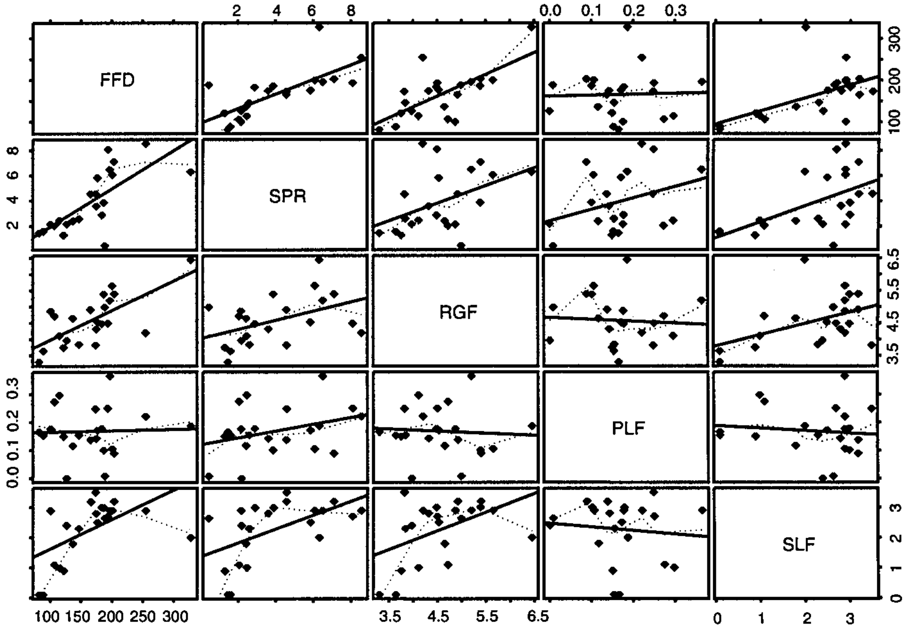


Figure 4.2 Scatterplot matrix of the variables in the jets data frame showing fitted lines and locally weighted regressions.

```
#finally lines and lowess are used to plot
#the results of a locally weighted regression
#with a different line type from the linear regression fit
```

The resulting diagram is shown in Figure 4.2.

In some of the panels the locally weighted regression fit differs considerably from the linear fit, confirming in some respect our suspicion about the form of the relationship between some pairs of variables. But for the moment, at least, we shall ignore this possible complication and find the results of the usual multiple regression model on the data. Using again the command line language, the model can be applied using the lm function.

```
jets.fit<-lm(FFD~SPR+RGF+PLF+SLF+CAR)
#stores the results of applying lm in jets.fit
summary(jets.fit)
```

The results are shown in Table 4.2. We see that the five explanatory variables account for about 80% (Multiple R-Squared is 0.7967) of the variability of FFD. The most predictive variables appear to be SPR, RGF, and CAR, although since the regression coefficients and their standard

Table 4.2 Fitting the Multiple Regression Model Using the lm Function

```
> jets.fit <- lm(FFD ~ SPR + RGF + PLF + SLF + CAR)
> summary(jets.fit)

Call: lm(formula = FFD ~ SPR + RGF + PLF + SLF + CAR)
Residuals:
   Min      1Q    Median     3Q    Max
–44.48  –13.85   0.04965  14.96  64.91

Coefficients:
                 Value  Std. Error   t value  Pr(>|t|)
(Intercept)   –89.4837     51.8632   –1.7254    0.1037
        SPR    15.8788      3.9359    4.0343    0.0010
        RGF    43.9766     11.2427    3.9116    0.0012
        PLF   –84.1065     85.1941   –0.9872    0.3382
        SLF     2.6411      8.3655    0.3157    0.7563
        CAR   –20.9991      7.9932   –2.6271    0.0183

Residual standard error: 29.41 on 16 degrees of freedom
Multiple R-Squared: 0.7967
F-statistic: 12.54 on 5 and 16 degrees of freedom, the p-value
  is 0.00004569

Correlation of Coefficients:
           (Intercept)       SPR       RGF      PLF      SLF
       SPR      0.1632
       RGF     –0.9042   –0.1540
       PLF     –0.3764   –0.4774    0.1328
       SLF     –0.0902   –0.4866   –0.2152   0.3039
       CAR      0.4949   –0.2474   –0.4388   0.0317   0.0157
```

errors are estimated *conditionally* on the other variables such an interpretation needs to be made with caution. Removing one of the nonsignificant explanatory variables and reestimating the remaining coefficients might lead to a different picture. We can investigate this further by fitting a variety of models and comparing their fits using the anova function; for example,

```
jets.fit1<-lm(FFD~SPR)
jets.fit2<-lm(FFD~SPR+RGF)
anova(jets.fit1,jets.fit2)
```

Table 4.3 Comparing Models Using the anova Function

```
> jets.fit1 <- lm(FFD ~ SPR)
> jets.fit2 <- lm(FFD ~ SPR + RGF)
> anova(jets.fit1, jets.fit2)
Analysis of Variance Table

Response: FFD

      Terms  Resid. Df      RSS    Test  Df  Sum of Sq   F Value        Pr(F)
1       SPR         20  32273.65
2  SPR + RGF        19  20896.87  +RGF    1   11376.78  10.34407  0.004545782
```

Table 4.4 Comparing Models

```
> anova(jets.fit2, jets.fit3)
Analysis of Variance Table

Response: FFD

              Terms  Resid. Df       RSS    Test  Df   Sum of Sq   F Value
1         SPR + RGF         19  20896.87
2   SPR + RGF + CAR         18  15043.81   +CAR   1    5853.064  7.003223
              Pr(F)
1
2        0.01641463
```

gives the output shown in Table 4.3. The addition of RGF after SPR reduces the residual sum of squares by 11,377 which has an associated p value of 0.0045 — highly significant. Now let's see if adding CAR is worthwhile:

```
jets.fit3<-lm(FFD~SPR+RGF+CAR)
anova(jets.fit2,jets.fit3)
```

Here the results shown in Table 4.4 confirm that CAR adds significantly to the prediction of FFD after SPR and RGF have been used.

Repeating this process with the remaining two variables, PLF and SLF, shows that neither contribute significantly after SPR, RGF, and CAR. We can now find the estimated parameters and their standard errors in this reduced model from

```
summary(jets.fit3)
```

Table 4.5 Estimated Regression Coefficients etc. for Selected Model

```
> summary(jets.fit3)

Call: lm(formula = FFD ~ SPR + RGF + CAR)
Residuals:
   Min       1Q   Median      3Q     Max
–58.58   –18.07    4.482   14.59   58.25

Coefficients:
                 Value   Std. Error   t value   Pr(>|t|)
(Intercept)  –109.6063     47.2135   –2.3215    0.0322
        SPR    14.9359      3.1038    4.8121    0.0001
        RGF    47.4005     10.5445    4.4953    0.0003
        CAR   –20.7819      7.8530   –2.6464    0.0164

Residual standard error: 28.91 on 18 degrees of freedom
Multiple R-Squared: 0.7791
F-statistic: 21.16 on 3 and 18 degrees of freedom, the p-
  value is 3.957e-006

Correlation of Coefficients:
        (Intercept)      SPR       RGF
 SPR      –0.0099
 RGF      –0.9590   –0.2439
CAR        0.5474   –0.2868   -0.4627
```

giving the results shown in Table 4.5. [Note that since S-PLUS codes the levels of CAR, 1 (can land) and –1 (cannot land) by default, the estimated parameter for CAR and its standard error need to be doubled to give the effect corresponding to a 1, 0 coding.]

The next stage in the analysis should be an examination of the residuals from fitting the chosen model to check on the normality and constant variance assumptions. The most useful plots of these residuals are as follows:

- A plot of residuals against each explanatory variable in the model. The presence of a nonlinear relationship, for example, may suggest that a higher-order term in the explanatory variable should be considered.
- A plot of residual against fitted values. If the variance of the residuals appears to increase with predicted value, a transformation of the response variable may be in order.

- A normal probability plot of the residuals. After all the systematic variation has been removed from the data, the residuals should look like a sample from a standard normal distribution. A plot of the ordered residuals against the expected order statistics from a normal distribution provides a graphical check of this assumption.

Unfortunately, the basic 'observed-fitted' residuals suffer from having a distribution that is scale dependent because their variance is a function of both σ^2 and the diagonal values of the so-called hat matrix, **H**, given by

$$\mathbf{H} = \mathbf{X}\left(\mathbf{X}'\mathbf{X}\right)^{-1}\mathbf{X}' \tag{4.3}$$

where **X** is the matrix introduced in Section 4.2. (See Cook and Weisberg, 1982, for a full explanation of the hat matrix.) Consequently, it is rather more useful to work with standardized residuals $r_i^{(\text{std})}$ given by

$$r_i^{(\text{std})} = \frac{y_i - \hat{y}_i}{s\sqrt{1 - h_{ii}}} \tag{4.4}$$

where s^2 is the usual estimate of σ^2 obtained as the residual mean square from the model fitting, y_i is the observed response value, $\hat{y}_i$ is the value predicted from the fitted model, and h_{ii} is the *i*th element in the main diagonal of **H**. These standardised residuals are easily calculated using the lm.influence function:

```
s<-summary(jets.fit3)$sigma
#gives the required value of s in 4.4
h<-lm.influence(jets.fit3)$hat
#gives the vector of the main diagonal elements
#of the hat matrix in 4.3
jets.res<-residuals(jets.fit3)/(s*sqrt(1-h))
#the residuals function gives the basic observed fitted
#residuals from jets.fit3
```

We may now plot these standardised residuals in a number of ways:

```
#construct plots of the standardised residuals
#against each of the three explanatory variables
par(mfrow=c(1,3))
#set up plotting area to take all three plots
```

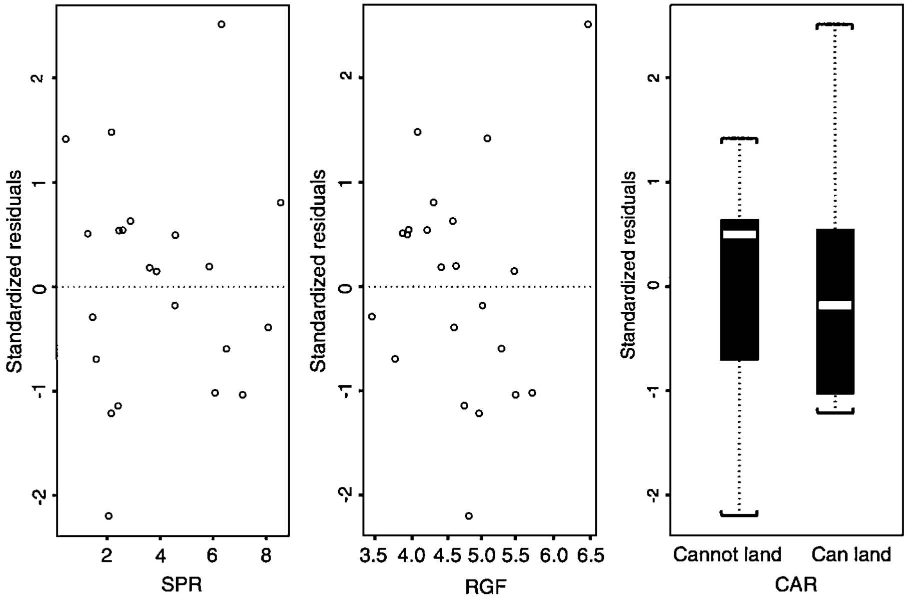


Figure 4.3 Standardised residuals for regression model fitted to jet fighter data plotted against variables SPR, RGF, and CAR.

```
plot(SPR,jets.res,ylab="Standardised residuals")
abline(h=0,lty=2)
#add dotted horizontal line at y=0
plot(RGF,jets.res,ylab="Standardised residuals")
abline(h=0,lty=2)
plot(CAR,jets.res,ylab="Standardised residuals")
```

This leads to Figure 4.3. It is also helpful to have the numerical values of the observed values, fitted values, and the standardised residuals; these are all given in Table 4.6 and were obtained using

```
cbind(FFD,predict(jets.fit3),jets.res)
#the predict function gives the fitted value from the
#model; the function cbind combines the three
#vectors into a matrix
```

It is standardised residuals outside of the interval (–2, 2) that give most cause for concern. Here there are two, aircraft number 4 (F9F-2), where the predicted value of FFD is considerably higher than the observed value,

Table 4.6 Observed and Predicted Values of FFD and the Corresponding Residual Values

```
> cbind(FFD, predict(jets.fit3), jets.res)
      FFD                    jets.res
  1    82     89.5231    –0.2887851
  2    89    107.6855    –0.6938394
  3   101    132.8333    –1.2158725
  4   107    165.5842    –2.1976956
  5   115    101.2748     0.5402804
  6   122    108.2545     0.5095121
  7   127     90.3969     1.4806494
  8   137    167.8224    –1.1429785
  9   147    132.1314     0.5431492
 10   166    171.0346    –0.1829026
 11   174    160.7714     0.4965961
 12   175    169.9838     0.1827579
 13   177    171.7859     0.1940028
 14   184    166.8140     0.6282893
 15   187    183.0519     0.1468159
 16   189    154.4998     1.4155201
 17   194    203.7158    –0.3911602
 18   197    213.2078    –0.5962569
 19   201    228.2499    –1.0206190
 20   204    231.6942    –1.0368842
 21   255    237.9299     0.8020890
 22   328    269.7550     2.5074932
```

and aircraft number 22 (F-111A), where the reverse is the case. Apart from these two outliers, the residuals in Figure 4.3 look reasonably well behaved.

Finally, we can look at a normal probability plot of the standardised residuals using

```
qqnorm(jets.res)
qqline(jets.res)
```

leading to Figure 4.4.

The interpretation of a normal probability plot is often unclear, particularly when, as with these data on jet fighters, there are only a relatively small number of observations. The plot can be made more informative by supplementing it with a confidence interval, as suggested in Atkinson

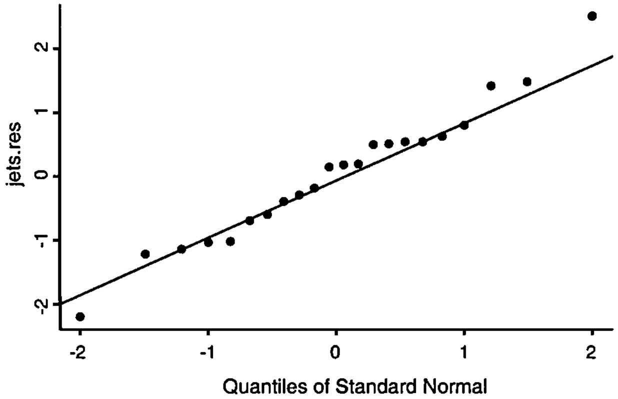


Figure 4.4 Normal probability plot of standardised residuals from model fitted to jet fighter data.

(1987) and Cook and Weisberg (1982). In essence, the procedure involves the generation of *m pseudo-residual* vectors, **e,** from

$$e_k = \left(\mathbf{I} - \mathbf{H}\right)\epsilon_k, \quad k = 1,\ldots,m \tag{4.5}$$

where the ϵ_k are $n \times 1$ vectors of standard normal variates.

Suitable code for the construction of such an enhanced probability plot using 100 simulations is as follows:

```
#first change strings for categories of CAR to 0 and 1
#
jets$CAR<-factor(jets$CAR,levels=c(“Can not land”,“Can land”),
labels=c(0,1))
#
#
jets.one<-cbind(rep(1,22),jets[,c(3,4,7)])
#store the three explanatory variables SPR, RGF and CAR
#chosen for the final model along with
#a column of ones to get the usual X matrix used in
#multiple regression
#
#
jets.one<-as.matrix(jets.one)
#
```

```
#get hat matrix as defined in Equation 4.3
#
jets.hat<-
jets.one%*%solve(t(jets.one)%*%jets.one)%*%t(jets.one)
#
#construct a diagonal matrix as required in Equation 4.5
#
ident<-diag(22)
#
#generate 100 sets of 22 standard normal variables, i.e., 2200
normal variates
#
set.seed(547)
epsilon<-matrix(rnorm(100*22,0,1),ncol=100)
#
#apply Equation 4.5 to get pseudo-residuals
#
e<-(ident-jets.hat)%*%epsilon
#
#now tranpose e and sort the elements in the columns
#save the 5th and 95th ranked values and then get the
#range of each column to give the required values for the
#95% CI for the probability plot
#
e<-t(e)
e<-apply(e,2,sort)
e<-e[5:95,]
E<-apply(e,2,range)
#
#now get a normal probability plot of the standardised residuals
#with the confidence limits
#
win.graph()
ylim<-range(jets.res,E[1,],E[2,])
qqnorm(jets.res,ylim=ylim,ylab=“Standardised residuals”)
par(new=T)
qqnorm(sort(E[1,]),type=“l”,axes=F,ylim=ylim,xlab=” “,ylab=“ ”)
par(new=T)
qqnorm(sort(E[2,]),type=“l”,axes=F,ylim=ylim,xlab=“ ”,ylab=“ ”)
```

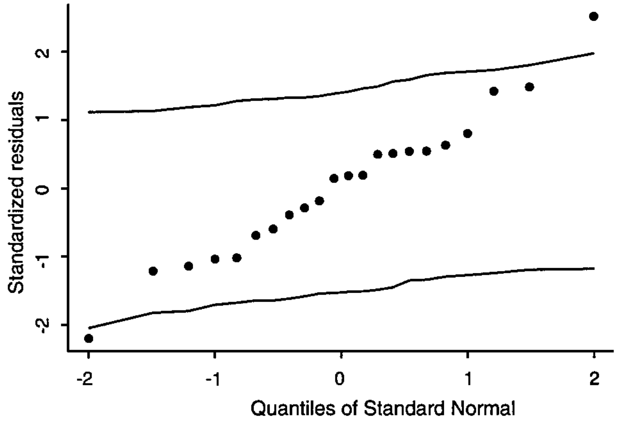


Figure 4.5 Normal probability plot of standardised residuals from model fitted to jet fighter data with added confidence interval.

The resulting plot is shown in Figure 4.5. The first and last observations fall outside the constructed confidence interval, and it may be worthwhile rerunning the regression analysis after removing these two observations.

Exercises

4.1. Investigate the use of the plot function with a regression object from using the lm function. Try, for example, both plot(jets.fit3) and plot(jets.fit3,ask=T).

4.2. Investigate the use of the **Stepwise Linear Regression** dialog for selecting a parsimonious model with which to describe the jet fighter data.

4.3. Other researchers dealing with the jets data have used a log transformation of FFD. Examine whether this approach leads to conclusions different from those reached in the text.

4.4. Many other regression diagnostics are available apart from those described in the text; see Rawlings (1988) for a good description. Use the **Linear Regression** dialog to investigate the use of some of these data, particularly *Cook's distance* and *partial residuals*, on the final model selected in the text for the jet fighter.

Chapter 5

Logistic Regression: Psychiatric Caseness and Mortgage Default

5.1 Description of Data

In this chapter we shall look at two data sets from very different application areas. The first, shown in Table 5.1, consists of data collected during a study of a psychiatric screening questionnaire, the *General Health Questionnaire* or GHQ (see Goldberg, 1972), designed to help identify possible psychiatric 'caseness'.

The second data set, kindly supplied by Professor David Hand and shown in Table 5.2, arises from an investigation into the reasons for mortgage default.

In the first of the two data sets, interest lies in assessing whether GHQ score is predictive of 'caseness' and whether the sex of a subject plays a role in this prediction. In the second data set the main question is whether any of the four explanatory variables might be used to identify mortgage loans at risk of default.

5.2 Logistic Regression and Generalised Linear Models

In essence, the same general question is addressed by both data sets introduced in the previous section, namely, 'can a particular response

Table 5.1 Psychiatric Data

ghqscore	sex	case	nocase
0	0	4	80
1	0	4	29
2	0	8	15
3	0	6	3
4	0	4	2
5	0	6	1
6	0	3	1
7	0	2	0
8	0	3	0
9	0	2	0
10	0	1	0
0	1	1	36
1	1	2	25
2	1	2	8
3	1	1	4
4	1	3	1
5	1	3	1
6	1	2	1
7	1	4	2
8	1	3	1
9	1	2	0
10	1	2	0

Gender is coded 0 for women and 1 for men.

variable be predicted from a set of explanatory variables?' This is the same question that is addressed by the multiple regression model that was the subject of the previous chapter, so readers might ask why are we considering it again here? The reason is that the response variable for each data set in Section 5.1 is now binary rather than continuous — case or not case for the data in Table 5.1 and defaulted on loan or not for the second. We could, of course, simply ignore this aspect of the data and, as in the previous chapter, model the expected value of the response as a linear function of the explanatory variables. For a binary variable this expected value is simply the probability of the 'one' category of the variable, so for the psychiatric data, for example, our model would be

$$p = \Pr(\text{of being a case}) = \beta_0 + \beta_1 \text{sex} + \beta_2 \text{ghq} \tag{5.1}$$

Table 5.2 Mortgage Default Data

	EVER90	FICO	LTV	INCOME	CA
1	1	576	0.86	5	0
2	1	678	0.90	3	1
3	1	693	0.80	5	0
4	1	669	0.75	4	0
5	1	542	0.95	4	0
6	1	566	0.95	3	0
7	1	643	0.84	5	0
8	0	785	0.58	5	0
9	1	461	0.80	4	0
10	0	785	0.85	5	0
11	1	620	0.95	3	0
12	0	792	0.79	3	0
13	0	748	0.90	4	0
14	1	661	0.75	5	0
15	0	753	0.70	5	0
16	0	747	0.95	4	0
17	0	720	0.88	5	0
18	0	717	0.89	4	0
19	0	763	0.90	5	0
20	1	782	0.90	4	1
21	0	758	0.42	5	0
22	0	697	0.80	5	0
23	1	690	0.75	2	0
24	0	746	0.90	5	1
25	0	679	0.70	5	0
26	0	767	0.80	2	0
27	0	733	0.88	5	0
28	0	679	0.75	2	0
29	0	765	0.36	3	0
30	0	678	0.95	5	0
31	0	782	0.62	4	0
32	0	777	0.80	5	0
33	0	765	0.63	5	0
34	0	769	0.59	5	0
35	0	720	0.38	5	0
36	0	758	0.90	4	0
37	0	724	0.70	5	0
38	1	611	0.90	5	0
39	0	639	0.61	5	0
40	0	761	0.50	3	0

Table 5.2 (Continued) Mortgage Default Data

	EVER90	FICO	LTV	INCOME	CA
41	1	549	0.66	3	0
42	0	639	0.68	6	0
43	0	719	0.61	5	0
44	0	801	0.73	2	0
45	0	765	0.90	5	0
46	1	598	0.95	5	0
47	1	603	0.95	4	0
48	0	710	0.67	2	0
49	0	774	0.48	5	0
50	0	738	0.73	5	0
51	1	676	0.73	3	0
52	0	768	0.78	5	0
53	0	765	0.90	5	0
54	0	766	0.87	5	0
55	0	729	0.90	4	0
56	0	766	0.68	5	0
57	1	671	0.75	1	0
58	0	782	0.80	2	0
59	1	756	0.75	2	0
60	0	791	0.89	4	0
61	1	650	0.85	3	0
62	0	704	0.75	3	0
63	1	664	0.80	8	1
64	0	762	0.62	4	0
65	0	733	0.70	3	0
66	1	634	0.95	5	1
67	0	797	0.26	3	1
68	1	624	0.90	5	1
69	0	749	0.70	2	0
70	0	687	0.95	3	0
71	0	732	0.72	4	1
72	0	669	0.80	5	0
73	0	692	0.79	5	0
74	0	777	0.80	3	1
75	0	682	0.47	4	1
76	0	772	0.80	5	0
77	0	809	0.75	5	0
78	0	728	0.74	5	0
79	0	669	0.67	5	1
80	1	692	0.75	4	0

Table 5.2 (Continued) Mortgage Default Data

	EVER90	FICO	LTV	INCOME	CA
81	0	721	0.75	5	0
82	1	742	0.69	5	0
83	0	687	0.79	2	0
84	0	696	0.83	5	1
85	1	586	0.90	5	0
86	0	727	0.80	3	1
87	0	725	0.80	7	0
88	1	652	0.95	5	1
89	1	722	0.80	5	1
90	1	606	0.80	4	0
91	0	761	0.80	5	0
92	0	777	0.80	5	0
93	0	629	0.29	5	0
94	1	742	0.74	3	0
95	0	752	0.61	2	0

EVER90: takes value 1 if loan has ever been 90 days past due date during a specified time period, 0 otherwise.
FICO: a credit score provided by Fair Isaac Company.
LTV: ratio of loan amount to value of home.
INCOME: income category of borrower.
CA takes value 1 if home in California, 0 otherwise.

We could then estimate the three regression coefficients, β_0, β_1, and β_2 by least squares as in the previous chapter. Unfortunately, this approach is not satisfactory for two reasons;

1. It can lead to fitted values for the probability of being a case outside the interval (0,1).
2. The normality assumption needed in Chapter 4 to derive significance tests for model parameters is clearly not reasonable for a binary response.

A more suitable approach to modelling a binary response is to use *logistic regression*. Here the expected value of the response variable is not modelled directly; instead, the *logistic function* of the expected value is used, so the model for the psychiatric data becomes

$$\log \frac{p}{1-p} = \beta_0 + \beta_1 \text{sex} + \beta_2 \text{ghq} \tag{5.2}$$

(β_0, β_1, and β_2 will not, of course, be the same as in Equation 5.1).

The logistic transformation gives the *log odds* of being a case, and by now assuming a *binomial distribution* for the observed response, the parameters in Equation 5.2 can be estimated by maximum likelihood (see Collett, 1991, for details). In terms of p, the model in Equation 5.2 can be rewritten as

$$p = \frac{\exp[\beta_0 + \beta_1 \text{sex} + \beta_2 \text{ghq}]}{1 + \exp[\beta_0 + \beta_1 \text{sex} + \beta_2 \text{ghq}]} \tag{5.3}$$

Fitted values of p will now lie in the interval (0,1) as required.

The estimated regression coefficients in a logistic regression model give the estimated change in the log odds corresponding to a unit change in the corresponding explanatory variable. For easier interpretation, the parameters are usually exponentiated to give the estimated change in the odds, conditional on the other variables remaining constant.

Logistic regression and the other modelling procedures used in earlier chapters, analysis of variance and multiple regression, can all be shown to be special cases of the *generalised linear model* formulation described in detail in McCullagh and Nelder (1989). In essence, this approach postulates a linear model for a suitable transformation of the expected value of a response variable and allows for a variety of different error distributions. The possible transformations are known as *link functions*. For multiple regression and analysis of variance, for example, the link function is simply the identity function, so the expected value is modelled directly, and the corresponding error distribution is normal. For logistic regression, the link function is logistic and the appropriate error distribution is the binomial. Many other possibilities are opened up by the generalised linear model formulation; see McCullagh and Nelder (1989) for full details.

5.3 Analysis Using S-PLUS

Logistic regression is available in S-PLUS via the generalised linear model function, glm, or by using the **Logistic Regression** dialog. Both possibilities will be used in the following subsections.

5.3.1 GHQ Data

We shall assume that the GHQ data are available as an S-PLUS data frame ghq, the contents of which are shown in Table 5.3. (Note that the data have been grouped to give the total number of cases and noncases for

Table 5.3 Contents of ghq Data Frame

```
> ghq
      ghqscore   sex   case   nocase
  1       0       0      4      80
  2       1       0      4      29
  3       2       0      8      15
  4       3       0      6       3
  5       4       0      4       2
  6       5       0      6       1
  7       6       0      3       1
  8       7       0      2       0
  9       8       0      3       0
 10       9       0      2       0
 11      10       0      1       0
 12       0       1      1      36
 13       1       1      2      25
 14       2       1      2       8
 15       3       1      1       4
 16       4       1      3       1
 17       5       1      3       1
 18       6       1      2       1
 19       7       1      4       2
 20       8       1      3       1
 21       9       1      2       0
 22      10       1      2       0
```

each combination of the two explanatory variables; originally, however, the data would have consisted of whether or not each subject was a case.)

We shall use the command language approach to analyse these data using the glm function to apply logistic regression. To begin, we shall consider only the single explanatory variable ghqscore.

```
p<-case/(case+nocase)
ghq<-data.frame(ghq,p)
attach(ghq)
#first calculate the proportion of cases and then
#insert into the ghq data frame
fit.lin<-glm(p~ghqscore)
#the default when using glm is the equivalent of
#using the lm function, i.e., simple linear or
#multiple regression. We fit this model first
```

```
#to be able to compare the results with those
#obtained from logistic regression using
fit.log<-glm(p~ghqscore,family=binomial,
weights=case+ncase)
#the argument family=binomial implements a
# binomial distribution and if no link is
#specified uses the logistic with the binomial choice.
#Since the observations are grouped the weights
#argument must be used to give the total number
#of observations on which each observed proportion is
#based.
summary(fit.lin)
summary(fit.log)
```

The results are shown in Table 5.4. In both models the regression coefficient for the GHQ variable is highly significant. The *deviance* term that occurs in Table 5.4 measure lack of fit. Specifically, it is minus twice the difference between the maximized log-likelihood of the model and the maximum likelihood achievable, i.e., the maximized likelihood of the full or saturated model. For normal distributions, the deviance is simply the well-known *residual sum of squares*. The difference in deviance between two competing models can be used to compare them, by referring its value to a chi-square distribution with degrees of freedom equal to the difference in the degrees of freedom of the two models.

Now we can use the predict function to look at the predicted values from each model:

```
lin.pred<-predict(fit.lin)
log.pred<-exp(predict(fit.log))/(1+exp(predict(fit.log)))
cbind(lin.pred,log.pred)
```

The fitted values are shown in Table 5.5. (Note that the first 11 equal the second 11 since they correspond to the same GHQ scores, 0 to 10.) A problem that immediately becomes apparent with the simple linear regression model is that some of its predictions are greater than 1. A graphical comparison of the fits along with the observed proportions is also helpful here, and can be obtained as follows:

```
Case<-case[1:11]+case[12:22]
Nocase<-nocase[1:11]+nocase[12:22]
P<-Case/(Case+Nocase)
#calculate the observed proportions of cases
```

Table 5.4 Linear and Logistic Regression Models for the Psychiatric Data

```
> fit.lin <- glm(p ~ ghqscore)
> fit.log <- glm(p ~ ghqscore, family = binomial, weights = case + nocase)
> summary(fit.lin)

Call: glm(formula = p ~ ghqscore)
Deviance Residuals:
      Min          1Q        Median          3Q         Max
-0.2150518  -0.1162369  -0.03278505  0.1217964  0.2516149

Coefficients:
                 Value   Std. Error    t value
(Intercept)  0.1143407  0.05922838   1.930505
  ghqscore   0.1002370  0.01001142  10.012266

(Dispersion Parameter for Gaussian family taken to be 0.0220503)
    Null Deviance: 2.651447 on 21 degrees of freedom
Residual Deviance: 0.4410058 on 20 degrees of freedom
Number of Fisher Scoring Iterations: 1

Correlation of Coefficients:
            (Intercept)
ghqscore   -0.8451543
> summary(fit.log)

Call: glm(formula = p ~ ghqscore, family = binomial, weights = case + nocase)
Deviance Residuals:
      Min          1Q       Median         3Q        Max
 -1.768974  -0.7230615  0.1255168  0.5306368  1.757787

Coefficients:
                  Value   Std. Error    t value
(Intercept)  -2.7107322  0.27243281  -9.950094
  ghqscore    0.7360353  0.09456846   7.783094

(Dispersion Parameter for Binomial family taken to be 1)
    Null Deviance: 130.3059 on 21 degrees of freedom
Residual Deviance: 16.23682 on 20 degrees of freedom
Number of Fisher Scoring Iterations: 5

Correlation of Coefficients:
                  (Intercept)
    ghqscore      -0.7324319
```

Table 5.5 Predicted Values for Linear and Logistic Regression Models Fitted to the Psychiatric Data

```
> lin.pred <- predict(fit.lin)
> log.pred <- exp(predict(fit.log))/(1 + exp(predict(fit.log)))
> cbind(lin.pred, log.pred)
     lin.pred     log.pred
 1   0.1143407   0.06234304
 2   0.2145777   0.12188529
 3   0.3148147   0.22466904
 4   0.4150518   0.37692367
 5   0.5152888   0.55808875
 6   0.6155258   0.72500870
 7   0.7157628   0.84624903
 8   0.8159999   0.91993872
 9   0.9162369   0.95998065
10   1.0164739   0.98042217
11   1.1167110   0.99052540
12   0.1143407   0.06234304
13   0.2145777   0.12188529
14   0.3148147   0.22466904
15   0.4150518   0.37692367
16   0.5152888   0.55808875
17   0.6155258   0.72500870
18   0.7157628   0.84624903
19   0.8159999   0.91993872
20   0.9162369   0.95998065
21   1.0164739   0.98042217
22   1.1167110   0.99052540
```

```
#corresponding to each GHQ score, after
#combining over males and females
par(pty=“s”)
ylim<-range(lin.pred,log.pred,P)
plot(ghqscore[1:11],lin.pred[1:11],xlab=“GHQ”,
ylab=“Probability of case”,type=“l”,ylim=ylim)
#plots ghqscore against the predictions made
#by the simple linear regression
#model and draws a line through the points.
lines(ghqscore[1:11],log.pred[1:11],lty=2)
#adds a dotted line for the logistic regression
```

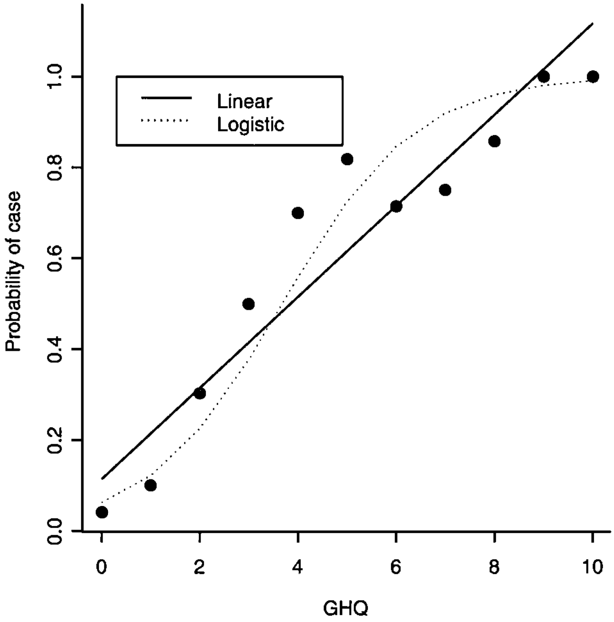


Figure 5.1 GHQ data showing observations and fitted linear and locally weighted regressions.

```
#predictions
points(ghqscore[1:11],P)
#adds the observed proportions to the plot
legend(0.3,1,c("Linear","Logistic"),lty=1:2)
#adds a legend at a convenient place on the plot.
```

The resulting graph is shown in Figure 5.1. We now see that in addition to giving predicted values greater than 1, the linear model provides a very poor description of the observed proportions.

Now let's consider sex as well as the GHQ score and compare the fit of the following three models.

1. GHQ score
2. GHQ score + sex
3. GHQ score + sex + sex × GHQ score

We now fit each of these three models using the glm function and then compare their fit using the anova function.

```
fit1<-glm(p~ghqscore,family=binomial,weights=case+nocase)
fit2<-glm
p~ghqscore+sex,family=binomial,weights=case+nocase)
fit3<-
glm(p~ghqscore*sex,family=binomial,weights=case+nocase)
anova(fit1,fit2,fit3)
#for logistic regression models the anova
#function will lead to an analysis of
#deviance table as described in McCullagh and Nelder.
```

The results are shown in Table 5.6. Comparing the difference in deviances of the models with a chi-square with a single degree of freedom indicates that both the GHQ score and gender are needed in the model but not their interaction. The estimated regression coefficients and their standard errors can be found using

```
summary(fit2)
```

and they are also shown in Table 5.6. The fitted models are

$$\log\left(\text{odds of being a case}\right) = -2.49 + 0.78\ \text{ghqscore} - 0.94\ \text{sex} \qquad (5.4)$$

The standard error of the regression coefficient for the GHQ score is 0.099, so an approximate 95% confidence interval for the coefficient is (0.58, 0.98). An increase of 1 in GHQ score raises the log odds of being a case by between 0.58 and 0.98, conditional on gender. This becomes easier to interpret after the two limits are exponentiated so that we can relate the change to odds rather than log (odds):

```
exp(c(0.58,0.98))
```

gives the interval (1.79, 2.66). So a 1-unit increase in GHQ score increases the odds of being a case by about twofold. The same series of calculations for gender leads to the confidence interval for the odds ratio of being a case in males and females of (0.25, 0.60), conditional on the GHQ score. Clearly, for a given GHQ score, men are less likely to be cases than women.

As with the multiple regression model considered in the previous chapter, fitting a logistic regression model is not complete without checking on model assumptions by examining the properties of some suitably defined residuals. There are a number of ways in which a fitted logistic model may be inadequate:

Table 5.6 Three Logistic Models for the Psychiatric Data Compared

```
> fit1 <- glm(p ~ ghqscore, family = binomial, weights = case +
nocase, data = ghq)
> fit2 <- glm(p ~ ghqscore + sex, family = binomial, weights = case +
      nocase, data = ghq)
> fit3 <- glm(p ~ ghqscore * sex, family = binomial, weights = case +
      nocase, data = ghq)
> anova(fit1, fit2, fit3)
Analysis of Deviance Table

Response: p

           Terms  Resid. Df  Resid. Dev             Test  Df  Deviance
1       ghqscore         20        16.2
2 ghqscore + sex         19        11.1             +sex   1      5.12
3 ghqscore * sex         18         8.8  +ghqscore:sex   1      2.35

> summary(fit2)

Call: glm(formula = p ~ ghqscore + sex, family = binomial, data =
ghq, weights = case + nocase)
Deviance Residuals:

 Min      1Q  Median     3Q   Max
-1.4  -0.394   0.188  0.432  1.33

Coefficients:

               Value  Std. Error  t value
(Intercept)  -2.494       0.282    -8.85
   ghqscore   0.779       0.099     7.87
        sex  -0.936       0.434    -2.16

(Dispersion Parameter for Binomial family taken to be 1)

    Null Deviance: 130 on 21 degrees of freedom

Residual Deviance: 11.1 on 19 degrees of freedom

Number of Fisher Scoring Iterations: 5

Correlation of Coefficients:
           (Intercept)  ghqscore
 ghqscore       -0.611
      sex       -0.220    -0.305
```

- The linear function of the explanatory variables may be inadequate; for example, one or more of the explanatory variables may need to be transformed.
- The logistic transformation of the response probability may not be appropriate.
- The data may contain outliers that are not well fitted by the model.
- The assumption of a binomial distribution may not be correct.

In logistic regression there are several types of residuals that may be useful for assessing one or other of those potential difficulties. Here, we shall define two and then illustrate their use on the GHQ data. We assume there are n observations of the form y_i/n_i, $i = 1, 2, \ldots, n$ and that the corresponding fitted value of y_i is $\hat{y}_i = n_i\hat{p}_i$. The ith row residual is then the difference $y_i - \hat{y}_i$ and provides information about how well the model fits each particular observation. But because they are based on different n_is and for other reasons explained in Collett (1991), the raw residuals are difficult to interpret. Better are the *Pearson residuals* and the *deviance residuals*:

- Pearson residuals

$$\frac{y_i - n_i\hat{p}_i}{\sqrt{n_i\hat{p}_i\left(1 - \hat{p}_i\right)}} \tag{5.5}$$

- Deviance residuals

$$\operatorname{sign}\left(y_i - \hat{y}_i\right)\left[2y_i\log\left(\frac{y_i}{\hat{y}_i}\right) + 2\left(n - y_i\right)\log\left(\frac{n - y_i}{n - \hat{y}_i}\right)\right]^{1/2} \tag{5.6}$$

where sign$(y_i - \hat{y}_i)$ is the function that makes d_i positive when $(y_i \geq \hat{y}_i)$ and negative when $(y_i > \hat{y}_i)$.

Both residuals are best used after standardising by dividing by $\sqrt{1 - h_i}$ where h_i is the ith diagonal element of the 'hat matrix' in logistic regression (see Collett, 1991).

There are various ways of plotting the residuals that give different insights into possible model inadequacies. Three possibilities are as follows:

- *Index plot*: plot of residuals against observation number or index. Useful for the detection of outliers.
- Plot of residuals against values of the linear predictor. The occurrence of a systematic pattern in the plot suggests the model is incorrect in some way.
- Plot of residuals against explanatory variables in the model may help to identify whether the variable needs to be transformed.

Suitable commands for constructing each of these plots for the deviance residuals from the logistic regression model with the explanatory variables ghqscore and sex are as follows

```
resid<-residuals(fit2,type="deviance")
#store deviance residuals from the
#fitted model in resid
resides<-resid/sqrt(1-lm.influence(fit2)$hat)
#uses lm.influence to get the diagonal
#elements of the logistic regression
#equivalent of the hat matrix introduced
#in Chapter 4
par(mfrow=c(1, 3))
#set up plotting area to take three plots
#side-by-side
plot(1:22,resides,xlab="Observation No.",
ylab="Standardised deviance residual")
plot(predict(fit2),resides,xlab="Predicted value",
ylab="Standardised deviance residual")
plot(ghqscore,resides,xlab="GHQ",ylab=
"Standardised deviance residual")
```

The resulting diagram is shown in Figure 5.2. There is no discernable pattern in these residuals that would give cause for concern.

5.3.2 Mortgage Default Data

We assume that the mortgage default data are available as the data frame credit, the contents of which are shown in Table 5.7. (The information about the income categories in the **INCOME** variable is confidential, although it is known that the category labels are monotone with increasing income. Here we shall simply use these labels as the values of a continuous variable in the modelling process.)

We shall now use the **Logistic Regression** dialog to undertake the logistic regression. To access this dialog:

- Click on **Statistics**.
- Select **Regression**.
- Select **Logistic**.

In the dialog choose the credit data frame. As the dependent variable, select **EVER90**, and as independent variables, highlight **FICO, LTV, INCOME**, and **CA**. The dialog box now appears as shown in Figure 5.3.

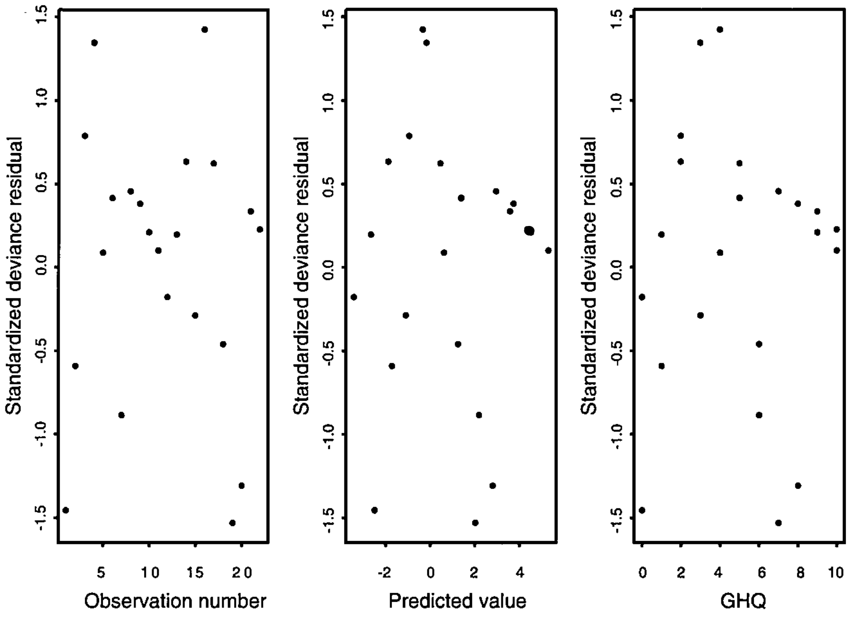
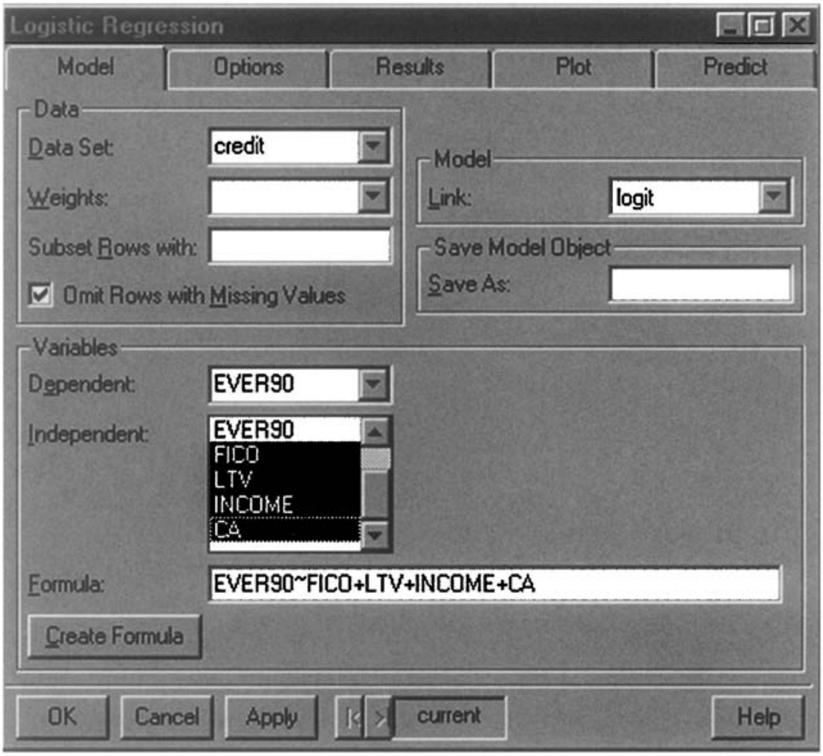


Figure 5.2 Residual plots for logistic regression model including ghqscore and sex fitted to GHQ data

Click **OK** to obtain the results shown in Table 5.8. It appears that the variables FICO and LTV are of most importance in predicting mortgage default. Largely as an exercise in using some other S-PLUS features, we will now demonstrate how to construct some informative graphics for displaying the relationships involved.

To display graphically the relationship between the variables FFCO and LTV and the probability of mortgage default, we first need to use the **Logistic Regression** dialog again to fit a model using only these two variables, and to save the fitted values.

- Click on **Statistics**.
- Select **Regression**.
- Select **Logistic**.
- Select **credit** data frame.
- Select **EVER90** as dependent variable.
- Select **FICO** and **LTV** as independent variables.
- Click on **Results** tab.
- In **Saved Results** section choose **Fitted Values**, and in **Save In** slot select **credit** data frame.
- Click **OK**.



Logistic Regression

Data

Data Set: credit

Weights:

Subset Rows with:

☑ Omit Rows with Missing Values

Model

Link: logit

Save Model Object

Save As:

Variables

Dependent: EVER90

Independent: EVER90
FICO
LTV
INCOME
CA

Formula: EVER90~FICO+LTV+INCOME+CA

Create Formula

Figure 5.3 Logistic Regression dialog showing a model for the mortgage default data.

The results will appear in a Report file and the new credit data frame, which now has the fitted values incorporated, is also shown:

- Highlight **FICO**.
- **Ctrl click** on **LTV**.
- **Ctrl click** on **fit**.
- Click on

  to access **3D graph** palette.
- Select **Drop Line Scatter** as shown in Figure 5.4.

The results shown in Figure 5.5, which shows the relationship between the probability of mortgage default and FICO and LTV. A somewhat clearer

Table 5.7 Contents of credit Data Frame

```
> credit
   row.labels EVER90 FICO  LTV INCOME         CA
 1          1      1  576 0.86      5      Other
 2          2      1  678 0.90      3 California
 3          3      1  693 0.80      5      Other
 4          4      1  669 0.75      4      Other
 5          5      1  542 0.95      4      Other
 6          6      1  566 0.95      3      Other
 7          7      1  643 0.84      5      Other
 8          8      0  785 0.58      5      Other
 9          9      1  461 0.80      4      Other
10         10      0  785 0.85      5      Other
11         11      1  620 0.95      3      Other
12         12      0  792 0.79      3      Other
13         13      0  748 0.90      4      Other
14         14      1  661 0.75      5      Other
15         15      0  753 0.70      5      Other
16         16      0  747 0.95      4      Other
17         17      0  720 0.88      5      Other
18         18      0  717 0.89      4      Other
19         19      0  763 0.90      5      Other
20         20      1  782 0.90      4 California
21         21      0  758 0.42      5      Other
22         22      0  697 0.80      5      Other
23         23      1  690 0.75      2      Other
24         24      0  746 0.90      5 California
25         25      0  679 0.70      5      Other
26         26      0  767 0.80      2      Other
27         27      0  733 0.88      5      Other
28         28      0  679 0.75      2      Other
29         29      0  765 0.36      3      Other
30         30      0  678 0.95      5      Other
31         31      0  782 0.62      4      Other
32         32      0  777 0.80      5      Other
33         33      0  765 0.63      5      Other
34         34      0  769 0.59      5      Other
35         35      0  720 0.38      5      Other
36         36      0  758 0.90      4      Other
37         37      0  724 0.70      5      Other
38         38      1  611 0.90      5      Other
39         39      0  639 0.61      5      Other
```

Table 5.7 (Continued)   Contents of credit Data Frame

```
> credit
     row.labels  EVER90  FICO   LTV  INCOME          CA
 40          40       0   761  0.50       3       Other
 41          41       1   549  0.66       3       Other
 42          42       0   639  0.68       6       Other
 43          43       0   719  0.61       5       Other
 44          44       0   801  0.73       2       Other
 45          45       0   765  0.90       5       Other
 46          46       1   598  0.95       5       Other
 47          47       1   603  0.95       4       Other
 48          48       0   710  0.67       2       Other
 49          49       0   774  0.48       5       Other
 50          50       0   738  0.73       5       Other
 51          51       1   676  0.73       3       Other
 52          52       0   768  0.78       5       Other
 53          53       0   765  0.90       5       Other
 54          54       0   766  0.87       5       Other
 55          55       0   729  0.90       4       Other
 56          56       0   766  0.68       5       Other
 57          57       1   671  0.75       1       Other
 58          58       0   782  0.80       2       Other
 59          59       1   756  0.75       2       Other
 60          60       0   791  0.89       4       Other
 61          61       1   650  0.85       3       Other
 62          62       0   704  0.75       3       Other
 63          63       1   664  0.80       8  California
 64          64       0   762  0.62       4       Other
 65          65       0   733  0.70       3       Other
 66          66       1   634  0.95       5  California
 67          67       0   797  0.26       3  California
 68          68       1   624  0.90       5  California
 69          69       0   749  0.70       2       Other
 70          70       0   687  0.95       3       Other
 71          71       0   732  0.72       4  California
 72          72       0   669  0.80       5       Other
 73          73       0   692  0.79       5       Other
 74          74       0   777  0.80       3  California
 75          75       0   682  0.47       4  California
 76          76       0   772  0.80       5       Other
 77          77       0   809  0.75       5       Other
 78          78       0   728  0.74       5       Other
```

Table 5.7 (Continued) Contents of credit Data Frame

> credit

	row.labels	EVER90	FICO	LTV	INCOME	CA
79	79	0	669	0.67	5	California
80	80	1	692	0.75	4	Other
81	81	0	721	0.75	5	Other
82	82	1	742	0.69	5	Other
83	83	0	687	0.79	2	Other
84	84	0	696	0.83	5	California
85	85	1	586	0.90	5	Other
86	86	0	727	0.80	3	California
87	87	0	725	0.80	7	Other
88	88	1	652	0.95	5	California
89	89	1	722	0.80	5	California
90	90	1	606	0.80	4	Other
91	91	0	761	0.80	5	Other
92	92	0	777	0.80	5	Other
93	93	0	629	0.29	5	Other
94	94	1	742	0.74	3	Other
95	95	0	752	0.61	2	Other

picture can be obtained by selecting **Spline Surface** from the **3D** graphics palette (Figure 5.6). Here the resulting diagram is shown in Figure 5.7. We see that as FICO and LTV increase, the probability of mortgage default decreases.

Table 5.8 Logistic Regression Model for Mortgage Default Data

```
*** Generalized Linear Model ***

Call: glm(formula = EVER90 ~ FICO + LTV + INCOME + CA, family =
binomial(link = logit), data = credit, na.action = na.exclude,
control = list(epsilon = 0.0001, maxit = 50, trace = F))

Deviance Residuals:
       Min          1Q        Median          3Q        Max
 –1.523824   –0.536522    –0.2340431   0.3169709   2.565638

Coefficients:
                    Value     Std. Error      t value
(Intercept)   19.07413721    5.564345576     3.427921
       FICO   –0.03189893    0.007279867    –4.381802
        LTV    5.69435393    2.800980222     2.032986
     INCOME   –0.40185724    0.246608000    –1.629539
         CA    0.57827914    0.389452398     1.484852

(Dispersion Parameter for Binomial family taken to be 1)
    Null Deviance: 118.4944 on 94 degrees of freedom
Residual Deviance: 64.35339 on 90 degrees of freedom
Number of Fisher Scoring Iterations: 5
```

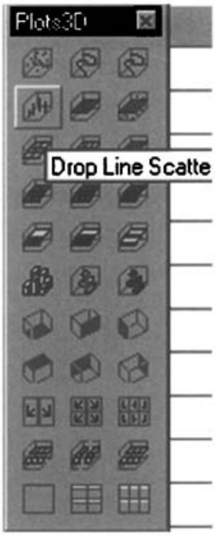


Figure 5.4 3D Graphic palette showing Drop Line scatter choice.

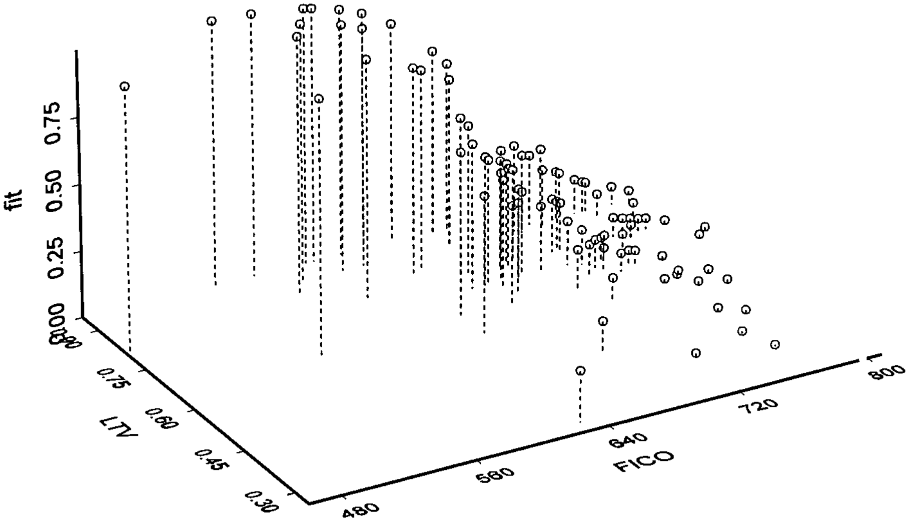


Figure 5.5 Plot of probability of mortgage default against FICO and LTV.

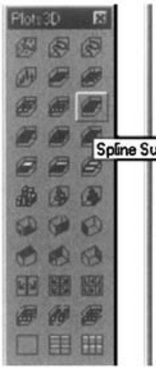


Figure 5.6 3D Graphic palette showing Spline Surface choice.

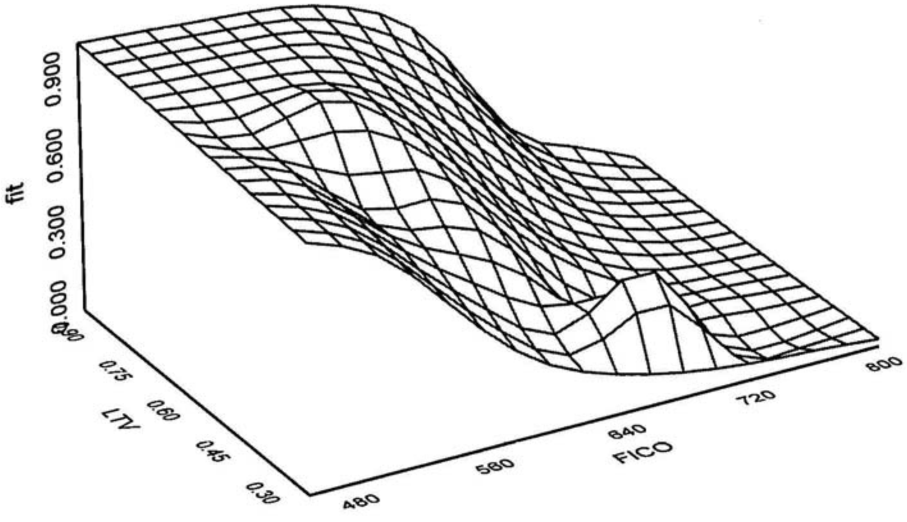


Figure 5.7 Spline surface for probability of mortgage default as a function of the variables FICO and LTV.

Exercises

5.1. In a logistic regression model for the GHQ data, which includes both the GHQ score and sex as explanatory variables, what would be the interpretation of the regression coefficient for sex?

5.2. Find the standard errors of the fitted values from the logistic regression model for the GHQ data, which includes only the single explanatory variable ghqscore. Plot the fitted values showing the 95% confidence interval.

Chapter 6

Analysing Longitudinal Data: Beating the Blues

6.1 Description of Data

The data to be used in this chapter arise from a study of an interactive, multimedia program designed to deliver *cognitive behavioural therapy* (CBT) to depressed patients via a computer terminal; the data are shown in Table 6.1. Patients were randomly allocated to receive either the computer therapy program, which was known as Beat the Blues (BtB), or treatment as usual (TAU). The trial protocol specified recording a measure of depression prior to the beginning of treatment and then again 2, 3, 5, and 8 months after the start of the treatment. Note that some patients in the trial 'drop-out' and do not have a full set of four post-randomisation depression recordings. (I am grateful to Dr. Judy Proudfoot for allowing me to use these data.)

The main question of interest about these data is whether or not the new computer approach for delivery of treatment for depression is effective or not.

6.2 Analysing Longitudinal Data

Longitudinal data arise when participants in a study are measured on the same variable on several different occasions. The data in Table 6.1 are an example in which depression is measured on five occasions, one before

Table 6.1 Beat the Blues Data

group	pre	m2	m3	m5	m8
0	25	12	5	7	7
0	13	12	11	11	10
0	17	17	15	14	14
1	20	20	16	15	12
1	23	12	4	6	5
1	42	10	8	10	6
1	16	10	7	9	2
0	18	12	11	10	NA
1	15	7	4	3	5
1	14	14	6	5	5
0	19	16	6	5	3
0	35	15	10	10	11
1	41	8	5	9	4
1	28	18	17	NA	NA
1	24	5	5	6	6
1	19	4	7	1	2
1	26	21	12	8	4
0	19	18	10	10	8
0	15	15	18	15	15
0	31	18	8	8	7
1	19	4	3	3	3
1	36	14	7	1	1
0	13	15	NA	NA	NA
1	35	12	10	8	10
0	26	29	25	23	20
0	19	18	23	23	23
1	16	1	0	0	NA
1	13	5	3	3	0
1	18	10	10	6	8
0	17	19	14	NA	NA
0	15	25	20	20	20
0	21	22	14	13	12
1	19	3	3	3	1
1	18	4	4	9	NA
0	22	10	13	12	14
0	15	12	5	5	4
0	21	15	17	8	13
0	16	15	14	15	12
0	22	22	22	23	24
1	13	10	6	2	4

treatment begins and four after the start of treatment. Analysis of such data has become something of a growth industry in statistics, largely because of its increasing importance in clinical trials (see Everitt and Pickles, 2000). There are a number of possible approaches to the analysis of such data:

- *Time-by-time analysis*: A series of *t*-tests are used to test for differences between the two groups at each time point. (In examples with more than two groups, a series of one-way analyses of variance might be used.) The procedure is straightforward but has a number of serious flaws and weaknesses that are detailed in Everitt (2001); consequently, it will not be pursued further here.
- *Response feature analysis — the use of summary measures*: Here the repeated measures for each participant are transformed into a single number considered to capture some important aspect of the participant's response profile. The summary measure to use has to be decided on before analysis of the data begins and must, of course, be relevant to the particular questions that are of interest in the study. Commonly used summary measures include
  1. Overall mean
  2. Maximum (minimum) value
  3. Time to maximum (minimum) response
  4. Slope of regression line on time
  5. Time to reach a particular value (for example, a fixed percentage of baseline)

  Having identified a suitable summary measure, a simple *t*-test (or analysis of variance) can be applied to assess between group differences.
- *Random effects model*: A detailed analysis of longitudinal data requires consideration of models that represent both the level and the shape of a group's profile of repeated measurements and also accounts adequately for the observed pattern of dependencies in these measurements. A flexible way to do this is to use regression-type models that include random effects for subjects, the presence of which allows for particular patterns of covariance between the repeated measures. For example, for the data in Table 6.1 we might first postulate a simple *random intercept model* of the form

$$y_{ijk} = \left(\beta_0 + \alpha_k\right) + \beta_1 \text{Time}_j + \beta_2 \text{Group}_i + \epsilon_{ijk} \qquad (6.1)$$

where y_{ijk} represents the depression score for the *k*th patient on the *j*th post-randomisation occasion (Time$_j$, taking values 2, 3, 5, or 8) in the *i*th treatment group (Group$_i$, a dummy variable coding group membership),

β_0, β_1, and β_2 are regression coefficients, and the ϵ_{ijk} are error terms assumed to be normally distributed with zero mean and variance σ^2. The α_k are the patient random effect terms that model the shift in intercept for each subject; these are also assumed to be normally distributed, again with zero mean but variance σ_a^2. Such a model implies *compound symmetry* for the covariance matrix of the repeated measures, i.e., equality of the correlation between each pair of repeated measures (see Everitt and Dunn, 2001, for details). Other covariates such as pre-treatment depression score could be included in the model if necessary. Random effects models are described in detail in Pinheiro and Bates (2000).

6.3 Analysis Using S-PLUS

We shall begin by using the summary measure approach in the depression data in Table 6.1, and then move on to consider the fitting of random effects models to the data. For both, we shall concentrate on the command language approach.

6.3.1 Summary Measure Analysis of the Depression Data

The data are available in the depress data frame as shown in Table 6.2. As the summary measure for these data we shall simply use the mean of the post-randomisation measures. To begin, we shall simply ignore the pretreatment depression score available for each patient.

One question that needs to be addressed before calculating the chosen summary measure for each patient is what to do about those patients who drop out before the 8-month time point and, consequently, do not have all four intended post-randomisation depression measures. There are three possibilities:

1. Consider only patients who *do* have all post-randomisation measures,
2. Use all patients and calculate the mean of their *available* post-randomisation measures.
3. *Impute* (estimate) the missing values in some way; for example, use the *last observation carried forward* approach (LOCF), in which the missing values are replaced by the last value recorded for a patient.

For reasons explained in Everitt and Pickles (2000), the second option is the one generally recommended, and it is the one we will use here (but see Exercise 6.1).

Table 6.2 Contents of the Depress Data Frame

```
> depress
   subject group pre m2 m3 m5 m8
1        1   TAU  25 12  5  7  7
2        2   TAU  13 12 11 11 10
3        3   TAU  17 17 15 14 14
4        4   BtB  20 20 16 15 12
5        5   BtB  23 12  4  6  5
6        6   BtB  42 10  8 10  6
7        7   BtB  16 10  7  9  2
8        8   TAU  18 12 11 10 NA
9        9   BtB  15  7  4  3  5
10      10   BtB  14 14  6  5  5
11      11   TAU  19 16  6  5  3
12      12   TAU  35 15 10 10 11
13      13   BtB  41  8  5  9  4
14      14   BtB  28 18 17 NA NA
15      15   BtB  24  5  5  6  6
16      16   BtB  19  4  7  1  2
17      17   BtB  26 21 12  8  4
18      18   TAU  19 18 10 10  8
19      19   TAU  15 15 18 15 15
20      20   TAU  31 18  8  8  7
21      21   BtB  19  4  3  3  3
22      22   BtB  36 14  7  1  1
23      23   TAU  13 15 NA NA NA
24      24   BtB  35 12 10  8 10
25      25   TAU  26 29 25 23 20
26      26   TAU  19 18 23 23 23
27      27   BtB  16  1  0  0 NA
28      28   BtB  13  5  3  3  0
29      29   BtB  18 10 10  6  8
30      30   TAU  17 19 14 NA NA
31      31   TAU  15 25 20 20 20
32      32   TAU  21 22 14 13 12
33      33   BtB  19  3  3  3  1
34      34   BtB  18  4  4  9 NA
35      35   TAU  22 10 13 12 14
36      36   TAU  15 12  5  5  4
37      37   TAU  21 15 17  8 13
38      38   TAU  16 15 14 15 12
39      39   TAU  22 22 22 23 24
40      40   BtB  13 10  6  2  4
```

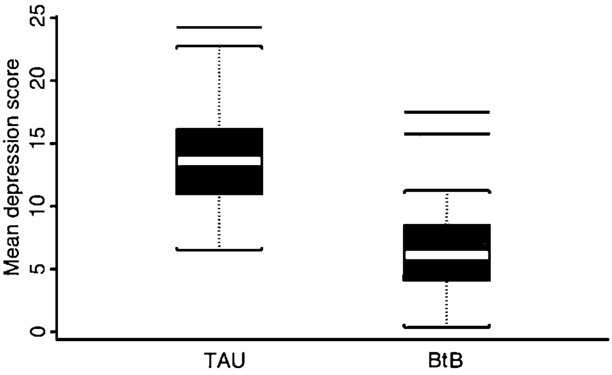


Figure 6.1 Box plots of mean summary measure for Beat the Blues data.

To begin, we shall calculate the chosen summary measure for each patient in the study and then use a box plot to display the measures graphically for each treatment group.

```
attach(depress)
depress.sm<-apply(depress[,4:7],1,mean,na.rm=T)
#use the apply function to get the mean of available
#post-randomization measurements for each patient
boxplot(depress.sm[group==“TAU”],depress.sm[group==“BtB”],
names=c(“TAU”,”BtB”),ylab=“Mean depression score”)
```

The resulting diagram is shown in Figure 6.1. This suggests that the depression score is higher for the subjects receiving treatment as usual; this can be tested formally with an independent samples *t*-test.

```
t.test(depress.sm[group==“TAU”],depress.sm[group==“BtB”])
```

The results are shown in Table 6.3. There is a very significant difference between treatment groups, with the average depression score for TAU being between 4 and 10 points higher than that of the BtB group.

We can take account of the pretreatment depression value in the summary measure approach by using the lm function to model the summary measure in terms of the pretreatment value and the treatment group.

```
summary(lm(depress.sm~pre+group))
```

The corresponding results are shown in Table 6.4. Since the default coding used by S-PLUS for the two levels of group is –1 for TAU and +1

Table 6.3 Results of Applying a *t*-Test to the Mean Summary Measure of Post-Randomisation Depression Values

```
> t.test(depress.sm[group == "TAU"], depress.sm[group == "BtB"])

        Standard Two-Sample t-Test

data: depress.sm[group == "TAU"] and depress.sm[group == "BtB"]
t = 4.91, df = 38, p-value = 0
alternative hypothesis: true difference in means is not equal to 0
95 percent confidence interval:
        4.27   10.26
sample estimates:
  mean of x   mean of y
       14.2        6.94
```

Table 6.4 Analysis of Mean Depression Score Taking Account of Pre-Randomisation Depression Value

```
> summary(lm(depress.sm ~ pre + group))

Call: lm(formula = depress.sm ~ pre + group)
Residuals:

   Min       1Q   Median     3Q    Max
–7.231   –3.032   –0.667  1.929  10.06

Coefficients:

                Value  Std. Error   t value  Pr(>|t|)
(Intercept)    8.5452      2.2530    3.7928    0.0005
        pre    0.0948      0.0997    0.9511    0.3477
      group   –3.7639      0.7542   –4.9907    0.0000

Residual standard error: 4.688 on 37 degrees of freedom
Multiple R-Squared: 0.4023
F-statistic: 12.45 on 2 and 37 degrees of freedom, the p-value
 is 0.00007319

Correlation of Coefficients:
         (Intercept)      pre
  pre        –0.9443
group         0.1747  –0.1850
```

for BtB, the regression coefficient for group and its standard error need to be doubled to give the estimated treatment effect adjusted for pretreatment depression, and the appropriate confidence interval for the effect. Consequently, a 95% confidence interval for treatment effect is (–7.53 – 1.96 × 1.51, –7.53 + 1.96 × 1.51), i.e., (–10.50, –4.57). Beat the Blues is estimated to reduce the depression score by between 10 and 5 points on average. Pretreatment score appears to have little effect on the scores post-treatment.

6.3.2 Random Effects Models for the Depression Data

Before undertaking the formal modelling of the depression data, it may be useful to consider some informative graphical displays. According to Diggle et al. (1994), there is no single prescription for making effective graphical displays of longitudinal data, although they do offer the following simple guidelines:

- Show as much of the relevant raw data as possible, rather than only data summaries.
- Highlight aggregate patterns of potential scientific interest.
- Identify both cross-sectional and longitudinal patterns.
- Make easy identification of unusual individuals or unusual observations.

Two graphical displays of the depression data that meet some of these requirements will now be constructed using the S-PLUS command language, the first a plot of individual patient profiles and the second a plot of group means and standard deviations:

```
lt<-rep(1,40)
lt[group=="BtB"]<-2
#set up vector lt with values 1 for TAU and 2 for BtB
matplot(c(0,2,3,5,8),t(depress[,3:7]),type="l",
lty=lt,axes=F,xlab="Visit",ylab="Depression",
col=1)
#use the matplot function to plot each patient's profile
#of depression values, setting the line type to 1 for TAU
#and to 2 for BtB using the previously constructed vector
#lt. Labels but does not draw x or y axes
axis(1,at=c(0,2,3,5,8),labels=c("pre","m2",
"m3","m5","m8"))
```

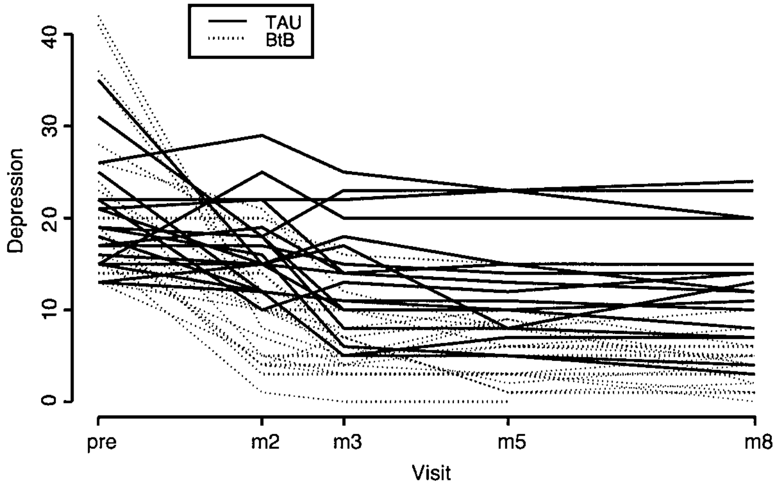


Figure 6.2 Individual participant profiles for the Beat the Blues data identifying treatment group.

```
#adds x-axis with tick marks at appropriate
#points and suitably labelled
axis(2)
legend(locator(1),c("TAU","BtB"),lty=1:2)
#adds y-axis and a legend interactively
```

The resulting plot is shown in Figure 6.2. The tendency for the profiles of the patients given the BtB treatment to be lower throughout the post-randomisation visits is clearly visible.

Now let us consider constructing a plot of the group means with standard deviation bars shown:

```
m1<-apply(depress[group=="TAU",3:7],2,mean,na.rm=T)
s1<-
sqrt(apply(depress[group=="TAU",3:7],2,var,na.action="omit")
m2<-apply(depress[group=="BtB",3:7],2,mean,na.rm=T)
s2<-sqrt(apply(depress[group=="BtB",3:7],2,var,
na.action="omit"))
#calculate means and standard deviations of
#each group
times <-c(0,2,3,5,8)
ylim<-range(m1+s1,m2+s2,m1-s1,m2-s2)
#store values for x-axis in times and a
```

```
#suitable range for the y-axis in ylim
plot(times,m1,type="l",axes=F,ylim=ylim,
xlab="Visit",ylab="Depression")
lines(times,m2,lty=2)
#plots the mean profiles of each group with
#different line types
axis(1,at=times,labels=c("pre","m2","m3","m5","m8"))
axis(2)
#add x and y axes
#now the segments function will be used to
#add standard deviation bars to the plot
#need to ensure that for the group with the highest
#mean value at a particular time point to
#standard deviation line goes upwards, and
#for the group with the lower mean downwards.
pm<-compare(m1,m2)
m1s1<-m1+pm*s1
m2s2<-m2-pm*s2
#compare returns a vector of +1, -1, and 0s
#depending on the differences between the corresponding
#elements of m1 and m2
segments(times,m1,times,m1s1)
segments(times–0.1,m1s1,times+0.1,m1s1)
segments(times,m2,times,m2s2)
segments(times–0.1,m2s2,times+0.1,m2s2)
legend(locator(1),c("TAU","BtB"),lty=1:2)
```

The resulting diagram is shown in Figure 6.3. On average, the depression values for patients given the BtB treatment are lower on each post-randomisation visit than those given treatment as usual.

Now we move on to consider the fitting of random effect models to the depression data using the lme function. The first step is to rearrange the data so that the values of the four post-randomisation depression measures of each patient are stacked into one long vector, and then the values of the subject identifier, time of measurement, treatment group, and pretreatment depression need to be replicated in accordance with this new arrangement of the response variable. Suitable commands are as follows:

```
Depression<-as.vector(as.matrix(t(depress[,4:7])))
#stacks the repeated depression values into a single vector
```

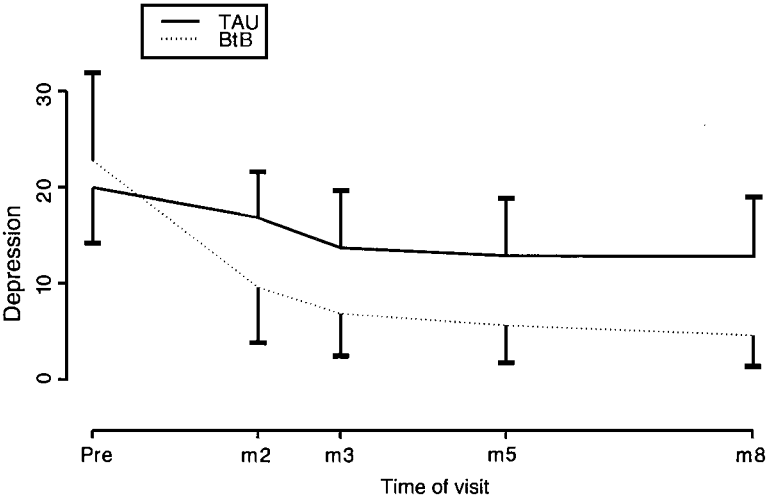


Figure 6.3 Plot of mean profiles and standard deviations for each treatment group in the Beat the Blues data.

```
#after transposing using the t function
Group<-rep(group,rep(4,40))
Pre<-rep(pre,rep(4,40))
Subject<-rep(subject,rep(4,40))
Time<-rep(c(2,3,5,8),40)
depress.new<-data.frame(Subject,Group,Pre,Time, Depression)
#the rep function is used to replicate the
#explanatory variables, subject number and
#time of measurement appropriately and then the
#rearranged values are combined into a new
#data frame.
```

The first 20 rows of depress.new are shown in Figure 6.5.

To begin, we shall fit the random effects model described by Equation 6.1 with the addition of the pretreatment depression value as an extra covariate.

```
fit1<-lme(Depression~Pre+Group+Time,method="ML",
random=~1|Subject,data=depress.new,na.action=
na.omit)
#Depression is modelled in terms of the pretreatment
#value, treatment group, and time of measurement
```

Table 6.5 Beat the Blues Data Rearranged for Fitting Random Effect Models (Data for Five Patients)

	Subject	Group	Pre	Time	Depression
1	1	TAU	25	2	12
2	1	TAU	25	3	5
3	1	TAU	25	5	7
4	1	TAU	25	8	7
5	2	TAU	13	2	12
6	2	TAU	13	3	11
7	2	TAU	13	5	11
8	2	TAU	13	8	10
9	3	TAU	17	2	17
10	3	TAU	17	3	15
11	3	TAU	17	5	14
12	3	TAU	17	8	14
13	4	BtB	20	2	20
14	4	BtB	20	3	16
15	4	BtB	20	5	15
16	4	BtB	20	8	12
17	5	BtB	23	2	12
18	5	BtB	23	3	4
19	5	BtB	23	5	6
20	5	BtB	23	8	5

```
#the random argument specifies a single random
#effect for each ‘group’ of response values
#the ‘group’ here being subject.
summary(fit1)
```

The results are shown in Table 6.6. Both the treatment group and time-fixed effects are very significant whilst the pretreatment score effect is again nonsignificant. The estimated standard deviation of the random intercept effects is 4.226 and the corresponding value for the residual terms is 2.738.

Now consider a model with a random intercept and random slope for each patient:

```
fit2<-lme(Depression~Pre+Group+Time,method=“ML”,
random~Time|Subject,data=depress.new,na.action =
na.omit)
summary(fit2)
```

Table 6.6 Results of Fitting Random Intercept Model to Beat the Blues Data

```
> summary(fit1)
Linear mixed-effects model fit by maximum likelihood
 Data: depress.new
      AIC        BIC      logLik
830.8885   848.9523   –409.4443

Random effects:
 Formula: ~ 1 | Subject
            (Intercept)   Residual
StdDev:         4.22594   2.737807

Fixed effects: Depression ~ Pre + Group + Time
                 Value   Std.Error    DF     t-value   p-value
(Intercept)   11.23785    2.215434   109    5.072525    <.0001
        Pre    0.10093    0.096079    37    1.050468    0.3003
      Group   –3.76292    0.727953    37   –5.169180    <.0001
       Time   –0.66767    0.102413   109   –6.519347    <.0001

Correlation:
          (Intr)     Pre    Group
   Pre    –0.925
 Group     0.164   –0.178
  Time    –0.186   –0.012   –0.001

Standardized Within-Group Residuals:
      Min           Q1           Med          Q3        Max
–1.825689   –0.5614503   –0.07627247   0.5261911   3.095711

Number of Observations: 150
Number of Groups: 40
```

The results are given in Table 6.7. The tests for the fixed effects in the model have results very similar to those for the random intercept model as do the estimated standard deviations for the random intercept terms and the residual terms. The estimated standard deviation of the random slope effects is 0.363.

Table 6.7 Results of Fitting Random Intercept and Random Slope Model to Beat the Blues Data

```
> summary(fit2)
Linear mixed-effects model fit by maximum likelihood
 Data: depress.new
     AIC        BIC       logLik
833.3486   857.4337   –408.6743

Random effects:
 Formula: ~ Time | Subject
 Structure: General positive-definite
                  StdDev      Corr
(Intercept)   4.4034190   (Inter
       Time   0.3632755   –0.277
   Residual   2.5745429

Fixed effects: Depression ~ Pre + Group + Time
                 Value   Std.Error    DF     t-value    p-value
(Intercept)   11.16996    2.215142   109    5.042547     <.0001
        Pre    0.10368    0.095911    37    1.081000     0.2867
      Group   –3.73918    0.726462    37   –5.147112     <.0001
       Time   –0.66474    0.114392   109   –5.811035     <.0001

Correlation:
          (Intr)      Pre    Group
    Pre   –0.924
  Group    0.164   –0.179
   Time   –0.196   –0.011   –0.002

Standardized Within-Group Residuals:
      Min          Q1           Med          Q3          Max
–1.938337   –0.5395204   –0.1078871   0.4987325   2.795758

Number of Observations: 150
Number of Groups: 40
```

We can assess whether the random intercept and random slopes model fits better than the simpler random intercepts model using the **anova** function.

```
anova(fit1,fit2)
```

Table 6.8 Comparing Random Effects Models

```
> anova(fit1, fit2)
     Model df      AIC      BIC    logLik   Test  L.Ratio p-value
fit1     1  6 830.8885 848.9523 –409.4443
fit2     2  8 833.3486 857.4337 –408.6743 1 vs 2  1.53987   0.463
```

Table 6.9 Confidence Intervals for Parameters in Random Intercept Model for Beat the Blues Data

```
> intervals(fit1)
Approximate 95% confidence intervals

 Fixed effects:
                  lower        est.      upper
(Intercept)  6.90586774  11.2378455 15.5698233
        Pre –0.09113376   0.1009282  0.2929902
      Group –5.21809383  –3.7629201 –2.3077463
       Time –0.86791956  –0.6676652 –0.4674108

 Random Effects:
  Level: Subject

                    lower    est.    upper
sd((Intercept)) 2.987841 4.22594 5.977081

 Within-group standard error:

  lower     est.    upper
 2.27141 2.737807 3.29997
```

giving the results in Table 6.8. Clearly, the more-complicated model does not represent an improvement in this case.

We can find confidence intervals for the parameters of the random intercept model using the intervals function.

```
intervals(fit1)
```

gives the confidence intervals shown in Table 6.9. (Remember that the confidence interval given for the treatment group is based on the –1,1 coding used by default.)

Now we need to examine the residuals from the fitted model to check the various assumptions made. A plot of standardised residuals against

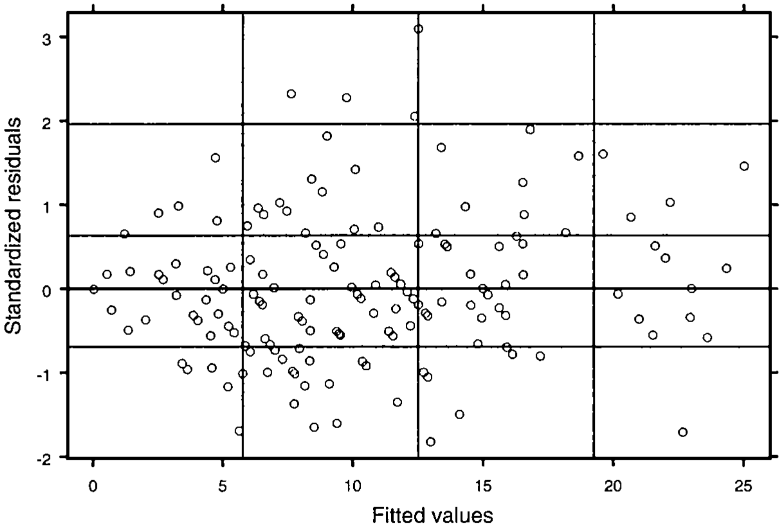


Figure 6.4 Plot of standardised residuals from random intercept model for Beat the Blues data.

fitted values, for example, can be used to assess the assumption of constant variance of the ϵ_{ij}:

```
plot(fit1)
```

The plot is shown in Figure 6.4. In this plot we are looking for a systematic increase (or, less commonly, a systematic decrease) in the variance of the residuals as the fitted values increase. If this is present, the residuals on the right-hand side of the plot will have a greater vertical spread than those on the left, forming a horizontal wedge-shaped pattern. There is no such pattern in Figure 6.4.

The assumption of normality for the error terms can be assessed by a normal probability plot of the residuals produced by the qqnorm function:

```
qqnorm(fit1,~resid(.)|Group)
#the second argument specifies the residuals
#from the fitted model and plotting by
#treatment group
```

The resulting plot is shown in Figure 6.5. There is little evidence of a departure from normality in either group.

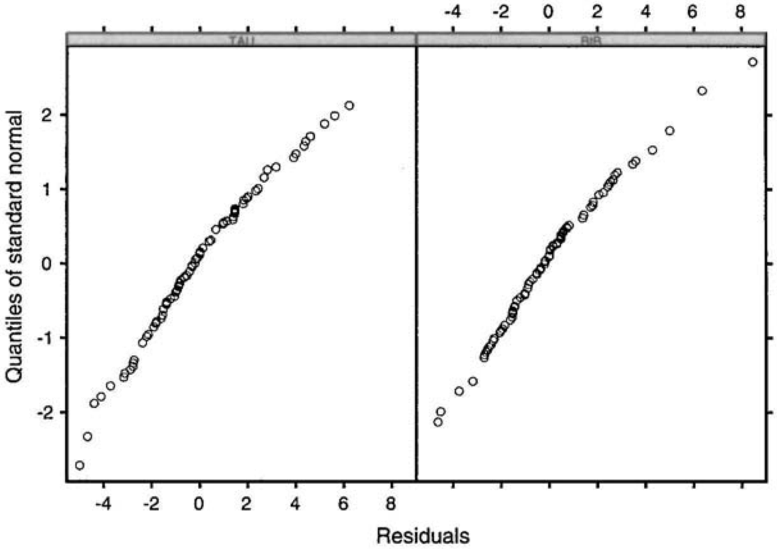


Figure 6.5 Normal probability plot of standardized residuals from a random intercept model fitted to the Beat the Blues data.

Lastly, we can assess the normality assumption of the estimated random effects (how these are estimated is described in Pinheiro and Bates, 2000), again by using the `qqnorm` function:

```
qqnorm(fit1,~ranef(.)|Group)
```

giving Figure 6.6. Again, there is no evidence of any serious departure from the assumption.

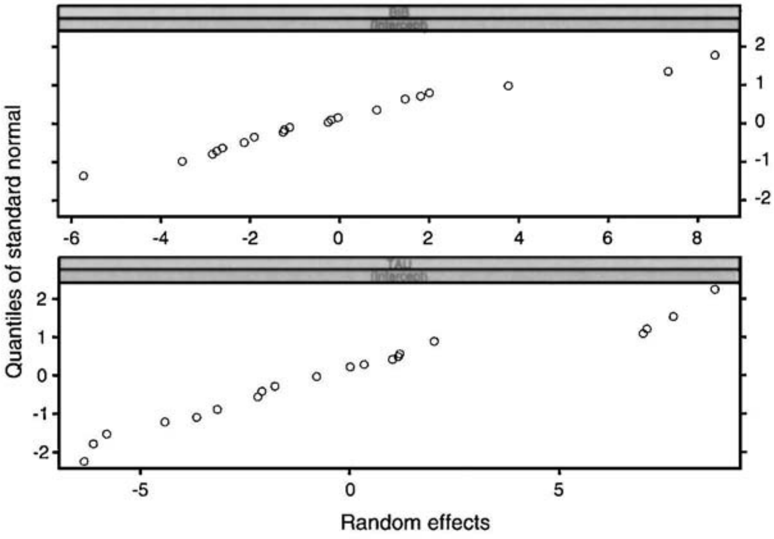


Figure 6.6 Normal probability plot of estimated random effects in a random intercepts model fitted to the Beat the Blues data.

Exercises

6.1. The box plot shown in Figure 6.1 suggests that the mean summary measure does not have the same variance in each treatment group and, consequently, violates at least one of the assumptions made by the *t*-test applied in the text. Investigate the use of the *t*-test function in a version that does not make this homogeneity of variance assumption.

6.2. Apply the mean summary measure approach to the depression data after excluding all patients who do not have all four intended post-randomisation depression values.

6.3. Apply the mean summary measure approach to the depression data after replacing missing values with the last observation carried forward.

Chapter 7

Nonlinear Regression and Maximum Likelihood Estimation: Athletes and Geysers

7.1 Description of Data

In this chapter we shall examine the functions available in S-PLUS for numerical optimisation in the context of both *nonlinear regression* and *maximum likelihood estimation*. To illustrate the former we shall use the data shown in Table 7.1, which show times in seconds recorded by the winners of the men's Olympic 1500-m event from 1900 to 2000 (there were no Olympic Games in 1916, 1940, and 1944). Interest here will centre on fitting a particular regression model to the data that might be used to predict future winning times, and the ultimate time achievable.

As an example of the application of maximum likelihood estimation in S-PLUS we shall estimate the parameters of a *normal mixture distribution* (see Everitt and Hand, 1981) fitted to the data in Table 7.2. These data consist of the waiting times between successive eruptions of the Old Faithful geyser in Yellowstone National Park, Wyoming, USA. There were 300 eruptions observed in the period of observation (August 1 to 15, 1985), so Table 7.2 contains 299 waiting times measured in minutes.

Table 7.1 Olympic 1500-m Winning Times (men)

Year	Time
1900	246.00
1904	245.40
1908	243.40
1912	236.80
1920	241.80
1924	233.60
1928	233.20
1932	231.20
1936	227.80
1948	225.20
1952	225.20
1956	221.20
1960	215.60
1964	218.10
1968	214.90
1972	216.30
1976	219.20
1980	218.40
1984	212.50
1988	215.96
1992	220.12
1996	215.78
2000	212.07

7.2 Nonlinear Regression and Maximum Likelihood Estimation

An examination of the 1500-m times shows that they are improving (decreasing) over time. From physiological consideration it is clear that there is a lower limit to the times. Such considerations led Chatterjee and Chatterjee (1982) to suggest the *three-parameter exponential* for modelling this type of athletic records data. The model is as follows:

$$E(\text{time}) = \theta_1 + \theta_2 \exp\left[\theta_3(\text{Year} - 1900)\right] \tag{7.1}$$

All three parameters in the model have meaningful interpretations:

Table 7.2 Waiting Times (minutes) for Eruption of Old Faithful

80	71	57	80	75	77	60	86	77	56	81	50	89	54	90	73
60	83	65	82	84	54	85	58	79	57	88	68	76	78	74	85
75	65	76	58	91	50	87	48	93	54	86	53	78	52	83	60
87	49	80	60	92	43	89	60	84	69	74	71	108	50	77	57
80	61	82	48	81	73	62	79	54	80	73	81	62	81	71	79
81	74	59	81	66	87	53	80	50	87	51	82	58	81	49	92
50	88	62	93	56	89	51	79	58	82	52	88	52	78	69	75
77	53	80	55	87	53	85	61	93	54	76	80	81	59	86	78
71	77	76	94	75	50	83	82	72	77	75	65	79	72	78	77
79	75	78	64	80	49	88	54	85	51	96	50	80	78	81	72
75	78	87	69	55	83	49	82	57	84	57	84	73	78	57	79
57	90	62	87	78	52	98	48	78	79	65	84	50	83	60	80
50	88	50	84	74	76	65	89	49	88	51	78	85	65	75	77
69	92	68	87	61	81	55	93	53	84	70	73	93	50	87	77
74	72	82	74	80	49	91	53	86	49	79	89	87	76	59	80
89	45	93	72	71	54	79	74	65	78	57	87	72	84	47	84
57	87	68	86	75	73	53	82	93	77	54	96	48	89	63	84
76	62	83	50	85	78	78	81	78	76	74	81	66	84	48	93
47	87	51	78	54	87	52	85	58	88	79					

- θ_1 is the ultimate limit.
- θ_2 is the amount by which the first record (i.e., for year 1900) exceeds the ultimate limit.
- θ_3 is the constant proportional rate of decline in the record series towards the ultimate limit.

The three parameters can be estimated by minimizing the sum of squares of the differences between the observed values of the 1500-m times and those predicted by the assumed model.

For the geyser eruption data we shall investigate whether there is any evidence of multimodality in the data by fitting a mixture of two normal densities, i.e., the density function given by

$$f(x) = N(x;\mu_1,\sigma_1) + (1-p)N(x;\mu_2,\sigma_2) \tag{7.2}$$

where

$$N(x;\mu_i,\sigma_i) = \frac{1}{\sigma_i\sqrt{2\pi}} e^{-\frac{1}{2}\left(\frac{x-\mu_i}{\sigma_i}\right)^2}$$

In this density there are five parameters to estimate: the mixing proportion, p, and the means, μ_1 and μ_2, and standard deviations, σ_1 and σ_2, of each component normal density. If such a density function does provide a good description of the eruption data, it implies something fundamental about the mechanism of the eruption process.

To estimate the five parameters in Equation 7.2 we shall use maximum likelihood, maximizing the log-likelihood of n observations $x_1, \ldots, x_n$ from $f(x)$, in (7.2) i.e.,

$$l = \sum_{i=1}^{n} \log\left\{N\left(x_i;\mu_1,\sigma_1\right) + \left(1-p\right)N\left(x_i;\mu_2,\sigma_2\right)\right\} \tag{7.3}$$

7.3 Analysis Using S-PLUS

Both the nonlinear regression and maximum likelihood estimation described in the previous section require the numerical optimisation of some specified function. In S-PLUS there are a number of functions available for such optimisation; here we illustrate the use of two of these, nls and nlminb.

7.3.1 Modelling the Olympic 1500-m Times

To estimate the three parameters in the nonlinear model specified in Equation 7.1 we shall use the nls function in S-PLUS. This function estimates parameters by minimizing the sum of squares of differences between the response and the model prediction. The data are available in an S-PLUS data frame Olympic. To begin, we shall store initial values of the three parameters, θ_1, θ_2, and θ_3 along with this data frame.

```
param(Olympic,"theta1") <-200
param(Olympic,"theta2") <-40
param(Olympic,"theta3")<- -0.01
#these starting values are suggested by the
#results in Chatterjee and Chatterjee, 1982.
```

The contents of the amended version of Olympic are shown in Table 7.3.

We can now estimate the parameters using the nls function:

```
Olympic.fit<-nls(Time~theta1+theta2*exp(theta3*(Year —
1900)),Olympic)
#Formula used to specify the nonlinear model
Olympic.fit$parameters
#this object contains final values of parameters.
```

Table 7.3 Contents of Olympic Data Frame

```
Parameters:
$theta1:
[1] 200

$theta2:
[1] 40

$theta3:
[1] -0.01

Variables:
          Year        Time
    1     1900      246.00
    2     1904      245.40
    3     1908      243.40
    4     1912      236.80
    5     1920      241.80
    6     1924      233.60
    7     1928      233.20
    8     1932      231.20
    9     1936      227.80
   10     1948      225.20
   11     1952      225.20
   12     1956      221.20
   13     1960      215.60
   14     1964      218.10
   15     1968      214.90
   16     1972      216.30
   17     1976      219.20
   18     1980      218.40
   19     1984      212.50
   20     1988      215.96
   21     1992      220.12
   22     1996      215.78
   23     2000      212.07
```

The results are shown in Table 7.4. To obtain parameter estimates using a different set of initial values we need to use the start argument of nls, for example,

Table 7.4 Final Parameter Estimates for Model Fitted to 1500-m Times Using Two Sets of Starting Values

	theta1	theta2	theta3
(1) Starting values 1: $\theta_1 = 200, \theta_2 = 40, \theta_3 = -0.01$			
Estimated values	206.0838	41.86718	–0.01733334
(2) Starting values 2: $\theta_1 = 180, \theta_2 = 30, \theta_3 = -0.02$			
Estimated values	206.0941	41.85928	–0.01734269

```
Olympic.fit1<-nls(Time~theta1+theta2*exp(theta3*(Year —
1900)),start = list(theta1 = 180,theta2 = 30,theta3 = -0.02),
Olympic)
Olympic.fit1$parameters
```

The results obtained with these starting values are also shown in Table 7.4. They are almost identical to those obtained with the first set of starting values.

We can now examine the fit of the model graphically by plotting the original observations and adding the predicted values from the fitted model.

```
attach(Olympic)
plot(Year,Time)
lines(Year,predict(Olympic.fit))
```

The graph is shown in Figure 7.1. The fit appears to be very good.

One way to obtain confidence intervals for the estimated parameters is to use the *bootstrap* approach, which is described in detail in Efron and Tibshirani (1993), but which consists essentially of repeated sampling of the data with replacement, followed by calculation of the parameters for each such *bootstrap sample*. In this way empirical distributions of the parameters can be constructed from which confidence intervals can be determined from the appropriate quantiles, i.e., 2.5 and 97.5% for a 95% confidence interval. In S-PLUS bootstrapping is available by using the **bootstrap** function

```
set.seed(962)
#to ensure readers have same set of random samples
Olympic.boot<-bootstrap(Olympic,nls(Time~theta1+
theta2*exp(theta3*(Year — 1900)),Olympic)$parameters, B =
1000)
#we use 1000 bootstrap samples; starting
```

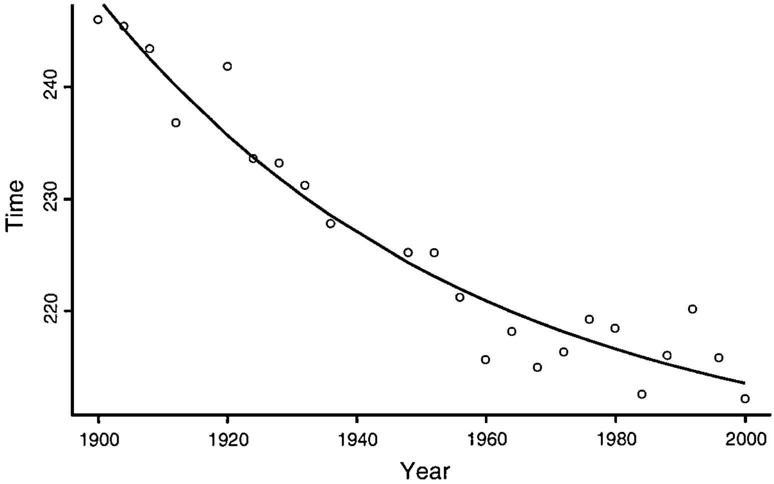


Figure 7.1 Plot of Olympic 1500-m times and three-parameter exponential prediction.

```
#values in each case will be the parameter
#values stored with the Olympic data frame
summary(Olympic.boot)
plot(Olympic.boot)
```

The numerical results are shown in Table 7.5 and the constructed distributions of the parameters are shown graphically in Figure 7.2. The empirical percentiles lead to 95% confidence intervals as follows:

θ_1: [192.79, 213.21]
θ_2: [35.59, 56.67]
θ_3: [–0.027, –0.011]

The BCa (*bias corrected accelerated*) confidence intervals, which are based on an improved procedure described in Efron and Tibshirani (1993), are very similar.

7.3.2 Estimating the Parameters in a Mixture Fitted to the Geyser Eruption Data

Here we shall use the nlminb function to estimate the parameters in a mixture of two normal densities fitted to the geyser eruption data, using maximum likelihood. First we need to write an S-PLUS function to evaluate

Table 7.5 Bootstrap Results for Olympic 1500-m Times

```
> summary(boot)
Call:
bootstrap(data = Olympic, statistic = nls(Time ~ theta1 + theta2 *
exp(theta3 * (Year - 1900)), Olympic)$parameters, B = 1000)

Number of Replications: 1000

Summary Statistics:
           Observed          Bias        Mean          SE
 theta1   206.08380    -0.6986649   205.38513    5.355482
 theta2    41.86718     1.3503861    43.21757    5.764726
 theta3    -0.01733    -0.0006773    -0.01801    0.004886

Empirical Percentiles:
               2.5%            5%         95%
 theta1   192.79244     196.08406   212.39022
 theta2    35.59040      36.70991    52.87415
 theta3    -0.02711      -0.02495    -0.01199

BCa Confidence Limits:
               2.5%            5%         95%       97.5%
 theta1   194.23732     196.88147   212.69860   213.82443
 theta2    34.71046      35.72474    50.23496    53.32543
 theta3    -0.02608      -0.02399    -0.01171    -0.01062

Correlation of Replicates:

         theta1   theta2   theta3
theta1   1.0000  -0.7339  -0.7976
theta2  -0.7339   1.0000   0.2300
theta3  -0.7976   0.2300   1.0000
```

the log-likelihood for any values of the five parameters. We shall call this function LL.

```
LL<-function(params,data){
#params contains the five parameter values of
#the mixture density in the order, p, mu1,
#sigma1, mu2, sigma2, and data contains
#the observed values — in our example the
#eruption waiting times
```

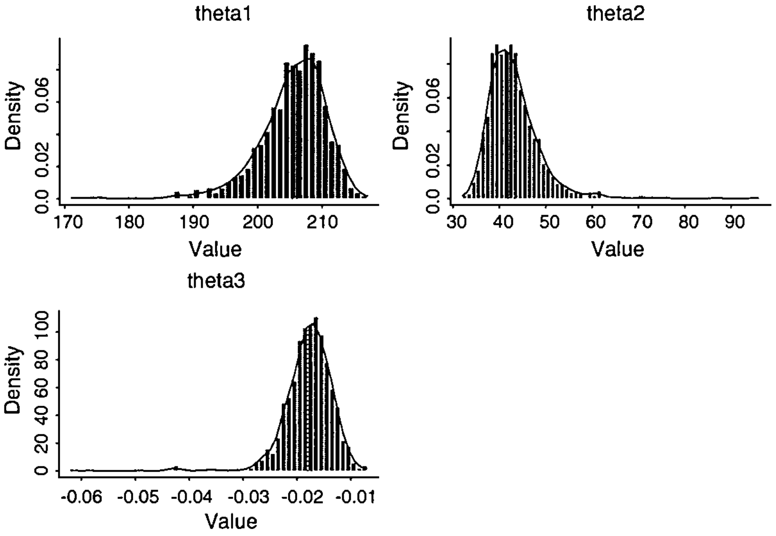


Figure 7.2 Bootstrap distributions of the three parameters in the three-parameter exponential distribution fitted to the Olympic 1500-m times (1000 bootstrap samples used).

```
t1<-dnorm(data,params[2],params[3])
t2<-dnorm(data,params[4],params[5])
#evaluate the two normal densities using the
#dnorm function
f<-params[1]*t1+(1-params[1])*t2
#evaluate the mixture density for all
#sample values
ll<-sum(log(f))
#evaluate the log-likelihood
-ll
#nlminb needs a function to minimize so
#we set the value returned by LL to
#minus the value of the log-likelihood
}
```

We assume the eruption waiting times are available in a vector geyser, and first we will need to examine a histogram of the data to get initial values for the five parameters in the mixture.

```
hist(geyser)
```

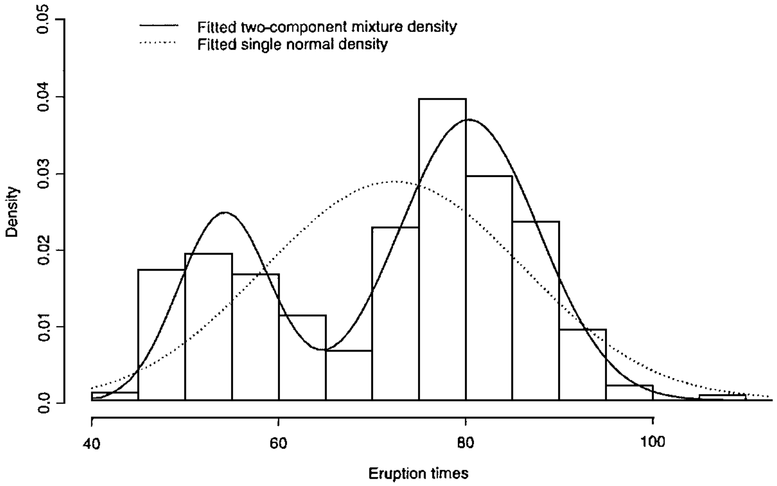


Figure 7.3 Fitted single normal distribution and two-component normal mixture for geyser eruption waiting times.

The resulting histogram is shown in Figure 7.3 (the fitted curves in the figure are explained later). Two modes are clearly visible, and reasonable starting values for the five parameters might be $p = 0.5$, $\mu_1 = 50$, $\sigma_1 = 10$, $\mu_2 = 80$, and $\sigma_2 = 10$.

Now we can fit the mixture distribution to the eruption waiting times, stored in the vector, geyser, using the nlminb function.

```
geyser.res<-nlminb(c(0.5,50,10,80,10),LL,
data = geyser,lower = c(0.0001,-Inf,0.0001,
-Inf,0.0001),upper = c(0.9999,Inf,Inf,Inf, Inf))
#starting values of p = 0.5, mu1 = 50, sigma1 = 10,
#mu2 = 80 and sigma2 = 10
#LL is the function to be minimized
#and data is the extra argument used
#by this function
#lower bound for p is set at 0.0001 and
#for sigma1 and sigma2 0.0001.
#an upper bound of 0.9999 is set for p
#all other bounds are set at infinity
```

This returns geyser.res, which is an S-PLUS list object containing a variety of information about the optimisation process. Of most interest are the values of the estimated parameters found from

```
geyser.res$parameters
```

giving

```
[1] 0.3075936 54.2026523 4.9520039 80.3603088 7.5076321
```

(Fewer decimal places could be obtained by using the options function, for example, options(digits = 3).)

The fit of the mixture can be assessed by superimposing the fitted density onto a histogram of the observed eruption times.

```
x<-seq(40,120,length = 100)
#use the seq function to create a vector
#of 100 values between 40 and 120 at which
#to plot estimated mixture density
p<-geyser.res$parameters[1]
mu1<-geyser.res$parameters[2]
sig1<-geyser.res$parameters[3]
mu2<-geyser.res$parameters[4]
sig2<-geyser.res$parameters[5]
f<-pdnorm(x,mu1,sig1)+(1-p)dnorm(x,mu2,sig2)
#f contains fitted mixture densities corresponding
#to the values in x
hist(geyser,probability = T,col = 0,ylab = “Density”,
ylim = c(0, 0.03),xlab = “Eruption waiting times”)
#constructs histogram without colour or shading
#and as a density function
lines(x,f)
#adds estimated density to histogram
```

The resulting curves are shown in Figure 7.3. It is clear that the fitted mixture describes the eruption waiting times very well.

We can estimate the standard errors of the five parameters by again using a bootstrap approach. We first construct an S-PLUS function that returns the values of the five parameters for each bootstrap sample taken:

```
fit1<-function(data,start){
#data is a vector of sample values
#start is a vector of 5 starting values for
#the five parameters of the mixture; the mixing
#proportion is constrained to be in the interval 0.0001
#0.9999
data.res<-nlminb(start,LL,data = data,lower = c
0.0001,NA,0.0001,NA,0.0001),upper = c(
0.9999,NA,NA,NA,NA))
#estimate the five parameters
result <- data.res$parameters
result
}
```

Now the bootstrap can be applied; here we shall use 500 samples (be patient when running this portion of code — it takes some time!).

```
set.seed(9831)
geyser.boot<-bootstrap(geyser,fit1,args.stat =
list(start = c(0.05, 50, 10, 80, 10)),B = 500)
#takes 500 bootstrap samples and estimates
#the mixture parameters for each using the
#same starting values for each
summary(geyser.boot)
plot(boot)
```

The results are shown in Figure 7.4 and Table 7.6. In this case the estimated 95% confidence intervals for the five parameters are

p: [0.245,0.365]
μ_1: [52.500, 55.732]
σ_1: [4.952, 0.527]
μ_2: [78.994, 81.674]
σ_2: [6.385, 8.792]

(Note that some samples cause problems for the estimation process because of the singularity problem described in Everitt and Hand, 1981; see also Exercise 7.3).

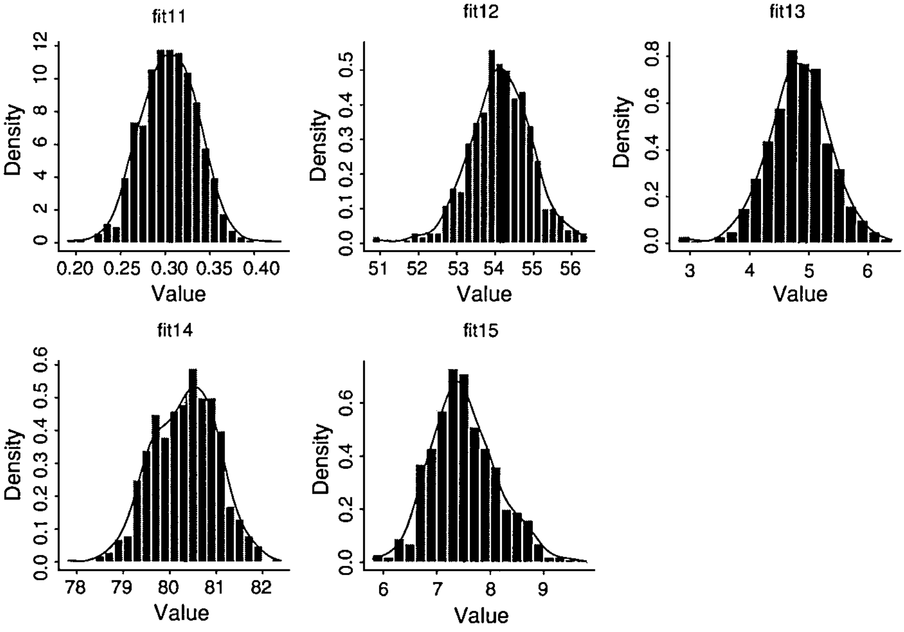


Figure 7.4 Bootstrap distributions for the five parameters in the two-component normal mixture fitted to the geyser eruption waiting time data; fit11 is the mixing proportion, fit12 is the mean of the first component, fit12 is the standard deviation of the first component, fit14 is the mean of the second component, and fit15 is the standard deviation of the second component.

Table 7.6 Bootstrap Results for Geyser Waiting Times

```
> summary(boot)
Call:
bootstrap(data = geyser, statistic = fit1, B = 500, args.stat = list(
        start = c(0.5, 50, 10, 80, 10)))

Number of Replications: 500

Summary Statistics:
        Observed        Bias      Mean         SE
fit11     0.3076   -0.002743    0.3049    0.03222
fit12    54.2027   -0.077846   54.1248    0.82236
fit13     4.9520   -0.129478    4.8225    0.52680
fit14    80.3603   -0.036408   80.3239    0.69097
fit15     7.5076    0.005208    7.5128    0.61591

Empirical Percentiles:
           2.5%         5%       95%     97.5%
fit11    0.2451     0.2541     0.354    0.3648
fit12   52.4997    52.7917    55.422   55.7321
fit13    3.8153     3.9642     5.675    5.8460
fit14   78.9938    79.2288    81.425   81.6744
fit15    6.3848     6.6201     8.654    8.7921

BCa Confidence Limits:
           2.5%         5%       95%     97.5%
fit11    0.2515     0.2606    0.3611     0.373
fit12   52.5957    52.8893   55.5269    55.765
fit13    4.0611     4.2227    5.9302     6.082
fit14   78.9484    79.2066   81.3629    81.539
fit15    6.6189     6.7132    8.7762     9.005

Correlation of Replicates:

          fit11      fit12      fit13      fit14      fit15
fit11    1.0000     0.4554     0.4573     0.3137    -0.3666
fit12    0.4554     1.0000     0.7401     0.4760    -0.4981
fit13    0.4573     0.7401     1.0000     0.4995    -0.5305
fit14    0.3137     0.4760     0.4995     1.0000    -0.4802
fit15   -0.3666    -0.4981    -0.5305    -0.4802     1.0000
```

Exercises

7.1. Investigate the residuals from fitting the model in Equation 7.1 to the Olympic records data. Is there any evidence of problems with the model?

7.2. Investigate the use of different numbers of bootstrap samples when finding confidence intervals for the parameters in the three parameter exponential model for the Olympic record data.

7.3. The mixture model in Equation 7.2 can give rise to singularity problems when fitted to data — essentially this means that the likelihood function tends towards infinity for reasons described in Everitt and Hand (1981). One solution is to constrain the two variances in the model to be the same. Fit such a model to the geyser eruption waiting times and construct a diagram showing a histogram of these times plus the two-fitted models (equal and unequal variances). Add an appropriate legend.

Chapter 8

Survival Analysis: Motion Sickness and Bird Survival

8.1 Description of Data

Two data sets will be used in this chapter. The first, shown in Table 8.1, arises from a research programme investigating motion sickness at sea. Human subjects were placed in a cubical cabin mounted on a hydraulic piston and subjected to vertical motion for 2 hours. The length of time until each subject first vomited was recorded. Some subjects requested an early stop to the experiment and some lasted the whole 2 hours without vomiting. (See Burns, 1984, for full details of the study.)

Our second data set is shown in Table 8.2. These data arise from 50 female black ducks from two locations in New Jersey that were captured and fitted with radios. The ducks were captured over a period of about 4 weeks and included 31 hatch-year birds (birds born during the previous breeding season) and 19 after-hatch birds (birds at least 1 year of age). The status (alive, missing, or dead) of each bird was recorded daily from the date of release until the end of the study. For some of the birds, death was not observed during the period of the study. Full details of the study are given in Pollock et al. (1989).

Both these data sets involve time to the occurrence of a particular event (vomiting in Table 8.1, death in Table 8.2). Such data are generally referred to by the generic term *survival data* even when the end point or event being considered is not death. Such data generally require special techniques for analysis for two main reasons:

Table 8.1 Data from Two Experiments on Motion Sickness: Time (minutes) to Vomiting

Experiment 1		Experiment 2	
1	30	1	5
2	50	2	6*
3	50*	3	11
4	51	4	11
5	66*	5	13
6	82	6	24
7	92	7	63
8	120*	8	65
9	120*	9	69
10	120*	10	69
11	120*	11	79
12	120*	12	82
13	120*	13	82
14	120*	14	102
15	120*	15	115
16	120*	16	120*
17	120*	17	120*
18	120*	18	120*
19	120*	19	120*
20	120*	20	120*
21	120*	21	120*
		22	120*
		23	120*
		24	120*
		25	120*
		26	120*
		27	120*
		28	120*

Experiment 1: 0.167 Hz frequency, 0.11 *g* acceleration.

Experiment 2: 0.333 Hz frequency, 0.222 *g* acceleration.

* Indicates a censored observation.

1. Survival data are usually not symmetrically distributed — they will often be positively skewed, with a few people surviving a very long time compared with the majority; so assuming, for example, a normal distribution will not be reasonable.

Table 8.2 Bird Survival

Bird	Time	Indicator	Age	Weight	Length
1	2	1	1	1160	277
2	6	0	0	1140	266
3	6	0	1	1260	280
4	7	1	0	1160	264
5	13	1	1	1080	267
6	14	0	0	1120	262
7	16	0	1	1140	277
8	16	1	1	1200	283
9	17	0	1	1100	264
10	17	1	1	1420	270
11	20	0	1	1120	272
12	21	1	1	1110	271
13	22	1	0	1070	268
14	26	1	0	940	252
15	26	1	0	1240	271
16	27	1	0	1120	265
17	28	0	1	1340	275
18	29	1	0	1010	272
19	32	1	0	1040	270
20	32	0	1	1250	276
21	34	1	0	1200	276
22	34	1	0	1280	270
23	37	1	0	1250	272
24	40	1	0	1090	275
25	41	1	1	1050	275
26	44	1	0	1040	255
27	49	0	0	1130	268
28	54	0	1	1320	285
29	56	0	0	1180	259
30	56	0	0	1070	267
31	57	0	1	1260	269
32	57	0	0	1270	276
33	58	0	0	1080	260
34	63	0	1	1110	270
35	63	0	0	1150	271
36	63	0	0	1030	265
37	63	0	0	1160	275
38	63	0	0	1180	263
39	63	0	0	1050	271
40	63	0	1	1280	281

Table 8.2 (Continued) Bird Survival

Bird	Time	Indicator	Age	Weight	Length
41	63	0	0	1050	275
42	63	0	0	1160	266
43	63	0	0	1150	263
44	63	0	1	1270	270
45	63	0	1	1370	275
46	63	0	1	1220	265
47	63	0	0	1220	268
48	63	0	0	1140	262
49	63	0	0	1140	270
50	63	0	0	1120	274

Time: days observed.
Indicator: 0 censored observation, 1: observed death
Age 0: hatch-year birds, 1: after-hatch-year birds.
Weight: weight of bird (g).
Length: wing length of bird (mm).

2. At the completion of the study, some participants may not have reached the end point of interest. Consequently, their exact survival times are not known. All that is known is that the survival times are greater than the amount of time the individual has been in the study. The survival times of these participants are said to be *censored* (more precisely, they are *right-censored*).

8.2 Describing Survival Times and Cox's Regression

Of central importance in the analysis of survival data are two functions describing the distribution of survival times, the *survival function* and the *hazard function.*

8.2.1 The Survival Function

Using T to denote survival time, the survival function, $S(t)$, is defined as the probability that an individual survives longer than t,

$$S(t) = Pr(T > t) \tag{8.1}$$

The graph of $S(t)$ against t is known as the survival curve. When there are no censored observations the survivor function can be estimated very simply as

$$\hat{S}(t) = \frac{\text{number of individuals with survival times} \geq t}{\text{number of individuals in the data set}} \tag{8.2}$$

But when the data contain censored observations a more complex estimator of $\hat{S}(t)$ is required, the one most commonly used is the *Kaplan–Meier estimator*, which is described in detail in Collett (1994).

For the data in Table 8.1 the main question of interest is whether the time to vomiting differs between the two experimental conditions. A graph of the estimated survival curves of each group will allow an informal assessment of this question; more formally, the survival experience of the two groups can be compared using what is known as the *log-rank test* (again, for details see Collett, 1994).

8.2.2 The Hazard Function

In the analysis of survival data, it is often of interest to assess which periods have high or low chances of the event of interest occurring amongst those alive at the time. Such risks can be quantified with the *hazard function*, defined as the probability that a participant experiences the event in a small time interval, s, given that the participant has survived up to the beginning of the interval, when the size of the time interval approaches zero, i.e.,

$$h(t) = \lim_{s \to 0} \Pr(t \leq T < t + s | T \geq t) \tag{8.3}$$

The conditioning aspect is very important. For example, the probability of dying at age 100 is very small because most people die before that age, but the probability of a person dying at age 100 given that the person has reached that age is much greater. (The hazard function is also often known as the *instantaneous failure rate*.)

The hazard function is of most use as the basis for modelling the dependence of survival time on a number of explanatory variables (compare multiple regression, Chapter 4). Since $h(t)$ is restricted to being positive, its logarithm is expressed as a linear function of the explanatory variables, plus an unspecified function of time $\alpha(t)$:

$$\log h(t) = \log \alpha(t) + \beta_1 x_1 + \ldots \beta_p x_p \tag{8.4}$$

where $x_1, \ldots, x_p$ are the explanatory variables of interest. This model was proposed by Cox (1972) and is known as either *Cox's regression* or the *proportional hazards model*. The latter name arises because for any two individuals at any point in time, the ratio of their hazard functions is a constant. Because the baseline hazard function $\alpha(t)$ does not have to be specified explicitly, the proportional hazards model is, essentially, nonparametric.

The estimated regression coefficients give the change in the log hazard produced by a change of one unit in the corresponding explanatory variable. Interpretation is aided by exponentiating the coefficients to give the effects in terms of the hazard function directly.

It is Cox's regression model we shall use to investigate the data in Table 8.2 to assess how survival time of the ducks is related to the other variables: weight, age, and length.

8.3 Analysis Using S-PLUS

S-PLUS has extensive features for the analysis of survival data, many of them described in detail in Therneau and Grambach (2000). Here we shall illustrate only the most commonly used of these.

8.3.1 Motion Sickness

The motion sickness data in Table 8.1 are available as the data frame motion the contents of which are shown in Table 8.3.

We begin by calculating the Kaplan–Meier estimates of the survival curves for the two experiments and plotting these curves. We will use the command language for this, in particular the S-PLUS functions Surv and survfit.

```
attach(motion)
motion.surv<-Surv(Time,Status)
#use surv to create an S-PLUS survival
#object for use in other survival analysis
#functions
survfit(motion.surv~Group)
#use survfit function to get information
#about survival time characteristics of each group
summary(survfit(motion.surv~Group))
#use summary to get details of the calculation of each
#group's survival curve
plot(survfit(motion.surv~Group),lty = 1:2)
legend(locator(1),c("Experiment 1","Experiment 2"),
lty = 1:2)
```

Table 8.3 Contents of motion Data Frame

< motion

	Subject	Group	Status	Time
1	1	0	1	30
2	2	0	1	50
3	3	0	0	50
4	4	0	1	51
5	5	0	0	66
6	6	0	1	82
7	7	0	1	92
8	8	0	0	120
9	9	0	0	120
10	10	0	0	120
11	11	0	0	120
12	12	0	0	120
13	13	0	0	120
14	14	0	0	120
15	15	0	0	120
16	16	0	0	120
17	17	0	0	120
18	18	0	0	120
19	19	0	0	120
20	20	0	0	120
21	21	0	0	120
22	22	1	1	5
23	23	1	0	6
24	24	1	1	11
25	25	1	1	11
26	26	1	1	13
27	27	1	1	24
28	28	1	1	63
29	29	1	1	65
30	30	1	1	69
31	31	1	1	69
32	32	1	1	79
33	33	1	1	82
34	34	1	1	82
35	35	1	1	102
36	36	1	1	115
37	37	1	0	120
38	38	1	0	120
39	39	1	0	120

Table 8.3 (continued) Contents of motion Data Frame

```
< motion
          Subject   Group   Status   Time
   40        40       1        0      120
   41        41       1        0      120
   42        42       1        0      120
   43        43       1        0      120
   44        44       1        0      120
   45        45       1        0      120
   46        46       1        0      120
   47        47       1        0      120
   48        48       1        0      120
   49        49       1        0      120
```

```
#plot the two survival curves and add a
#suitable legend
```

The numerical results are shown in Table 8.4 and the plot in Figure 8.1. The plotted survival curves suggest perhaps that the time to vomiting is longer under the conditions of experiment 1 than experiment 2, although the large number of censored observations in each experiment makes this interpretation problematical.

A formal test of the difference between the survival curves of the two groups can be made using the log-rank test implemented using the **survdiff** function. This test operates by first computing the expected number of ‘deaths’ for each unique death time, or failure time in the data set, assuming that the chances of dying, given that participants are at risk, is the same in both groups. The total number of expected deaths is then calculated for each group by adding the expected number of deaths for each failure time. The test then compares the observed number of deaths in each group with the expected number of deaths via a chi-squared statistic.

```
survdiff(motion.surv~Group)
```

The results of applying the test are shown in Table 8.5. There is no strong evidence for a real difference in the survival distributions in the two experiments. Time to vomiting in each experiment appears to have the same distribution.

The log-rank test weights the contributions from all failure times equally, regardless of when they occurred. However, we have more precise information at the beginning when a larger proportion of participants are

Table 8.4 Characteristics of Motion Sickness Data and Details of Kaplan–Meier Estimation of Survival Curves

```
> motion.surv <- Surv(Time, Status)
> survfit(motion.surv ~ Group)
Call: survfit(formula = motion.surv ~ Group)

             n   events   mean   se(mean)   median   0.95LCL   0.95UCL
Group = 0   21        5  105.4       6.12       NA        NA        NA
Group = 1   28       14   87.1       7.80      115        79        NA

> summary(survfit(motion.surv ~ Group))
Call: survfit(formula = motion.surv ~ Group)

                       Group = 0
time   n.risk   n.event   survival   std.err   lower 95% CI   upper 95% CI
  30       21         1      0.952    0.0465          0.866          1.000
  50       20         1      0.905    0.0641          0.788          1.000
  51       18         1      0.854    0.0778          0.715          1.000
  82       16         1      0.801    0.0894          0.644          0.997
  92       15         1      0.748    0.0981          0.578          0.967

                       Group = 1
time   n.risk   n.event   survival   std.err   lower 95% CI   upper 95% CI
   5       28         1      0.964    0.0351          0.898          1.000
  11       26         2      0.890    0.0599          0.780          1.000
  13       24         1      0.853    0.0679          0.730          0.997
  24       23         1      0.816    0.0744          0.682          0.976
  63       22         1      0.779    0.0797          0.637          0.952
  65       21         1      0.742    0.0841          0.594          0.926
  69       20         2      0.668    0.0906          0.512          0.871
  79       18         1      0.630    0.0928          0.472          0.841
  82       17         2      0.556    0.0956          0.397          0.779
 102       15         1      0.519    0.0961          0.361          0.746
 115       14         1      0.482    0.0962          0.326          0.713
```

still ‘alive’. Various tests have been proposed that give greater weight to earlier survival times. The *Peto–Wilcoxon* method, for example, weights observations by the Kaplan–Meier estimate of the proportion of participants still alive at each failure time. This method can be applied using the survdiff function but now including the argument rho = 1.

```
survidiff(motion.surv~Group, rho = 1)
```

The results of this test are also given in Table 8.5. They are very similar in this case to those from the log-rank test.

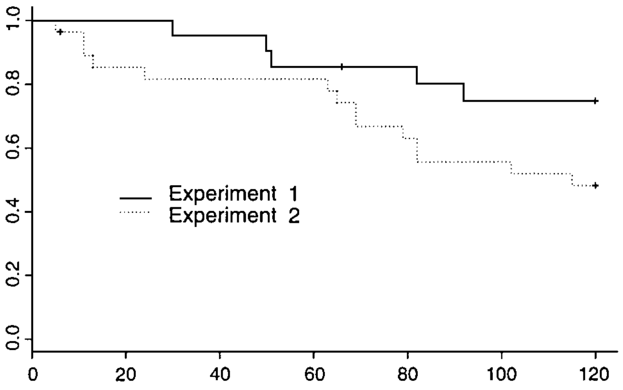


Figure 8.1 Survival curves for the data from each experiment in the motion sickness study.

Table 8.5 Results of Two Versions of the Log-Rank Test for the Motion Sickness Data

```
> survdiff(Surv(Time, Status) ~ Group)
Call:
survdiff(formula = Surv(Time, Status) ~ Group)
             N  Observed  Expected  (O-E)^2/E  (O-E)^2/V
Group = 0   21         5      8.86       1.68       3.21
Group = 1   28        14     10.14       1.47       3.21

  Chisq = 3.2 on 1 degrees of freedom, p = 0.0733
> survdiff(Surv(Time, Status) ~ Group, rho = 1)
Call:
survdiff(formula = Surv(Time, Status) ~ Group, rho = 1)

             N  Observed  Expected  (O-E)^2/E  (O-E)^2/V
Group = 0   21      4.01       7.2       1.41       3.22
Group = 1   28     11.49       8.3       1.22       3.22

Chisq = 3.2 on 1 degrees of freedom, p = 0.0728
```

8.3.2 Bird Deaths

The data in Table 8.2 are available as the data frame bird, the contents of which are given in Table 8.6.

Here we shall use the **Cox Proportional Hazards** dialog to fit a Cox's regression model to assess the effects of Age, Weight, and Length on a bird's survival time.

Table 8.6 Contents of bird Data Frame

```
> bird
    Bird  Time  Indicator  Age  Weight  Length
1      1     2          1    1    1160     277
2      2     6          0    0    1140     266
3      3     6          0    1    1260     280
4      4     7          1    0    1160     264
5      5    13          1    1    1080     267
6      6    14          0    0    1120     262
7      7    16          0    1    1140     277
8      8    16          1    1    1200     283
9      9    17          0    1    1100     264
10    10    17          1    1    1420     270
11    11    20          0    1    1120     272
12    12    21          1    1    1110     271
13    13    22          1    0    1070     268
14    14    26          1    0     940     252
15    15    26          1    0    1240     271
16    16    27          1    0    1120     265
17    17    28          0    1    1340     275
18    18    29          1    0    1010     272
19    19    32          1    0    1040     270
20    20    32          0    1    1250     276
21    21    34          1    0    1200     276
22    22    34          1    0    1280     270
23    23    37          1    0    1250     272
24    24    40          1    0    1090     275
25    25    41          1    1    1050     275
26    26    44          1    0    1040     255
27    27    49          0    0    1130     268
28    28    54          0    1    1320     285
29    29    56          0    0    1180     259
30    30    56          0    0    1070     267
31    31    57          0    1    1260     269
32    32    57          0    0    1270     276
33    33    58          0    0    1080     260
34    34    63          0    1    1110     270
35    35    63          0    0    1150     271
36    36    63          0    0    1030     265
37    37    63          0    0    1160     275
38    38    63          0    0    1180     263
39    39    63          0    0    1050     271
```

Table 8.6 (Continued) Contents of bird Data Frame

```
> bird
     Bird  Time  Indicator  Age  Weight  Length
40    40    63       0       1    1280     281
41    41    63       0       0    1050     275
42    42    63       0       0    1160     266
43    43    63       0       0    1150     263
44    44    63       0       1    1270     270
45    45    63       0       1    1370     275
46    46    63       0       1    1220     265
47    47    63       0       0    1220     268
48    48    63       0       0    1140     262
49    49    63       0       0    1140     270
50    50    63       0       0    1120     274
```

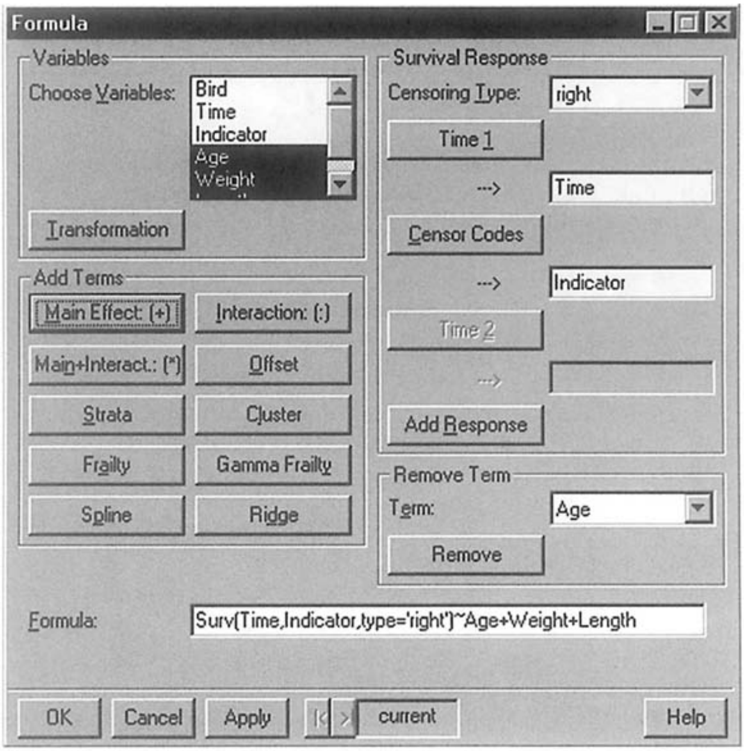
- Click on **Statistics**.
- Select **Survival**.
- Select **Cox Proportional Hazards**.

The **Cox Proportional Hazards** dialog now appears. Select **bird** as the data set and then click on **Create Formula**. The **Formula** dialog now become available.

- Highlight **Time** and click on the **Time 1** tab.
- Highlight **Indicator** and click on the **Censor Codes** tab.
- Click on the **Add Response** tab.

This creates a suitable S-PLUS survival object as the response. Now highlight Age, Weight, and Length and click in the **Main Effect (+)** tab. The **Formula** dialog now appears as shown in Figure 8.2.

Click **OK** to recover the **Cox Proportional Hazards** dialog and again click **OK**. The results of fitting the model are given in Table 8.7. Here the tests of the individual regression coefficients suggest that none is significantly different from zero. This is confirmed by Wald's and the other two tests that assess the three coefficients simultaneously. The *p*-values associated with each of these indicate that here the three explanatory variables have no effect on the survival times of the ducks.



Choose Variables: Bird
Time
Indicator
Age
Weight

Censoring Type: right

Time 1 --> Time

Censor Codes --> Indicator

Term: Age

Formula: Surv(Time,Indicator,type='right')~Age+Weight+Length

Figure 8.2 **Completed Formula dialog in the Cox Proportional Hazards dialog.**

Table 8.7 Results of Fitting Proportional Hazards Model to Bird Survival Data

```
        *** Cox Proportional Hazards ***
Call:
coxph(formula = Surv(Time, Indicator, type = "right") ~ Age + Weight
+ Length, data = bird, na.action = na.exclude, eps = 0.0001,
iter.max = 10, method = "efron", robust = F)

   n = 50

            coef  exp(coef)  se(coef)       z     p
   Age    0.4637      1.590   0.57810   0.802  0.42
Weight   -0.0042      0.996   0.00289  -1.451  0.15
Length    0.0125      1.013   0.04087   0.306  0.76

         exp(coef)  exp(-coef)  lower .95  upper .95
   Age       1.590       0.629      0.512       4.94
Weight       0.996       1.004      0.990       1.00
Length       1.013       0.988      0.935       1.10

Rsquare = 0.043 (max possible = 0.923)
Likelihood ratio test = 2.2 on 3 df,  p = 0.532
Wald test             = 2.25 on 3 df, p = 0.522
Score (logrank) test  = 2.28 on 3 df, p = 0.517
```

Exercises

8.1. Construct separate plots of the survival curves of the data from each experiment on motion sickness, showing in each case the estimated 95% confidence interval.

8.2. Plot the estimated survival curves of the hatch-year and after-hatch-year birds obtained from the bird data frame.

8.3. Fit a stratified Cox's model to the data in the bird data frame to explore the possibility that there should be separate baseline hazards for hatch-year and after-hatch-year birds.

Chapter 9

Exploring Multivariate Data: Male Egyptian Skulls

9.1 Description of Data

In this chapter we shall analyse the data shown in Table 9.1. These data show four measurements on male Egyptian skulls from five epochs. The measurements are

MB: Maximum Breadth
BH: Basibregmatic Height
BL: Basialiveolar Length
NH: Nasal Height

One question about these data is whether there is evidence of any change in the skulls over time? A steady change of head shape with time would indicate interbreeding with immigrant populations.

9.2 Exploring Multivariate Data

In this chapter we shall use a variety of primarily informal graphical methods to explore the structure of the data in Table 9.1 keeping in mind the main question of interest about the data. Some of these methods will have been used in previous chapters, but here we shall also use *principal components analysis* (see Everitt and Dunn, 2001) to help simplify the

Table 9.1 Data on Male Egyptian Skulls

c 4000 BC				c 3300 BC				c 1850 BC				c 200 BC				c AD 150			
MB	BH	BL	NH	MB	BH	BL	NH	MB	BH	BL	NH	MB	BH	BL	NH	MB	BH	BL	NH
131	138	89	49	124	138	101	48	137	141	96	52	137	134	107	54	137	123	91	50
125	131	92	48	133	134	97	48	129	133	92	47	141	128	95	53	136	131	95	49
131	132	99	50	138	134	98	45	132	138	87	48	141	130	87	49	128	126	91	57
119	132	96	44	148	129	104	51	130	134	106	50	135	131	99	51	130	134	92	52
136	143	100	54	126	124	95	45	134	134	96	45	133	120	91	46	138	127	86	47
138	137	89	56	135	136	98	52	140	133	98	50	131	135	90	50	126	138	101	52
139	130	108	48	132	145	100	54	138	138	95	47	140	137	94	60	136	138	97	58
125	136	93	48	133	130	102	48	136	145	99	55	139	130	90	48	126	126	92	45
131	134	102	51	131	134	96	50	136	131	92	46	140	134	90	51	132	132	99	55
134	134	99	51	133	125	94	46	126	136	95	56	138	140	100	52	139	135	92	54
129	138	95	50	133	136	103	53	137	129	100	53	132	133	90	53	143	120	95	51
134	121	95	53	131	139	98	51	137	139	97	50	134	134	97	54	141	136	101	54
126	129	109	51	131	136	99	56	136	126	101	50	135	135	99	50	135	135	95	56
132	136	100	50	138	134	98	49	137	133	90	49	133	136	95	52	137	134	93	53

141	140	100	51	130	136	104	53	129	142	104	47	136	130	99	55	142	135	96	52
131	134	97	54	131	128	98	45	135	138	102	55	134	137	93	542	139	134	95	47
135	137	103	50	138	129	107	53	129	135	92	50	131	141	99	55	138	125	99	51
132	133	93	53	123	131	101	51	134	125	90	60	129	135	95	47	137	135	96	54
139	136	96	50	130	129	105	47	138	134	96	51	136	128	93	54	133	125	92	50
132	131	101	49	134	130	93	54	136	135	94	53	131	125	88	48	145	129	89	47
126	133	102	51	137	136	106	49	132	130	91	52	139	130	94	53	138	136	92	46
135	135	103	47	126	131	100	48	133	131	100	50	144	124	86	50	131	129	97	44
134	124	93	53	135	136	97	52	138	137	94	51	141	131	97	53	143	126	88	54
128	134	103	50	129	126	91	50	130	127	99	45	130	131	98	53	131	124	91	55
130	130	104	49	134	139	101	49	136	133	91	49	133	128	92	51	132	127	97	52
138	135	100	55	131	134	90	53	134	123	95	52	138	126	97	54	137	125	85	57
128	132	93	53	132	130	104	50	136	137	101	54	131	142	95	53	129	128	81	52
127	129	106	48	130	132	93	52	133	131	96	49	136	138	94	55	140	135	103	48
131	136	114	54	135	132	98	54	138	133	100	55	132	136	92	52	147	129	87	48
124	138	101	46	130	128	101	51	138	133	91	46	135	130	100	51	136	133	97	51

data, and *multidimensional scaling* (see Everitt and Rabe-Hesketh, 1999) to display graphically *Mahalanobis distances* (see Chapter 2) between the five epochs.

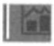
Principal components analysis seeks linear compounds of the original variables, which are uncorrelated and which account for maximal amounts of the variation in these variables. By using these new variables it may be possible to achieve a parsimonious summary of the data in a reduced number of dimensions.

Multidimensional scaling attempts to find a low-dimensional representation of an observed distance matrix so that the Euclidean distances in this representation match as closely as possible in some sense the observed distances. In this way it may be possible to find an adequate graphical representation of the distances that enables any structure or pattern to be discovered.

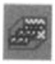
9.3 Analysis Using S-PLUS

We assume that the data in Table 9.1 are available as an S-PLUS data frame skulls, which as well as the four measurements described in the previous section, contains a factor variable, EPOCH, with five levels labelling the epoch at which the measurements were made. The contents of skulls is shown in Table 9.2.

To begin we shall construct some simple, but nonetheless informative graphics using the two graphics palettes which we remind readers can be made visible by clicking

 (2D)

and

 (3D)

We shall also make use of the 'conditioning' feature of S-PLUS that allows any type of graph to be plotted, conditional on the values of some variable (or variables). Here the conditioning will involve the categorical variable, EPOCH, but continuous variables may also be used, in which case the variable values are divided into a small number of intervals. This conditioning feature of S-PLUS has the potential to be very powerful, and we suggest readers experiment with the possibilities.

Table 9.2 Contents of skulls Data Frame

```
> skulls
      EPOCH    MB   BH   BL  NH
 1  c4000BC   131  138   89  49
 2  c4000BC   125  131   92  48
 3  c4000BC   131  132   99  50
 4  c4000BC   119  132   96  44
 5  c4000BC   136  143  100  54
 6  c4000BC   138  137   89  56
 7  c4000BC   139  130  108  48
 8  c4000BC   125  136   93  48
 9  c4000BC   131  134  102  51
10  c4000BC   134  134   99  51
11  c4000BC   129  138   95  50
12  c4000BC   134  121   95  53
13  c4000BC   126  129  109  51
14  c4000BC   132  136  100  50
15  c4000BC   141  140  100  51
16  c4000BC   131  134   97  54
17  c4000BC   135  137  103  50
18  c4000BC   132  133   93  53
19  c4000BC   139  136   96  50
20  c4000BC   132  131  101  49
21  c4000BC   126  133  102  51
22  c4000BC   135  135  103  47
23  c4000BC   134  124   93  53
24  c4000BC   128  134  103  50
25  c4000BC   130  130  104  49
26  c4000BC   138  135  100  55
27  c4000BC   128  132   93  53
28  c4000BC   127  129  106  48
29  c4000BC   131  136  114  54
30  c4000BC   124  138  101  46
31  c3300BC   124  138  101  48
32  c3300BC   133  134   97  48
33  c3300BC   138  134   98  45
34  c3300BC   148  129  104  51
35  c3300BC   126  124   95  45
36  c3300BC   135  136   98  52
37  c3300BC   132  145  100  54
38  c3300BC   133  130  102  48
39  c3300BC   131  134   96  50
```

Table 9.2 (Continued) Contents of skulls Data Frame

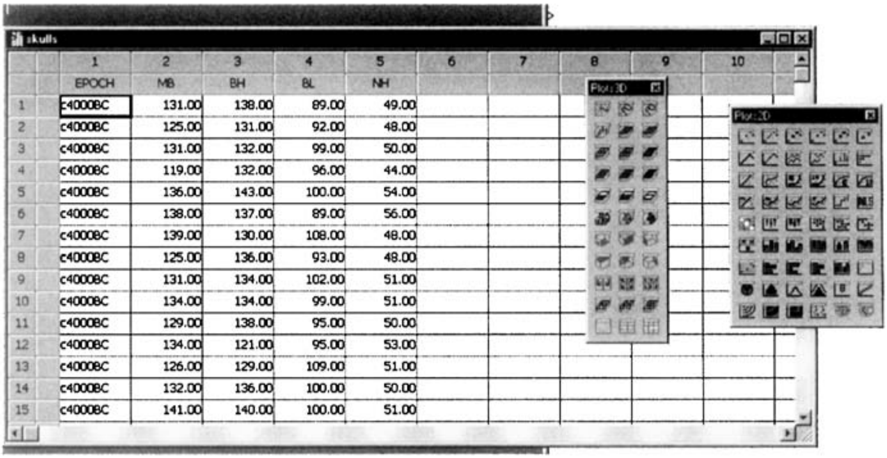
```
> skulls
        EPOCH     MB    BH    BL    NH
  40   c3300BC   133   125    94    46
  41   c3300BC   133   136   103    53
  42   c3300BC   131   139    98    51
  43   c3300BC   131   136    99    56
  44   c3300BC   138   134    98    49
  45   c3300BC   130   136   104    53
  46   c3300BC   131   128    98    45
  47   c3300BC   138   129   107    53
  48   c3300BC   123   131   101    51
  49   c3300BC   130   129   105    47
  50   c3300BC   134   130    93    54
  51   c3300BC   137   136   106    49
  52   c3300BC   126   131   100    48
  53   c3300BC   135   136    97    52
  54   c3300BC   129   126    91    50
  55   c3300BC   134   139   101    49
  56   c3300BC   131   134    90    53
  57   c3300BC   132   130   104    50
  58   c3300BC   130   132    93    52
  59   c3300BC   135   132    98    54
  60   c3300BC   130   128   101    51
  61   c1850BC   137   141    96    52
  62   c1850BC   129   133    93    47
  63   c1850BC   132   138    87    48
  64   c1850BC   130   134   106    50
  65   c1850BC   134   134    96    45
  66   c1850BC   140   133    98    50
  67   c1850BC   138   138    95    47
  68   c1850BC   136   145    99    55
  69   c1850BC   136   131    92    46
  70   c1850BC   126   136    95    56
  71   c1850BC   137   129   100    53
  72   c1850BC   137   139    97    50
  73   c1850BC   136   126   101    50
  74   c1850BC   137   133    90    49
  75   c1850BC   129   142   104    47
  76   c1850BC   135   138   102    55
```

Table 9.2 (Continued) Contents of skulls Data Frame

```
> skulls
        EPOCH     MB    BH    BL    NH
 77   c1850BC    129   135    92    50
 78   c1850BC    134   125    90    60
 79   c1850BC    138   134    96    51
 80   c1850BC    136   135    94    53
 81   c1850BC    132   130    91    52
 82   c1850BC    133   131   100    50
 83   c1850BC    138   137    94    51
 84   c1850BC    130   127    99    45
 85   c1850BC    136   133    91    49
 86   c1850BC    134   123    95    52
 87   c1850BC    136   137   101    54
 88   c1850BC    133   131    96    49
 89   c1850BC    138   133   100    55
 90   c1850BC    138   133    91    46
 91    c200BC    137   134   107    54
 92    c200BC    141   128    95    53
 93    c200BC    141   130    87    49
 94    c200BC    135   131    99    51
 95    c200BC    133   120    91    46
 96    c200BC    131   135    90    50
 97    c200BC    140   137    94    60
 98    c200BC    139   130    90    48
 99    c200BC    140   134    90    51
100    c200BC    138   140   100    52
101    c200BC    132   133    90    53
102    c200BC    134   134    97    54
103    c200BC    135   135    99    50
104    c200BC    133   136    95    52
105    c200BC    136   130    99    55
106    c200BC    134   137    93    52
107    c200BC    131   141    99    55
108    c200BC    129   135    95    47
109    c200BC    136   128    93    54
110    c200BC    131   125    88    48
111    c200BC    139   130    94    53
112    c200BC    144   124    86    50
113    c200BC    141   131    97    53
```

Table 9.2 (Continued) Contents of skulls Data Frame

```
> skulls
        EPOCH    MB   BH   BL  NH
 114   c200BC   130  131   98  53
 115   c200BC   133  128   92  51
 116   c200BC   138  126   97  54
 117   c200BC   131  142   95  53
 118   c200BC   136  138   94  55
 119   c200BC   132  136   92  52
 120   c200BC   135  130  100  51
 121   cAD150   137  123   91  50
 122   cAD150   136  131   95  49
 123   cAD150   128  126   91  57
 124   cAD150   130  134   92  52
 125   cAD150   138  127   86  47
 126   cAD150   126  138  101  52
 127   cAD150   136  138   97  58
 128   cAD150   126  126   92  45
 129   cAD150   132  132   99  55
 130   cAD150   139  135   92  54
 131   cAD150   143  120   95  51
 132   cAD150   141  136  101  54
 133   cAD150   135  135   95  56
 134   cAD150   137  134   93  53
 135   cAD150   142  135   96  52
 136   cAD150   139  134   95  47
 137   cAD150   138  125   99  51
 138   cAD150   137  135   96  54
 139   cAD150   133  125   92  50
 140   cAD150   145  129   89  47
 141   cAD150   138  136   92  46
 142   cAD150   131  129   97  44
 143   cAD150   143  126   88  54
 144   cAD150   134  124   91  55
 145   cAD150   132  127   97  52
 146   cAD150   137  125   85  57
 147   cAD150   129  128   81  52
 148   cAD150   140  135  103  48
 149   cAD150   147  129   87  48
 150   cAD150   136  133   97  51
```



skulls

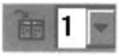
	1	2	3	4	5	6	7	8	9	10
	EPOCH	MB	BH	BL	NH					
1	c4000BC	131.00	138.00	89.00	49.00					
2	c4000BC	125.00	131.00	92.00	48.00					
3	c4000BC	131.00	132.00	99.00	50.00					
4	c4000BC	119.00	132.00	96.00	44.00					
5	c4000BC	136.00	143.00	100.00	54.00					
6	c4000BC	138.00	137.00	89.00	56.00					
7	c4000BC	139.00	130.00	108.00	48.00					
8	c4000BC	125.00	136.00	93.00	48.00					
9	c4000BC	131.00	134.00	102.00	51.00					
10	c4000BC	134.00	134.00	99.00	51.00					
11	c4000BC	129.00	138.00	95.00	50.00					
12	c4000BC	134.00	121.00	95.00	53.00					
13	c4000BC	126.00	129.00	109.00	51.00					
14	c4000BC	132.00	136.00	100.00	50.00					
15	c4000BC	141.00	140.00	100.00	51.00					

Figure 9.1 Skulls data and 2D and 3D graphics.

To access the skulls data frame for use with the two graphics palettes:

- Click on **Data**.
- Choose **Select Data**.
- In the **Select Data** dialog that now appears choose skulls in the **Existing Data** box and then click **OK**.

The skulls data frame appears, and we now make the two graphics palettes available by clicking on the appropriate buttons. Also, we need to turn the condition mode on by clicking on



(this button "toggles" between conditioning on and off and the 1 refers to the number of conditioning variables, which can be altered). The screen now looks something like Figure 9.1.

To begin, suppose we require histograms of, say, MB for each epoch.

- Highlight the **MB** column by clicking on the name.
- Now **Ctrl click** the **EPOCH** column.
- Select the **Histogram** option on the **2D Graph palette**.

This leads to a coloured version of Figure 9.2. The first variable highlighted is the one that forms the histograms, the second is the conditioning variable. There is perhaps some evidence that MB increases over the epochs. Similar graphs could now be constructed for the other three measurements in the data set.

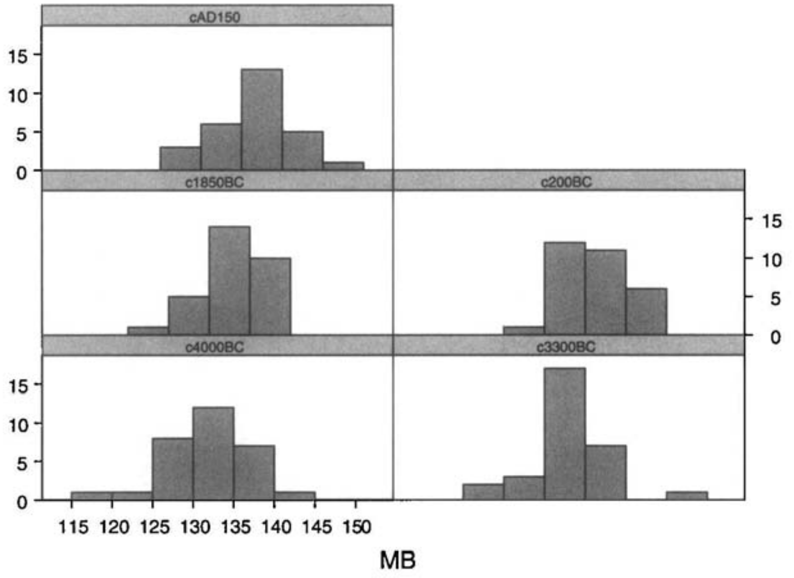


Figure 9.2 Histograms of the variable MB for each epoch.

Now suppose we would like a scatterplot of BH against MG for each epoch, with a locally weighted regression fit drawn on each graph.

- Highlight **MB** (this will be the *x* variable).
- **Ctrl click** on **BH** (this will be the *y* variable).
- **Ctrl click** on **EPOCH** (since the conditioning mode is on, this will be the conditioning variable).
- Select **Loess** on the **2D Graph palette**.

This series of operations leads to the graph in Figure 9.3. Is there a different relationship between MB and BH in the different epochs? It is perhaps difficult to judge, although there appears to be a small but definite negative relationship in c200BC that is not present in the other epochs.

Again, similar diagrams could be produced for all other pairs of variables. All such diagrams can be summarized conveniently by constructing a scatterplot matrix for each of the epochs.

- Highlight **MB** and the **Ctrl click** on each of the other three measurement variables.
- **Ctrl click** on **EPOCH**.
- Select the **Scatter Matrix** option in the **2D Graph palette**.

This leads to Figure 9.4. Although this is a rather 'busy' diagram, it does enable all the pairwise scatterplots for the five different epochs to be

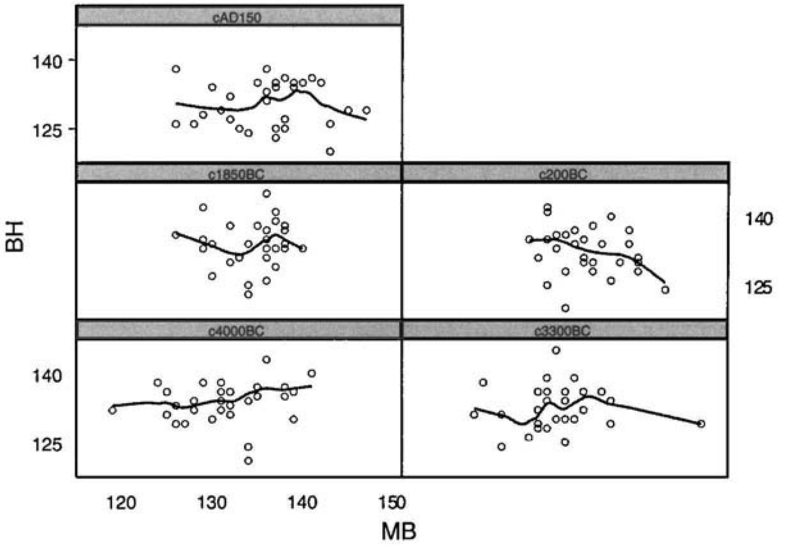


Figure 9.3 Scatterplots of the variables MB and BH for each epoch, showing a locally weighted regression fit.

viewed together, which might be helpful to an experienced archaeologist if not to the author!

Now let us consider two examples of using the **3D graph palette**, very much as exercises in the use of this feature of S-PLUS, rather than particularly helpful graphics for exploring the skulls data. To get two, three-dimensional graphs of the variables MB, BH, and BL (here we do not want the plots to be conditioned on epoch and so the conditioning button must be in the off position):

- Highlight **MB**.
- **Ctrl click** on **BH** and on **BL**.
- Select **3D Scatter** in the **3D Graph palette**.

This gives Figure 9.5. Such diagrams are often made clearer by 'dropping' lines from the plotted points to a plane through the origin. To construct this diagram, proceed as for Figure 9.5 but Select **Drop Line Scatter** in the **3D Graph palette** to get Figure 9.6.

Now let us consider some more complex methods for exploring the structure of the skulls data. To begin, we shall apply principal components to the data. This technique, described fully in Everitt and Dunn (2001) attempts to reduce the dimensionality of multivariate data by finding uncorrelated linear combinations of the original variables that account for maximal proportions of the variation in the data. Such variables can be

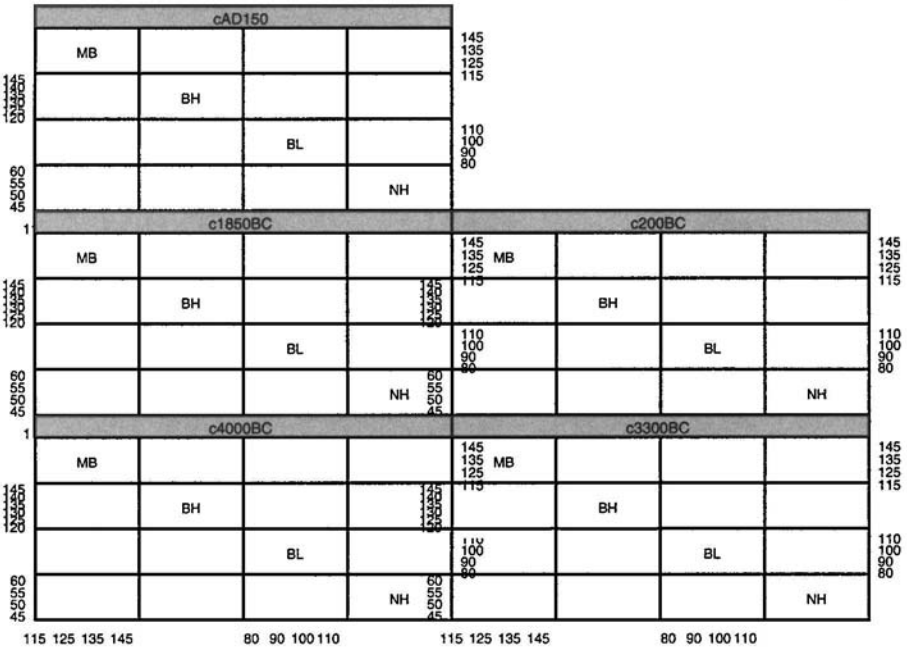


Figure 9.4 Scatterplot matrix of variables in the skulls data frame for each epoch.

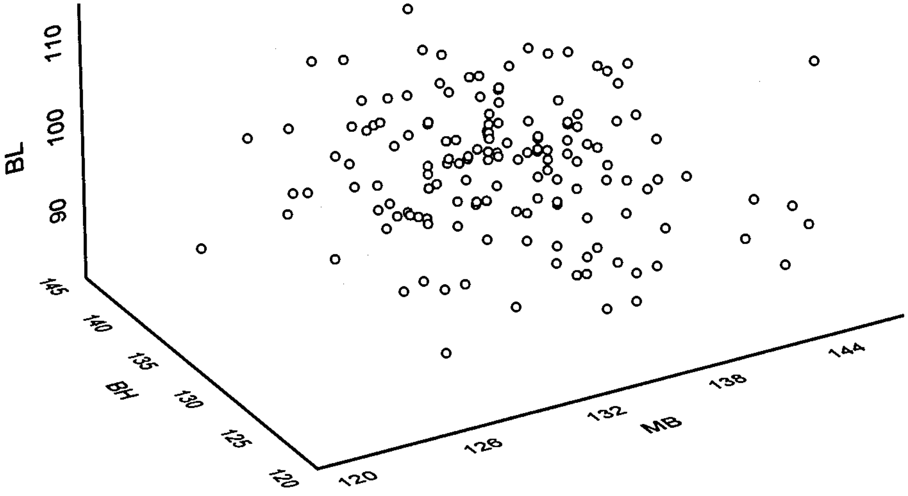


Figure 9.5 Three-dimensional scatter of the variables BH, MB, and BL.

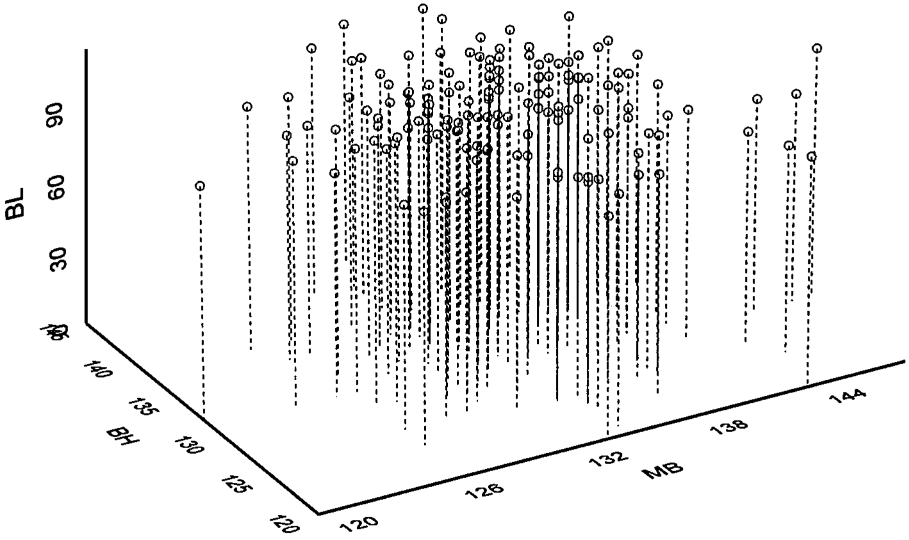


Figure 9.6 Three-dimensional drop-line scatter of the three variables BH, MB, and BL.

used in a variety of ways, but here our main interest will be in using the derived components to obtain an informative graphical display of the data. For this analysis we shall use the command language approach.

```
skulls.pc<-princomp(skulls[,-1],cor=T)
#produces a principal components of the skulls
#data after removing EPOCH. Components are
#derived from the correlation matrix
summary(skulls.pc)
```

This gives the results shown in Table 9.3. The first component accounts for just over 33% of the variance; the first two for 64%.

The loadings of the four observed variables on each component are displayed using the command:

```
skulls.pc$loadings
```

The results appear in Table 9.4.

The first component is a contrast between MB on the one hand and BH and BL on the other. The second component is simply a weighted average of MB, BH, and NH. Interpretation of the components is not our

Table 9.3 Standard Deviations of Principal Components of the Egyptian Skulls Data

```
> skulls.pc <- princomp(skulls[, -1], cor = T)
> summary(skulls.pc)
Importance of components:
                           Comp. 1     Comp. 2     Comp. 3     Comp. 4
     Standard deviation  1.1564147   1.0983595   0.8731551   0.8330136
 Proportion of Variance  0.3343237   0.3015984   0.1906000   0.1734779
 Cumulative Proportion   0.3343237   0.6359221   0.8265221   1.0000000
```

Table 9.4 Coefficients Defining the Principal Components of the Egyptian Skulls Data

```
> skulls.pc$loadings
      Comp. 1   Comp. 2   Comp. 3   Comp. 4
MB     -0.407     0.567    -0.710
BH      0.617     0.345              -0.707
 BL     0.672              -0.469     0.572
NH                0.748     0.525     0.405
```

main aim here, however; rather we shall use the scores of each skull on the first two components to display the data graphically.

```
skulls.pcx<-skull.pc$scores[,1]
skulls.pcy<-skull.pc$scores[,2]
#skulls.pcx and skulls.pcy now contain the
#first and second principal components scores
#for each skull
par(pty=“s”)
#select a square plotting area
xlim<-range(skulls.pcx)
#find range of x values to use in plotting
#the data
plot(skulls.pcx,skulls.pcy,xlim=xlim,
ylim=xlim,xlab=“PC1”,ylab=“PC2”,
type=“n”)
#set up axes of plot and label axis but do
#not plot the data
```

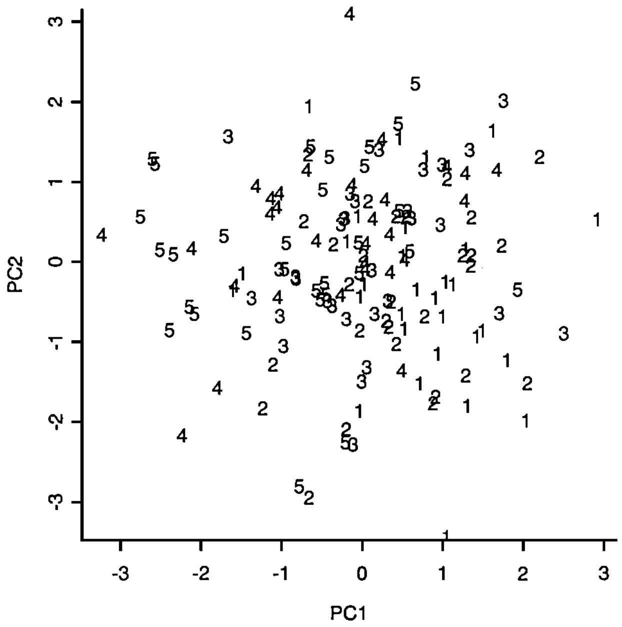


Figure 9.7 Plot of skulls data in the space of the first two principal component scores, with points labelled by epoch.

```
labs<-rep(1:5,rep(30,5))
#labs contains values 1 to 5 in sets of 30 and
#will be used to label the plot according to epoch
#since the EPOCH labels themselves would make
#the plot too messy
text(skulls.pcx,skulls.pcy,labels=labs)
```

The resulting diagram is shown in Figure 9.7. There does appear to be some distinction between epochs 1 (c4000BC) and 5(cAD150) in this diagram, but the observations for the remaining three epochs overlap to a considerable extent.

Finally, we shall calculate Mahalanobis distances (see Chapter 2) between each pair of epochs, and then try to represent the distances by Euclidean distances in two dimensions using *classical multidimensional scaling*. This technique is described in detail in Everitt and Rabe-Hesketh (1997), but in essence it tries to represent, in low-dimensional space, an observed distance matrix, by deriving coordinates for each observation (epochs in this case) so that the Euclidean distances defined by these coordinates approximate the elements of the observed distance matrix. Again, we shall use the command language, and we need in particular to use the apply function to obtain the mean vectors of each epoch, the var function to obtain the covariance matrix of each epoch, the Mahalanobis function to calculate the required distance matrix, and the cmdscale function to apply multidimensional scaling. In this calculation we shall use the following estimate of the assumed common covariance matrix, **S**,

$$\mathbf{S} = \frac{29\mathbf{S}_1 + 29\mathbf{S}_2 + 29\mathbf{S}_3 + 29\mathbf{S}_4 + 29\mathbf{S}_5}{145} \qquad (9.1)$$

where $\mathbf{S}_1, \ldots, \mathbf{S}_5$, are the covariance matrices within each epoch.

```
#Mahalanobis distances
centres<-matrix(0,5,4)
S <-matrix(0,4,4)
#set up matrices to take mean vectors
#of each epoch and covariance matrix
for(i in 1:5) {
      centres[i,]<-apply(skulls[labs==i,-1],2,mean)
      S<-S+29*var(skulls[,-1])
}
#use for loop to calculate all mean vectors and the
#combined covariance matrix
S<-S/145
mahal<-matrix(0,5,5)
for(i in 1:5) {
      mahal[i,]<-mahalanobis(centres,centres[i,],S)
}
#calculate required matrix of Mahalanobis distances
#between epoch means
par(pty=“s”)
coords<-cmdscale(mahal)
xlim<-range(coords[, 1])
plot(coords,xlab=“C1”,ylab=“C2”,type=“n”,xlim=xlim,
ylim=xlim)
text(coords,labels=c(“c4000BC”,”c3300BC”,”c1850BC”,
“c200BC”,”cAD150”))
```

The Mahalanobis distance matrix is shown in Table 9.5. The resulting diagram is shown in Figure 9.8. Here there is a very striking confirmation of a steady change of head shape with time.

Table 9.5 Mahalanobis Distances between Epochs

	[,1]	[,2]	[,3]	[,4]	[,5]
[1,]	0.00000000	0.08544641	0.7040863	1.3632193	1.9644964
[2,]	0.08544641	0.00000000	0.5923855	1.1838453	1.5724978
[3,]	0.70408633	0.59238550	0.0000000	0.3679117	0.7388707
[4,]	1.36321930	1.18384525	0.3679117	0.0000000	0.2009955
[5,]	1.96449636	1.57249782	0.7388707	0.2009955	0.0000000

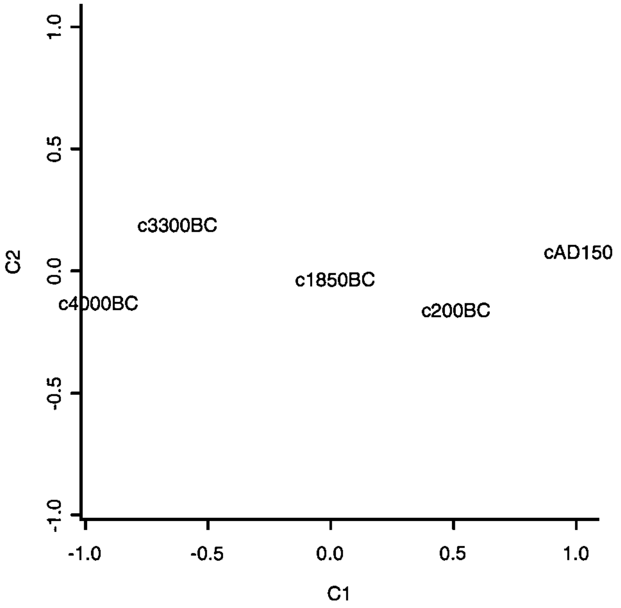


Figure 9.8 Two-dimensional solution from classical multidimensional scaling applied to the Mahalanobis distances between epochs.

Exercises

9.1. Construct a scatterplot matrix of all the principal component scores of the skulls data with the points in each panel labelled in some way by epoch.

9.2. Use the **Select Data** and **2D Graph palette** options to construct a contour plot of the bivariate density of the first two principal component scores of the skulls data.

9.3. Plot the convex hull of the observations of each epoch onto the plot of the data in the space of the first two principal components. (This will involve finding out about and then using the following S-PLUS functions: chull and polygon.)

Chapter 10

Cluster Analysis: Low Temperatures and Voting in Congress

10.1 Description of Data

Two sets of data will be of concern in this chapter. The first, shown in Table 10.1, gives the lowest temperatures (in °F) recorded for various cities in the United States. The second, in Table 10.2, records the number of times 15 congresspeople from New Jersey voted differently in the House of Representatives on 19 environmental bills.

One question of interest about the lowest temperatures data is whether the temperatures can be used to group the cities into distinct classes? And classification is also of interest for the voting data as an aid to see if the data imply party affiliations in the voting records of the 15 congresspeople.

10.2 Cluster Analysis

Cluster analysis is a generic term for a large number of relatively disparate techniques that seek to determine whether or not a data set contains distinct groups or clusters of observations and, if so, to find these groups. A detailed review of the area is given in Everitt et al. (2001).

Table 10.1 Lowest Temperatures in a Number of Cities in the United States

January	April	July	October
–8	26	53	28
–7	20	51	25
–44	–12	35	5
–12	16	54	28
–27	7	40	17
4	30	59	29
–25	–2	43	3
–8	23	57	25
53	57	67	64
12	31	62	33
–22	6	36	11
23	39	49	41
30	46	69	51
–17	23	51	26
–6	12	52	28
–23	5	44	13
17	32	61	34
–26	8	40	15
–16	13	33	8
24	31	43	34
0	29	43	28
–5	24	55	29

The most commonly used subset of clustering methods is that generally referred to as *agglomerative hierarchical methods.* These produce a series of hierarchical partitions of the observations, beginning at the stage of n separate single-member 'groups' (where n is the sample size), and ending with a single group containing all the observations. The series of steps is usually summarized in a tree-like diagram known as a *dendrogram.* In most applications, users will be interested in selecting one or two partitions from the series that in some sense best describe the data. A number of informal indicators of number of groups when using this type of clustering procedure are described in Everitt et al. (2001).

Most agglomerative hierarchical clustering methods operate on an $n \times n$ *distance* or *dissimilarity matrix* for the objects being clustered. In general, this will be calculated from the multivariate observations available for each object, and the most commonly used distance measure is *Euclidean* defined as

Table 10.2 Voting in Congress

Name (Party)	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
1 Hunt (R)	0	8	15	15	10	9	7	15	16	14	15	16	7	11	13
2 Sandman (R)	8	0	17	12	13	13	12	16	17	15	16	17	13	12	16
3 Howard (D)	15	17	0	9	16	12	15	5	5	6	5	4	11	10	7
4 Thompson (D)	15	12	9	0	14	12	13	10	8	8	8	6	15	10	7
5 Freylinghuysen (R)	10	13	16	14	0	8	9	13	14	12	12	12	10	11	11
6 Forsythe (R)	9	13	12	12	8	0	7	12	11	10	9	10	6	6	10
7 Widnall (R)	7	12	15	13	9	7	0	17	16	15	14	15	10	11	13
8 Roe (D)	15	16	5	10	13	12	17	0	4	5	5	3	12	7	6
9 Heltoski (D)	16	17	5	8	14	11	16	4	0	3	2	1	13	7	5
10 Rodino (D)	14	15	6	8	12	10	15	5	3	0	1	2	11	4	6
11 Minish (D)	15	16	5	8	12	9	14	5	2	1	0	1	12	5	5
12 Rinaldo (R)	16	17	4	6	12	10	15	3	1	2	1	0	12	6	4
13 Maraziti (R)	7	13	11	15	10	6	10	12	13	11	12	12	0	9	13
14 Daniels (D)	11	12	10	10	11	6	11	7	7	4	5	6	9	0	9
15 Patten (D)	13	16	7	7	11	10	13	6	5	6	5	4	13	9	0

$$d_{ij} = \sqrt{\sum_{k=1}^{p} \left(x_{ik} - x_{jk}\right)^2} \tag{10.1}$$

where x_{ik} and x_{jk} represent the value of the kth variable for objects i and j, respectively. The number of variables is p. Occasionally, however, the dissimilarity matrix, which is to be the basis of clustering, can arise directly, as with the voting data described previously.

Differences between agglomerative hierarchical techniques occur because of the variety of ways in which distance between a group and a single object, or between two groups, can be defined. Three methods that are commonly used are

- Distance between two groups taken as the distance between their two closest members — results in *single linkage clustering.*
- Distance between two groups taken as the distance between their two most remote members — results in *complete linkage clustering.*
- Distance between two groups taken as the distance between the average of the intergroup pairwise distances — results in *average linkage.*

All these methods and their properties are described in Everitt et al. (2001).

Another frequently used type of cluster analysis is based on finding a partition of the observations into a particular number of groups so as to optimise some numerical measure, small (or large for some measures) values of which indicate a 'good' clustering. One such method is *k-means* which, given an initial partition into the required number of groups, attempts to find an improved solution by searching for the partition that minimises the total within-group sum of squares of the observations. Again, there are various possibilities for deciding on the 'best' number of groups for a data set — see Everitt et al. (2001) for details. One simple method is to plot the within-clusters sum of squares against number of clusters. This sum of squares decreases monotonically as the number of clusters increases, but in many cases the decrease flattens markedly from some value onwards. The location of such an 'elbow' in the plot is often taken to indicate the appropriate number of clusters. Tibshirani et al. (2001) attempt to make this approach to identifying the number of clusters more formal with the introduction of the so-called 'gap' statistic, which for a sample of size n and a particular number of clusters k is defined as

$$\text{Gap}_n(k) = E_n^*\{\log(W_k)\} - \log(W_k) \tag{10.2}$$

where W_k is the within-clusters sum of squares, and E_n^* denotes expectation from a reference distribution, for which Tibshirani et al. (2001) make two suggestions;

1. A uniform distribution in which each variable is generated from a uniform distribution over the range of the observed values for that variable.
2. A uniform distribution over a box aligned with the principal components of the data (see Tibshirani et al. (2001) for more details).

$E_n^*\{\log(W_k)\}$ is estimated by the average of B copies $\log(W_k^*)$ found by drawing a number of samples from the reference distribution, and the number of clusters is chosen using the following: $\hat{k}$ = smallest k such that Gap $(k) \geq$ Gap $(k + 1) - s_{k+1}$, where $s_k = \sqrt{(1 + 1/B)}\,\text{SD}(k)$ and SD(k) is the standard deviation of the B replicates of log (W_k^*). Further details are given in Tibshirani et al. (2001).

This approach will be explored in Section 10.3.1.

10.3 Analysis Using S-PLUS

In the following two subsections we will describe the application of k-means clustering to the temperature data on U.S. cities, and then the application of a number of hierarchical clustering procedures to the voting in Congress data.

10.3.1 Clustering Cities in the United States on the Basis of their Year-Round Lowest Temperature

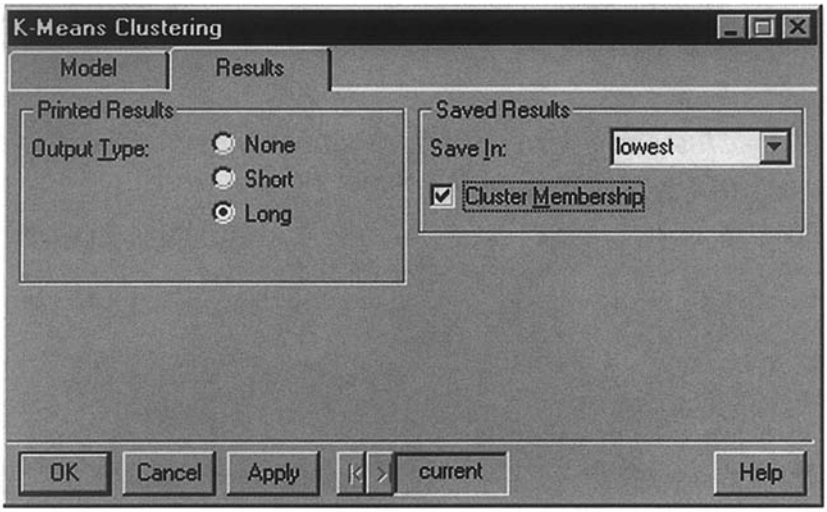
The data in Table 10.1 are available as an S-PLUS data frame lowest, the contents of which are shown in Table 10.3.

We shall apply the *k*-means method to these data using the appropriate dialog, which can be accessed as follows:

- Click on **Statistics**.
- Select **Cluster Analysis**.
- Select **K-Means**.

Table 10.3 Contents of the lowest Data Frame

```
> lowest
          Cities  January  April  July  October
 1       Atlanta       –8     26    53       28
 2     Baltimore       –7     20    51       25
 3      Bismark       –44    –12    35        5
 4        Boston      –12     16    54       28
 5       Chicago      –27      7    40       17
 6        Dallas        4     30    59       29
 7        Denver      –25     –2    43        3
 8       El Paso       –8     23    57       25
 9      Honolulu       53     57    67       64
10       Houston       12     31    62       33
11        Juneau      –22      6    36       11
12            LA       23     39    49       41
13         Miami       30     46    69       51
14     Nashville      –17     23    51       26
15            NY       –6     12    52       28
16         Omaha      –23      5    44       13
17       Phoenix       17     32    61       34
18      Portland      –26      8    40       15
19          Reno      –16     13    33        8
20            SF       24     31    43       34
21       Seattle        0     29    43       28
22    Washington       –5     24    55       29
```



Output Type: ○ None ○ Short ● Long

Save In: lowest

☑ Cluster Membership

Figure 10.1 Part of *K*-Means Clustering dialog.

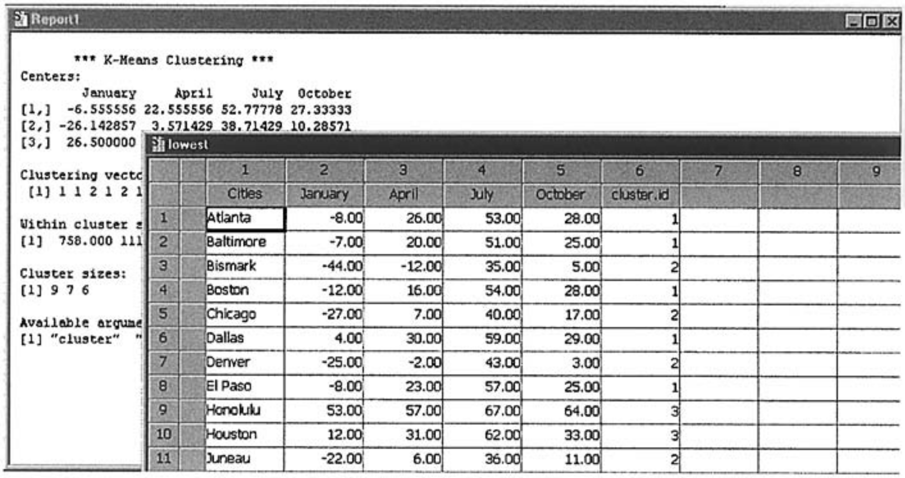
In the *k*-means clustering dialog that appears, select lowest as the data set and January, April, July, and October as the variables. Set the **Num of Clusters** to 3 and the **Max Iterations** to 50. Now click on the **Results** tab, choose **Long** for **Output Type**, check the **Cluster Membership** box, and save the cluster labels in the lowest data frame by selecting this data frame in the **Save In** slot. The dialog now looks as shown in Figure 10.1.

Click **OK** and the screen now looks like that shown in Figure 10.2 with the Report file giving the results of the cluster analysis and the lowest data frame now including the cluster.id variable both visible.

The results are shown in Table 10.4. The three clusters correspond to the following cities:

Cluster 1: Atlanta, Baltimore, Boston, Dallas, El Paso, Nashville, New York, Seattle, Washington, D.C.
Cluster 2: Bismarck, Chicago, Denver, Juneau, Omaha, Portland, Reno
Cluster 3: Honolulu, Houston, Los Angeles, Miami, Phoenix, San Francisco

The cities in the second cluster are definitely to be avoided by those people fond of warm weather! Cluster 3 provides cities with much more appeal for such people. The cities in cluster 1 are intermediate in temperature between the other two clusters.



```
        *** K-Means Clustering ***
Centers:
          January     April      July  October
[1,]  -6.555556 22.555556 52.77778 27.33333
[2,] -26.142857  3.571429 38.71429 10.28571
[3,]  26.500000

Clustering vectc
 [1] 1 1 2 1 2 1

Within cluster s
[1]  758.000 111

Cluster sizes:
[1] 9 7 6

Available argume
[1] "cluster"  "
```

		1	2	3	4	5	6	7	8	9
		Cities	January	April	July	October	cluster.id			
1		Atlanta	-8.00	26.00	53.00	28.00	1			
2		Baltimore	-7.00	20.00	51.00	25.00	1			
3		Bismark	-44.00	-12.00	35.00	5.00	2			
4		Boston	-12.00	16.00	54.00	28.00	1			
5		Chicago	-27.00	7.00	40.00	17.00	2			
6		Dallas	4.00	30.00	59.00	29.00	1			
7		Denver	-25.00	-2.00	43.00	3.00	2			
8		El Paso	-8.00	23.00	57.00	25.00	1			
9		Honolulu	53.00	57.00	67.00	64.00	3			
10		Houston	12.00	31.00	62.00	33.00	3			
11		Juneau	-22.00	6.00	36.00	11.00	2			

Figure 10.2 Screen showing the revised lowest **data frame now including cluster labels.**

Table 10.4 Results of *K*-Means Clustering on Lowest Temperature Data

```
*** K-Means Clustering ***

Centers:
          January      April      July   October
[1,]    –6.555556  22.555556  52.77778  27.33333
[2,]   –26.142857   3.571429  38.71429  10.28571
[3,]    26.500000  39.333333  58.50000  42.83333

Clustering vector:
[1] 1 1 2 1 2 1 2 1 3 3 2 3 3 1 1 2 3 2 2 3 1 1

Within cluster sum of squares:
[1]  758.000  1117.429  2885.167

Cluster sizes:
[1]  9  7  6

Available arguments:
[1]  "cluster"  "centers"  "withinss"  "size"
```

We can use the scatterplot matrix display to enable us to see the position of the three clusters graphically.

- Click on **Graph**.
- Select **2D Plot**.
- Choose **Matrix** in the **Axes Type** slot.
- Select the **lowest** data frame in the **Scatter Plot Matrix** dialog.
- Choose **January**, **April**, **July**, and **October** as *x* columns.
- Choose **cluster.id** as *y* columns.
- Check **Symbol** tab.
- Tick **Use Text As Symbol** box.
- As **Text to Use**, specify *y* column.
- Change **Height** to 0.15.
- Click **OK**.

The resulting plot is shown in Figure 10.3. The plot shows clearly the division into low-, medium-, and high-temperature cities.

The value of three for the number of clusters was chosen arbitrarily. It would be useful if the data themselves could provide some information

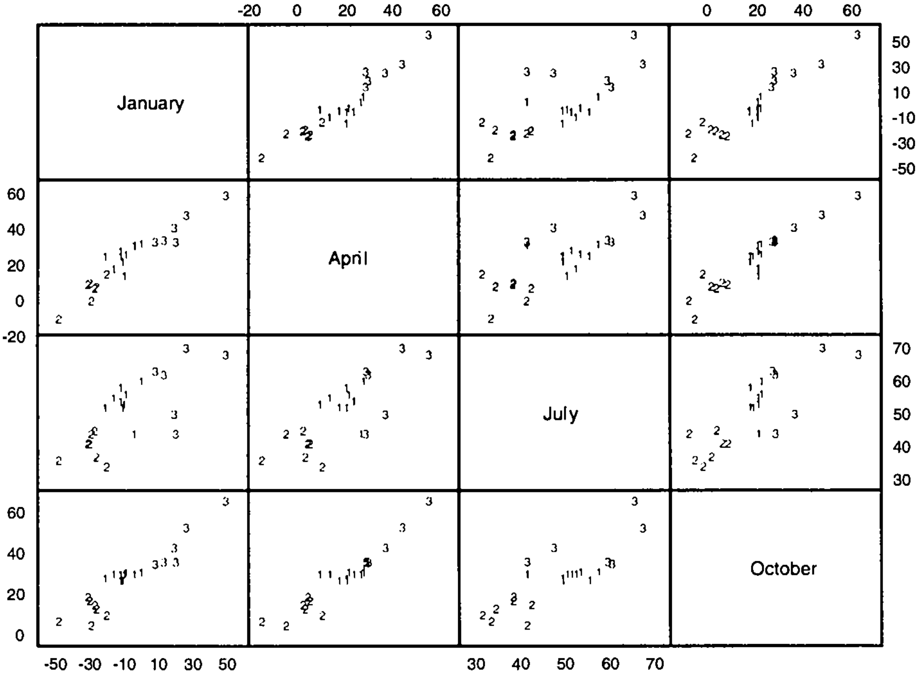


Figure 10.3 Scatterplot matrix of low-temperature data showing cluster labels.

regarding the likely number of clusters that best describes the data. To investigate this we shall use the suggestion made by Tibshirani et al. (2001), described in Section 10.2. A probably very inefficient S-PLUS function for computing the 'gap' statistic is as follows:

```
gap<-function(x,B=100,K=8,method="uniform") {
#
#K is the upper limit of number of clusters
#B is the number of samples from the reference distribution
#method="pc" if principal components approach wanted.
#
#get within cluster sums of squares for observed data
#for the requested upper limit of number of clusters
#
n<-length(x[,1])
p<-length(x[1,])
S<-var(x)
wss1<-(n-1)*sum(diag(S))
wsso<-numeric(0)
for(i in 2:K) {W<-sum(kmeans(x,i)$withinss)
               wsso<-c(wsso,W)
               }
wsso<-c(wss1,wsso)
#
if(method=="pc") {X <- sweep(x,2,apply(x,2,mean))
               X.svd<-svd(X)
               Xprime<-X%*%X.svd$v
                                     }
#
#get range of values for generating samples from the
reference distribution
#
if(method=="pc") rang<-apply(Xprime,2,range)
     else rang<-apply(x,2,range)
#
xstar<-matrix(0,n,p)
wk.exp<-matrix(0,B,K)
#
#now generate B samples from the reference distribution
#and cluster each, calculating the within cluster sum of
#squares for each solution
#
for(j in 1:B){
for(i in 1:n) xstar[i,]<-runif(p,rang[1,],rang[2,])
     if(method==“pc”) xstar<-xstar%*%t(X.svd$v)
wss1<-(n-1)*sum(apply(xstar,2,var))
wss<-numeric(0)
for(i in 2:K) {W<-sum(kmeans(xstar,i)$withinss)
               wss<-c(wss,W)
               }
wss<-c(wss1,wss)
#
wk.exp[j,]<-wss
}
#
term<-apply(log(wk.exp),2,mean)
gap<-term-log(wsso)
#
sdk<-sqrt(apply(log(wk.exp),2,var))
#
sk<-sqrt(1+1/B)*sdk
#
#
                diff<-gap[2:K]-sk[2:K]
                diff<-gap[1:(K-1)]-diff
              values<-seq(1:(K-1))[diff>=0]
              nclust.est<-min(values)
results<-
list(gap=gap,sk=sk,lwss=log(wsso),lwkexp=term,B=B,K=K,
nclust.est=nclust.est)
results
}
```

A function to produce two useful plots from the object resulting from the gap function is as follows:

```
plotgap<-function(gapobj) {
    par(mfrow=c(1,2))
    ylim<-range(gapobj$lwss,gapobj$lwkexp)
```

```
        plot(1:gapobj$K,gapobj$lwss,ylim=ylim,
        ylab="Observed and expected log(wss)",
        xlab="Number of clusters",type="l")
        lines(1:gapobj$K,gapobj$lwkexp,lty=2)
        legend(locator(1),c("Observed","Expected"),lty=1:2)
        plot(1:gapobj$K,gapobj$gap,
        xlab="Number of clusters",ylab="Gap statistic",type="l")
}
```

We can now apply these two functions to the low-temperature data:

```
#store numerical part of lowest data frame as a matrix
#
low<-as.matrix(lowest[,-1])
#apply gap statistic using each type of reference
   distribution in turn
set.seed(9251)
gap.res<-gap(low,B=50,K=6)
gap.res
plotgap(gap.res)
#
gap.res1<-gap(low,B=50,K=6,method="pc")
gap.res1
plotgap(gap.res1)
```

The results are shown in Table 10.5 and the plots in Figures 10.4 and 10.5. We see that the 'uniform' method estimates the number of clusters to be four, but the 'pc' method indicates that the observations are best regarded as a single homogeneous set. A detailed investigation of the gap statistic is given in Everitt (2002).

10.3.2 Classifying New Jersey Congresspeople on the Basis of their Voting Behaviour

We assume that the voting behaviour data are available as an S-PLUS matrix object congress and the names and party affiliations of the congresspeople as a vector names; see Table 10.6.

Here we shall use the command language approach to apply the three agglomerative hierarchical clustering methods mentioned in Section 10.2

Table 10.5 Results from Applying the gap Function to the Low-Temperature Data Using Both the 'Uniform' and the 'pc' Approach

```
> set.seed(9251)
> gap.res <- gap(low, B = 50, K = 6)
> gap.res
$gap:
[1]  0.378   0.629   1.113   1.401   1.458   1.466

$sk:
[1]  0.1075   0.0979   0.1115   0.1305   0.1421   0.1385

$lwss:
[1]  10.04   9.28   8.47   7.91   7.61   7.38

$lwkexp:
[1]  10.41   9.91   9.58   9.31   9.07   8.85

$B:
[1]  50

$K:
[1]  6

$nclust.est:
[1]  4

> gap.res1 <- gap(low, B = 50, K = 6, method = "pc")
> gap.res1
$gap:
[1]  0.3336   –0.1611   –0.0519   0.1055   0.1146   0.1082

$sk:
[1]  0.201   0.176   0.165   0.132   0.136   0.161

$lwss:
[1]  10.04   9.28   8.47   7.91   7.61   7.38

$lwkexp:
[1]  10.37   9.12   8.42   8.02   7.73   7.49

$B:
[1]  50

$K:
[1]  6

$nclust.est:
[1]  1
```

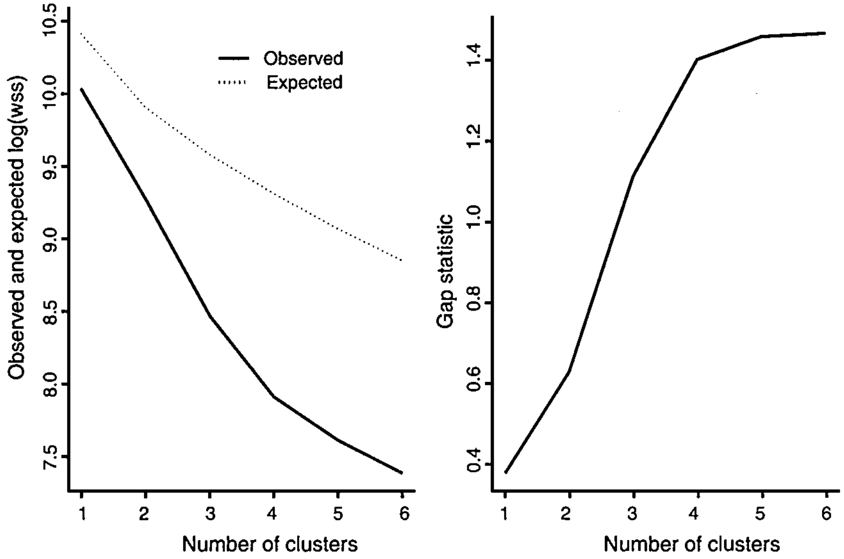


Figure 10.4 Plot of observed and expected log(wss) and gap statistic for low-temperature data using a uniform reference distribution.

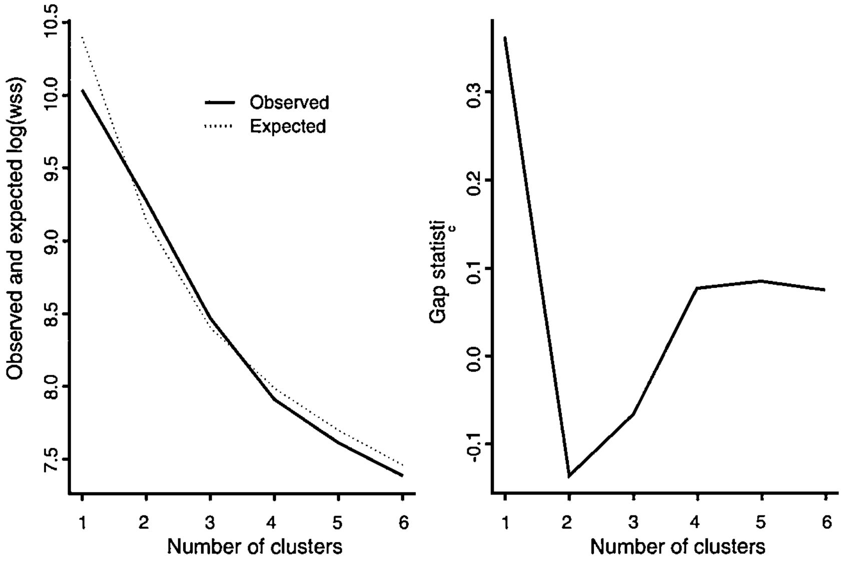


Figure 10.5 Plot of observed and expected log(wss) and gap statistic for low-temperature data using principal components reference distribution.

Table 10.6 Voting Data as Stored in S-PLUS

```
> congress
       [,1]  [,2]  [,3]  [,4]  [,5]  [,6]  [,7]  [,8]  [,9]  [,10]  [,11]  [,12]
 [1,]    0     8    15    15    10     9     7    15    16    14     15     16
 [2,]    8     0    17    12    13    13    12    16    17    15     16     17
 [3,]   15    17     0     9    16    12    15     5     5     6      5      4
 [4,]   15    12     9     0    14    12    13    10     8     8      8      6
 [5,]   10    13    16    14     0     8     9    13    14    12     12     12
 [6,]    9    13    12    12     8     0     7    12    11    10      9     10
 [7,]    7    12    15    13     9     7     0    17    16    15     14     15
 [8,]   15    16     5    10    13    12    17     0     4     5      5      3
 [9,]   16    17     5     8    14    11    16     4     0     3      2      1
[10,]   14    15     6     8    12    10    15     5     3     0      1      2
[11,]   15    16     5     8    12     9    14     5     2     1      0      1
[12,]   16    17     4     6    12    10    15     3     1     2      1      0
[13,]    7    13    11    15    10     6    10    12    13    11     12     12
[14,]   11    12    10    10    11     6    11     7     7     4      5      6
[15,]   13    16     7     7    11    10    13     6     5     6      5      4
      [,13]  [,14]  [,15]
 [1,]    7    11    13
 [2,]   13    12    16
 [3,]   11    10     7
 [4,]   15    10     7
 [5,]   10    11    11
 [6,]    6     6    10
 [7,]   10    11    13
 [8,]   12     7     6
 [9,]   13     7     5
[10,]   11     4     6
[11,]   12     5     5
[12,]   12     6     4
[13,]    0     9    13
[14,]    9     0     9
[15,]   13     9     0
> names
 [1] "Hunt(R)"         "Sandman(R)"          "Howard(D)"
 [4] "Thompson(D)"     "Freylinghuysen(R)"   "Forsythe(R)"
 [7] "Widnall(R)"      "Roe(D)"              "Heltoski(D)"
[10] "Rodino(D)"       "Minish(D)"           "Rinaldo(R)"
[13] "Maraziti(R)"     "Daniels(D)"          "Patten(D)"
```

to the data and to produce the resulting dendrograms. The two S-PLUS functions needed are hclust and plclust.

```
par(mfrow=c(1,3))
plclust(hclust(congress,method="connected"),
labels=names)
plclust(hclust(congress,method="compact"),
labels=names)
plclust(hclust(congress,method="average"),
labels=names)
#hclust takes a distance or dissimilarity matrix
#and applies either single linkage, method="connected",
#complete linkage, method="compact" or
#average linkage, method "average".
#plclust takes the result of hclust and produces
#the corresponding dendrogram, labelled
#here with the names of the congressmen
```

The resulting diagram showing the three dendrograms is given in Figure 10.6.

There are similarities but also differences in the three dendrograms, a situation that is not uncommon when applying different methods of cluster analysis to the same data set! Since single linkage is well known to have some practical problems (see Everitt et al., 2001), we shall confine more detailed attention to the results from complete and average linkage. Both dendrograms seem most consistent with a two-group solution, and the names of the congresspeople in each group can easily be extracted from Figure 10.6. But in applications with a larger number of observations, groups may be found using the cuttree function.

```
g<-cuttree(hclus(congress,method="compact"),k=2)
#stores labels for 2 cluster solution from
#complete linkage in g
names[g==1]
names[g==2]
#gives names of congressmen in two group
#solution
```

By simply changing to method="average" in the above, the names of the congresspeople in the two-group solution from average linkage are obtained. Both solutions are shown in Table 10.7. The two solutions are

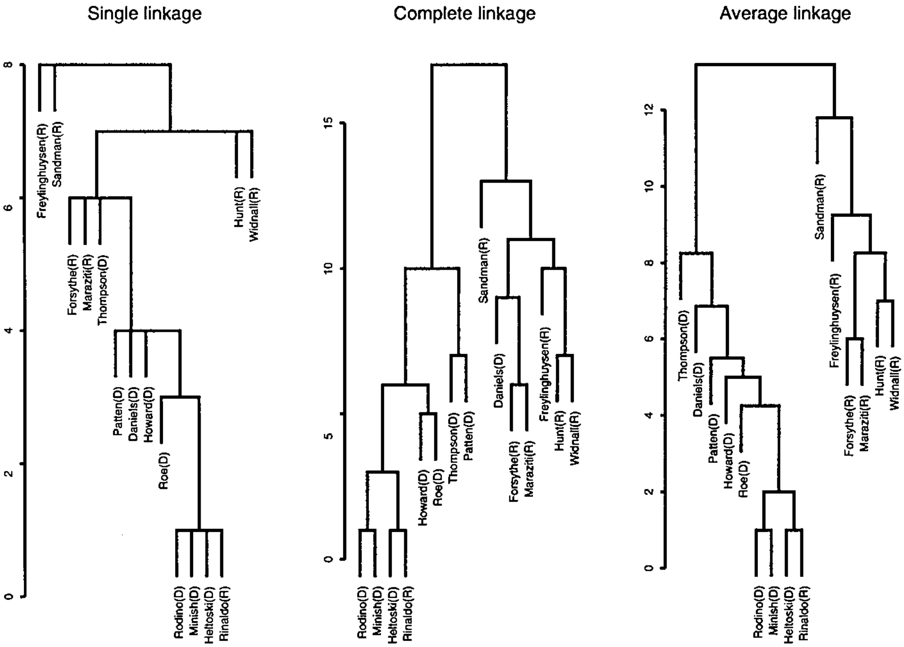


Figure 10.6 Dendrograms for single linkage, complete linkage, and average linkage for voting behaviour data.

very similar with only Daniels being placed in different clusters by the two clustering procedures. Both solutions show very definite evidence of party applications in voting.

The clustering results for these data can usefully be compared with the two-dimensional solution obtained by applying classical multidimensional scaling to the voting matrix

```
par(pty=“s”)
cords<-cmdscale(congress)
#gets 2D classical MDS solution
xlim<-range(cords[,1])
plot(cords,xlab=“c1”,ylab=“c2”,type=“n”,
xlim=xlim,ylim=xlim)
text(cords,labels=abbreviate(names))
#uses the abbreviate function to get unique
#shorter labels for each Congressman.
```

Table 10.7 Two Cluster Solutions from Complete Linkage and Average Linkage for the Voting in Congress Data

```
> g <- cutree(hclust(congress, method = “compact”), k = 2)
> names[g==1]
[1]   “Hunt(R)”                 “Sandman(R)”              “Freylinghuysen(R)”
[4]   “Forsythe(R)”             “Widnall(R)”              “Maraziti(R)”
[7]   “Daniels(D)”
> names[g==2]
[1]   “Howard(D)”   “Thompson(D)”   “Roe(D)”        “Heltoski(D)”
[5]   “Rodino(D)”   “Minish(D)”     “Rinaldo(R)”    “Patten(D)”
> g <- cutree(hclust(congress, method = “average”), k = 2)
> names[g==1]
[1]   “Hunt(R)”                 “Sandman(R)”              “Freylinghuysen(R)”
[4]   “Forsythe(R)”             “Widnall(R)”              “Maraziti(R)”
> names[g==2]
[1]   “Howard(D)”   “Thompson(D)”   “Roe(D)”        “Heltoski(D)”
[5]   “Rodino(D)”   “Minish(D)”     “Rinaldo(R)”    “Daniels(D)”
[9]   “Patten(D)”
```

The plot is shown in Figure 10.7. The Democrat/Republican division is clearly visible, as is the fact that Sandman is a distinct outlier. In fact, this particular congressperson had a greater tendency to abstain than the others.

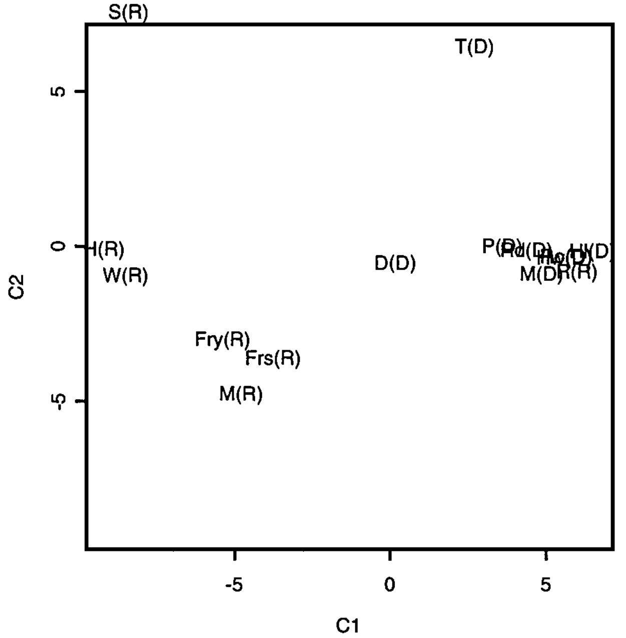


Figure 10.7 Two-dimensional solution from classical multidimensional scaling applied to voting behaviour data.

Exercises

10.1. A suggestion that has been made for deciding on the number of groups when using *k*-means clustering is to plot the values of within-group variance against the number of clusters and to take the number corresponding to any distinct 'elbow' in this plot. Investigate this possibility for the lowest temperature data.

10.2. Display the lowest temperature data in the space of their first two principal component scores, indicating on the plot the three-group cluster solution from *k*-means.

10.3. Investigate whether the two-dimensional solution for the voting data from classical multidimensional scaling is adequate for the data.

Chapter 11

Bivariate Density Estimation and Discriminant Analysis: Blood Fat Concentration

11.1 Description of Data

In a study of 371 males with chest pain, data were collected on the concentration of plasma cholesterol and plasma triglycerides (mg/dl). The data are shown in Table 11.1. For 51 patients there was no evidence of heart disease; for the remaining 320 there was evidence of narrowing of the arteries. Interest lies in assessing whether the two measurements made can be used to discriminate between men with and men without heart disease.

11.2 Bivariate Density Estimation and Discriminant Function Analysis

The data in Table 11.1 will first be explored by plotting a scattergram of the two variables and estimating their *bivariate density function.* Density estimation is described in detail in Silverman (1986), but for bivariate data it generally involves use of a *kernel estimator* of the form

Table 11.1 Blood Fat Data (Plasma cholesterol, plasma triglycerides)

51 patients with no evidence of heart disease

195,348	237,174	205,158	201,171	190,85	180,82	193,210
170,90	150,167	200,154	228,119	169,86	178,166	251,211
234,143	222,284	116,87	157,134	194,121	130,64	206,99
158,87	167,177	217,114	234,116	190,132	178,157	265,73
219,98	266,486	190,108	156,126	187,109	149,146	147,95
155,48	207,195	238,172	168,71	210,91	208,139	160,116
243,101	209,97	221,156	178,116	289,120	201,72	168,100
168,227	207,160					

320 patients with evidence of heart disease

184,145	263,142	185,115	271,128	173,56	230,304	222,151
215,168	233,340	212,171	221,140	239,97	168,131	231,145
221,432	131,137	211,124	232,258	313,256	240,221	176,166
210,92	251,189	175,148	185,256	184,222	198,149	198,333
208,112	284,245	231,181	171,165	258,210	164,76	230,492
197,87	216,112	230,90	265,156	197,158	230,146	233,142
250,118	243,50	175,489	200,68	240,196	185,116	213,130
180,80	208,220	386,162	236,152	230,162	188,220	200,101
212,130	193,188	230,158	169,112	181,104	189,84	180,202
297,232	232,328	150,426	239,154	178,100	242,144	323,196
168,208	197,291	417,198	172,140	240,441	191,115	217,327
208,262	220,75	191,115	119,84	171,170	179,126	208,149
180,102	254,153	191,136	176,217	283,424	253,222	220,172
268,154	248,312	245,120	171,108	239,92	196,141	247,137
219,454	159,125	200,152	233,127	232,131	189,135	237,400
319,418	171,78	194,183	244,108	236,148	260,144	254,170
250,161	196,130	298,143	306,408	175,153	251,117	256,271
285,930	184,255	228,142	171,120	229,242	195,137	214,223
221,268	204,150	276,199	165,121	211,91	264,259	245,446
227,146	197,265	196,103	193,170	211,122	185,120	157,59
224,124	209,82	223,80	278,152	251,152	140,164	197,101
172,106	174,117	192,101	221,179	283,199	178,109	185,168
181,119	191,233	185,130	206,133	210,217	226,72	219,267
215,325	228,130	245,257	186,273	242,85	201,297	239,137
179,126	218,123	279,317	234,135	264,269	237,88	162,91
245,166	191,90	207,316	248,142	139,173	246,87	247,91
193,290	332,250	194,116	195,363	243,112	271,89	197,347
242,179	175,246	138,91	244,177	206,201	191,149	223,154
172,207	190,120	144,125	194,125	105,36	201,92	193,259
262,88	211,304	178,84	331,134	235,144	267,199	227,202

Table 11.1 (Continued) Blood Fat Data (Plasma cholesterol, plasma triglycerides)

243,126	261,174	185,100	171,90	222,229	231,161	258,328
211,306	249,256	209,89	177,133	165,151	299,93	274,323
219,163	233,101	220,153	348,154	194,400	230,137	250,160
173,300	260,127	258,151	131,61	168,91	208,77	287,209
308,260	227,172	168,126	178,101	164,80	151,73	165,155
249,146	258,145	194,196	140,99	187,390	171,135	221,156
294,135	167,80	208,201	208,148	185,231	159,82	222,108
266,164	217,227	249,200	218,207	245,322	242,180	262,169
169,158	204,84	184,182	206,148	198,124	242,248	189,176
260,98	199,153	207,150	206,107	210,95	229,296	232,583
267,192	228,149	187,115	304,149	140,102	209,376	198,105
270,110	188,148	160,125	218,96	257,402	259,240	139,54
213,261	178,125	172,146	198,103	222,348	238,156	273,146
131,96	233,141	269,84	170,284	149,237	194,272	142,111
218,567	194,278	252,233	184,184	203,170	239,38	232,161
225,240	280,218	185,110	163,156	216,101		

$$\hat{f}(x, y) = \frac{1}{nh_x h_y} \sum_{i=1}^{n} K\left[\frac{x - X_i}{h_x}, \frac{y - Y_i}{h_y}\right] \tag{11.1}$$

where $(X_1, Y_1) \cdots (X_n, Y_n)$ are the sample bivariate observations, h_x and h_y are smoothing parameters usually known as *bandwidth*, and K is a *kernel function*, commonly, the standard bivariate normal density, i.e.,

$$K(x, y) = \frac{1}{2\pi} \exp\left[-\frac{1}{2}\left(x^2 + y^2\right)\right] \tag{11.2}$$

In essence, the estimator is a sum of 'bumps' placed at the observations. The kernel function determines the shape of the bumps, and the bandwidth determines their width. A value often suggested for the bandwidth is $n^{-1/5}$ (see Venables and Ripley, 1999), for each dimension.

Following this initial exploration various discriminant function procedures will be applied to investigate the possibility of using the cholesterol and triglyceride measurements to discriminate between people with heart disease and those without. Details of such techniques are given in Everitt and Dunn (2001), but the simplest, linear discriminant function analysis consists of finding a linear function of the two variables that best distinguishes between members of the two groups. The coefficients that define this function, a_1 and a_2, can be shown to be given by

$$\boldsymbol{a} = \boldsymbol{S}^{-1}(\bar{\boldsymbol{x}}_1 - \bar{\boldsymbol{x}}_2) \qquad (11.3)$$

where $\boldsymbol{a}' = [a_1, a_2]$, **S** is the estimator of the assumed common covariance matrix of the two groups, and $\bar{\boldsymbol{x}}_1$ and $\bar{\boldsymbol{x}}_2$ their mean vectors. Having found the vector, **a**, a discriminant score can be found for each individual as

$$z = a_1 \text{ Cholesterol} + a_2 \text{ Triglycerides} \qquad (11.4)$$

Individuals can now be assigned to one of the two groups on the basis of their discriminant score by comparing it to the threshold value ½($\bar{z}_1 + \bar{z}_2$), where $\bar{z}_1$ and $\bar{z}_2$ are the mean discriminant scores of each group. If a score is larger than the threshold, the individual is classified into one group; if lower than the threshold, into the other. (This rule is based on the assumption that the *prior probabilities* of being in either group are the same. It is this rather unrealistic assumption that we shall make in this chapter, although in designing a classification rule for use in practice, realistic estimates of the prior probabilities would clearly be needed. For the adjusted classification rule in this case, see Everitt and Dunn, 2001.)

The performance of a discriminant analysis classification rule is assessed by estimating the *misclassification rate* of the rule. One possible estimator is the misclassification rate of the rule based on the data from which it was derived. This is, however, well known to be a very poor estimator and there are several alternatives that are preferred (see Hand, 1998, for details). The most commonly used of the available methods is the so-called leaving-one-out method, in which the discriminant function is derived from just $n - 1$ members of the sample and then used to classify the member left out. The process is repeated n times, leaving out each sample member in turn.

11.3 Analysis Using S-PLUS

The blood fat data are available as the data frame bf, the contents of which are shown in Table 11.2.

11.3.1 Bivariate Density Estimation

We begin by constructing a scatterplot of the data in which the members of the no heart disease group are identified by a minus sign and the members of the heart disease group by a plus sign.

Table 11.2 Contents of bf Data Frame

```
> bf
              Group   Cholesterol  Triglycerides
 1  No heart disease      195           348
 2  No heart disease      237           174
 3  No heart disease      205           158
 4  No heart disease      201           171
 5  No heart disease      190            85
 6  No heart disease      180            82
 7  No heart disease      193           210
 8  No heart disease      170            90
 9  No heart disease      150           167
10  No heart disease      200           154
11  No heart disease      228           119
12  No heart disease      169            86
13  No heart disease      178           166
14  No heart disease      251           211
15  No heart disease      234           143
16  No heart disease      222           284
17  No heart disease      116            87
18  No heart disease      157           134
19  No heart disease      194           121
20  No heart disease      130            64
21  No heart disease      206            99
22  No heart disease      158            87
23  No heart disease      167           177
24  No heart disease      217           114
25  No heart disease      234           116
26  No heart disease      190           132
27  No heart disease      178           157
28  No heart disease      265            73
29  No heart disease      219            98
30  No heart disease      266           486
31  No heart disease      190           108
32  No heart disease      156           126
33  No heart disease      187           109
34  No heart disease      149           146
35  No heart disease      147            95
36  No heart disease      155            48
37  No heart disease      207           195
38  No heart disease      238           172
39  No heart disease      168            71
```

Table 11.2 (Continued) Contents of bf Data Frame

```
> bf
               Group      Cholesterol  Triglycerides
40    No heart disease        210            91
41    No heart disease        208           139
42    No heart disease        160           116
43    No heart disease        243           101
44    No heart disease        209            97
45    No heart disease        221           156
46    No heart disease        178           116
47    No heart disease        289           120
48    No heart disease        201            72
49    No heart disease        168           100
50    No heart disease        168           227
51    No heart disease        207           160
52    Heart disease           184           145
53    Heart disease           263           142
54    Heart disease           185           115
55    Heart disease           271           128
56    Heart disease           173            56
57    Heart disease           230           304
58    Heart disease           222           151
59    Heart disease           215           168
60    Heart disease           233           340
61    Heart disease           212           171
62    Heart disease           221           140
63    Heart disease           239            97
64    Heart disease           168           131
65    Heart disease           231           145
66    Heart disease           221           432
67    Heart disease           131           137
68    Heart disease           211           124
69    Heart disease           232           258
70    Heart disease           313           256
71    Heart disease           240           221
72    Heart disease           176           166
73    Heart disease           210            92
74    Heart disease           251           189
75    Heart disease           175           148
76    Heart disease           185           256
77    Heart disease           184           222
78    Heart disease           198           149
```

Table 11.2 (Continued) Contents of bf Data Frame

```
> bf
            Group        Cholesterol  Triglycerides
 79   Heart disease          198            333
 80   Heart disease          208            112
 81   Heart disease          284            245
 82   Heart disease          231            181
 83   Heart disease          171            165
 84   Heart disease          258            210
 85   Heart disease          164             76
 86   Heart disease          230            492
 87   Heart disease          197             87
 88   Heart disease          216            112
 89   Heart disease          230             90
 90   Heart disease          265            156
 91   Heart disease          197            158
 92   Heart disease          230            146
 93   Heart disease          233            142
 94   Heart disease          250            118
 95   Heart disease          243             50
 96   Heart disease          175            489
 97   Heart disease          200             68
 98   Heart disease          240            196
 99   Heart disease          185            116
100   Heart disease          213            130
101   Heart disease          180             80
102   Heart disease          208            220
103   Heart disease          386            162
104   Heart disease          236            152
105   Heart disease          230            162
106   Heart disease          188            220
107   Heart disease          200            101
108   Heart disease          212            130
109   Heart disease          193            188
110   Heart disease          230            158
111   Heart disease          169            112
112   Heart disease          181            104
113   Heart disease          189             84
114   Heart disease          180            202
115   Heart disease          297            232
116   Heart disease          232            328
117   Heart disease          150            426
```

Table 11.2 (Continued) Contents of bf Data Frame

```
> bf
              Group       Cholesterol   Triglycerides
118   Heart disease           239             154
119   Heart disease           178             100
120   Heart disease           242             144
121   Heart disease           323             196
122   Heart disease           168             208
123   Heart disease           197             291
124   Heart disease           417             198
125   Heart disease           172             140
126   Heart disease           240             441
127   Heart disease           191             115
128   Heart disease           217             327
129   Heart disease           208             262
130   Heart disease           220              75
131   Heart disease           191             115
132   Heart disease           119              84
133   Heart disease           171             170
134   Heart disease           179             126
135   Heart disease           208             149
136   Heart disease           180             102
137   Heart disease           254             153
138   Heart disease           191             136
139   Heart disease           176             217
140   Heart disease           283             424
141   Heart disease           253             222
142   Heart disease           220             172
143   Heart disease           268             154
144   Heart disease           248             312
145   Heart disease           245             120
146   Heart disease           171             108
147   Heart disease           239              92
148   Heart disease           196             141
149   Heart disease           247             137
150   Heart disease           219             454
151   Heart disease           159             125
152   Heart disease           200             152
153   Heart disease           233             127
154   Heart disease           232             131
155   Heart disease           189             135
156   Heart disease           237             400
```

Table 11.2 (Continued) Contents of bf Data Frame

```
> bf
            Group        Cholesterol  Triglycerides
157    Heart disease         319          418
158    Heart disease         171           78
159    Heart disease         194          183
160    Heart disease         244          108
161    Heart disease         236          148
162    Heart disease         260          144
163    Heart disease         254          170
164    Heart disease         250          161
165    Heart disease         196          130
166    Heart disease         298          143
167    Heart disease         306          408
168    Heart disease         175          153
169    Heart disease         251          117
170    Heart disease         256          271
171    Heart disease         285          930
172    Heart disease         184          255
173    Heart disease         228          142
174    Heart disease         171          120
175    Heart disease         229          242
176    Heart disease         195          137
177    Heart disease         214          223
178    Heart disease         221          268
179    Heart disease         204          150
180    Heart disease         276          199
181    Heart disease         165          121
182    Heart disease         211           91
183    Heart disease         264          259
184    Heart disease         245          446
185    Heart disease         227          146
186    Heart disease         197          265
187    Heart disease         196          103
188    Heart disease         193          170
189    Heart disease         211          122
190    Heart disease         185          120
191    Heart disease         157           59
192    Heart disease         224          124
193    Heart disease         209           82
194    Heart disease         223           80
195    Heart disease         278          152
```

Table 11.2 (Continued) Contents of bf Data Frame

```
> bf
              Group     Cholesterol  Triglycerides
196   Heart disease         251           152
197   Heart disease         140           164
198   Heart disease         197           101
199   Heart disease         172           106
200   Heart disease         174           117
201   Heart disease         192           101
202   Heart disease         221           179
203   Heart disease         283           199
204   Heart disease         178           109
205   Heart disease         185           168
206   Heart disease         181           119
207   Heart disease         191           233
208   Heart disease         185           130
209   Heart disease         206           133
210   Heart disease         210           217
211   Heart disease         226            72
212   Heart disease         219           267
213   Heart disease         215           325
214   Heart disease         228           130
215   Heart disease         245           257
216   Heart disease         186           273
217   Heart disease         242            85
218   Heart disease         201           297
219   Heart disease         239           137
220   Heart disease         179           126
221   Heart disease         218           123
222   Heart disease         279           317
223   Heart disease         234           135
224   Heart disease         264           269
225   Heart disease         237            88
226   Heart disease         162            91
227   Heart disease         245           166
228   Heart disease         191            90
229   Heart disease         207           316
230   Heart disease         248           142
231   Heart disease         139           173
232   Heart disease         246            87
233   Heart disease         247            91
234   Heart disease         193           290
```

Table 11.2 (Continued) Contents of bf Data Frame

```
> bf
              Group    Cholesterol  Triglycerides
235   Heart disease            332            250
236   Heart disease            194            116
237   Heart disease            195            363
238   Heart disease            243            112
239   Heart disease            271             89
240   Heart disease            197            347
241   Heart disease            242            179
242   Heart disease            175            246
243   Heart disease            138             91
244   Heart disease            244            177
245   Heart disease            206            201
246   Heart disease            191            149
247   Heart disease            223            154
248   Heart disease            172            207
249   Heart disease            190            120
250   Heart disease            144            125
251   Heart disease            194            125
252   Heart disease            105             36
253   Heart disease            201             92
254   Heart disease            193            259
255   Heart disease            262             88
256   Heart disease            211            304
257   Heart disease            178             84
258   Heart disease            331            134
259   Heart disease            235            144
260   Heart disease            267            199
261   Heart disease            227            202
262   Heart disease            243            126
263   Heart disease            261            174
264   Heart disease            185            100
265   Heart disease            171             90
266   Heart disease            222            229
267   Heart disease            231            161
268   Heart disease            258            328
269   Heart disease            211            306
270   Heart disease            249            256
271   Heart disease            209             89
272   Heart disease            177            133
273   Heart disease            165            151
```

Table 11.2 (Continued) Contents of bf Data Frame

```
> bf
              Group       Cholesterol  Triglycerides
274    Heart disease          299             93
275    Heart disease          274            323
276    Heart disease          219            163
277    Heart disease          233            101
278    Heart disease          220            153
279    Heart disease          348            154
280    Heart disease          194            400
281    Heart disease          230            137
282    Heart disease          250            160
283    Heart disease          173            300
284    Heart disease          260            127
285    Heart disease          258            151
286    Heart disease          131             61
287    Heart disease          168             91
288    Heart disease          208             77
289    Heart disease          287            209
290    Heart disease          308            260
291    Heart disease          227            172
292    Heart disease          168            126
293    Heart disease          178            101
294    Heart disease          164             80
295    Heart disease          151             73
296    Heart disease          165            155
297    Heart disease          249            146
298    Heart disease          258            145
299    Heart disease          194            196
300    Heart disease          140             99
301    Heart disease          187            390
302    Heart disease          171            135
303    Heart disease          221            156
304    Heart disease          294            135
305    Heart disease          167             80
306    Heart disease          208            201
307    Heart disease          208            148
308    Heart disease          185            231
309    Heart disease          159             82
310    Heart disease          222            108
311    Heart disease          266            164
312    Heart disease          217            227
```

Table 11.2 (Continued) Contents of bf Data Frame

```
> bf
           Group        Cholesterol   Triglycerides
313   Heart disease         249            200
314   Heart disease         218            207
315   Heart disease         245            322
316   Heart disease         242            180
317   Heart disease         262            169
318   Heart disease         169            158
319   Heart disease         204             84
320   Heart disease         184            182
321   Heart disease         206            148
322   Heart disease         198            124
323   Heart disease         242            248
324   Heart disease         189            176
325   Heart disease         260             98
326   Heart disease         199            153
327   Heart disease         207            150
328   Heart disease         206            107
329   Heart disease         210             95
330   Heart disease         229            296
331   Heart disease         232            583
332   Heart disease         267            192
333   Heart disease         228            149
334   Heart disease         187            115
335   Heart disease         304            149
336   Heart disease         140            102
337   Heart disease         209            376
338   Heart disease         198            105
339   Heart disease         270            110
340   Heart disease         188            148
341   Heart disease         160            125
342   Heart disease         218             96
343   Heart disease         257            402
344   Heart disease         259            240
345   Heart disease         139             54
346   Heart disease         213            261
347   Heart disease         178            125
348   Heart disease         172            146
349   Heart disease         198            103
350   Heart disease         222            348
351   Heart disease         238            156
```

Table 11.2 (Continued) Contents of bf Data Frame

> bf

	Group	Cholesterol	Triglycerides
352	Heart disease	273	146
353	Heart disease	131	96
354	Heart disease	233	141
355	Heart disease	269	84
356	Heart disease	170	284
357	Heart disease	149	237
358	Heart disease	194	272
359	Heart disease	142	111
360	Heart disease	218	567
361	Heart disease	194	278
362	Heart disease	252	233
363	Heart disease	184	184
364	Heart disease	203	170
365	Heart disease	239	38
366	Heart disease	232	161
367	Heart disease	225	240
368	Heart disease	280	218
369	Heart disease	185	110
370	Heart disease	163	156
371	Heart disease	216	101

```
attach(bf)
plot(Cholesterol,Triglycerides,type="n")
text(Cholesterol,Triglycerides,labels=
rep("-","+"),c(51,320)))
legend(locator(1),c("No heart disease","Heart
disease"),pch="-+")
```

The resulting diagram is shown in Figure 11.1. The main features in this diagram are the considerable overlap between the two groups and the presence of an individual with an extremely high triglyceride value. This is individual number 171. Since the value is so extreme, this individual will be removed from further analyses.

A first, very crude, estimate of the bivariate density of the two variables can be obtained using the **hist2d** function in S-PLUS, which simply counts the number of observations in each cell of a grid constructed for the data. The resulting counts can be viewed graphically using the **persp** function.

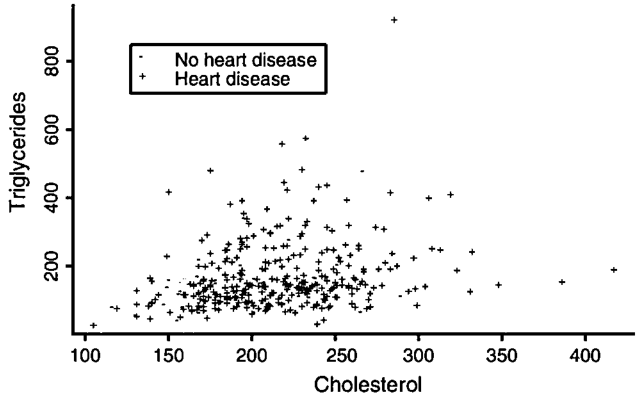


Figure 11.1 Scatterplot of cholesterol and triglycerides identifying those men with heart disease and those without.

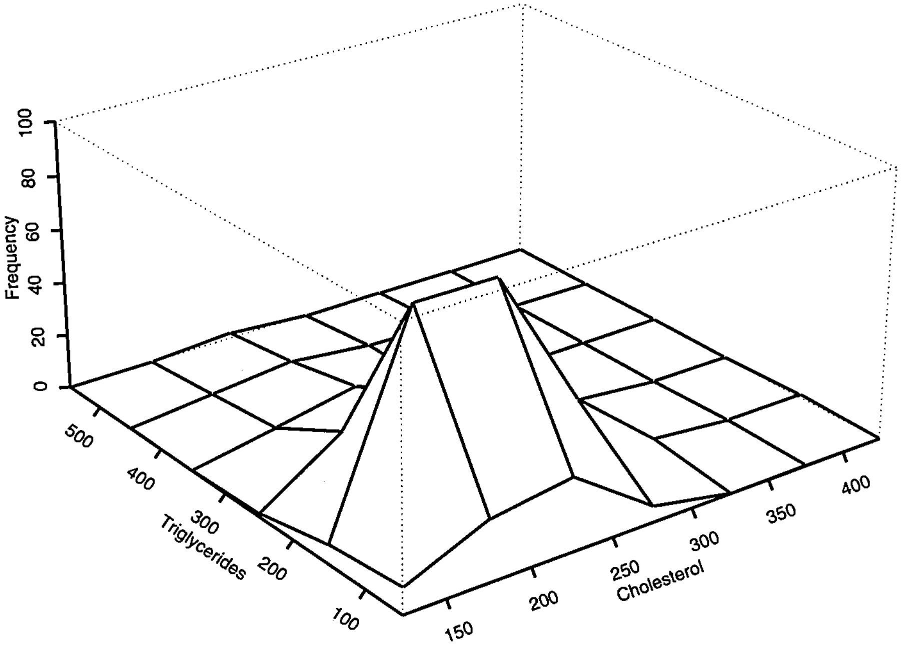


Figure 11.2 Two-dimensional histogram of blood fat data.

```
persp(hist2d(Cholesterol[-171],Triglycerides [-171]),
zlab="Frequency",xlab="Cholesterol",ylab="Triglycerides")
```

The resulting diagram is shown in Figure 11.2.

A far 'smoother' estimate of the bivariate density can be obtained by using the kernel estimator approach outlined in Section 11.2. A relatively crude function to implement this procedure is easily constructed making use of, in particular, the S-PLUS outer function.

```
kden<-function(x, y, ngridx=30, ngridy=30, constant.x
=1, constant.y=1)
    {
#x and y are vectors containing the bivariate data
#ngridx and ngridy are the number of points in the grid
#
    mx <- mean(x)
    sdx <- sqrt(var(x))
    my <- mean(y)
    sdy <- sqrt(var(y))
#standardize x and y before estimation using the scale
#function
    x <- scale(x)
    y <- scale(y)
    den <- matrix(0, ngridx, ngridy)
#
#find possible value for bandwidth
#
    n <- length(x)
    hx <- constant.x * n^(-0.2)
    hy <- constant.y * n^(-0.2)
    h <- hx * hy
    hsqrt <- sqrt(h)
#set up grid at which to calculate densities
#use the outer function to compute densities
#and accumulate over the n observations
    seqx <- seq(range(x)[1], range(x)[2], length=ngridx)
    seqy <- seq(range(y)[1], range(y)[2], length=ngridy)
    for(i in 1:n) {
        X <- x[i]
        Y <- y[i]
        xx <- (seqx - X)/hsqrt
        yy <- (seqy - Y)/hsqrt
        den <- den + outer(xx, yy, function(x, y)
             exp(-0.5 * (x^2 + y^2)))
             }
    den <- den/(n * 2 * pi * h)
    seqx <- sdx * seqx + mx
    seqy <- sdy * seqy + my
    result <- list(seqx=seqx, seqy=seqy, den=den)
    result
}
```

We can now use the function **kden** to estimate the required bivariate density and then view the estimate using **persp.**

```
den<-kden(Cholesterol[-171],Triglycerides[-171])
persp(den$seqx,den$seqy,den$den,xlab="Cholesterol",ylab=
"Triglycerides",zlab="Density")
```

The resulting diagram appears in Figure 11.3. The bivariate density looks relatively 'normal' apart from perhaps a slight 'bumpiness' for triglyceride values above 200, but there is no obvious bimodality that would indicate relatively clear separation between the with and without heart disease groups.

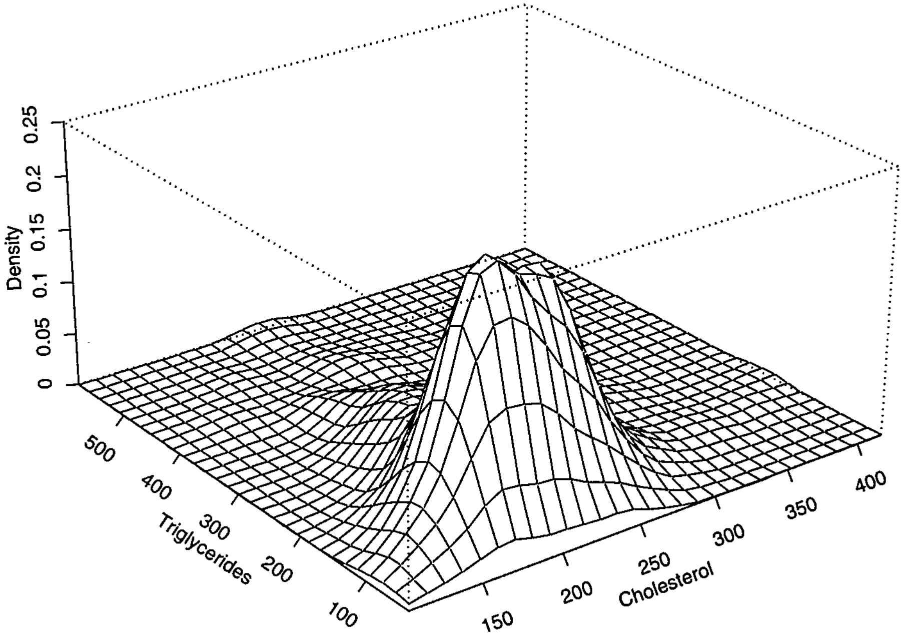


Figure 11.3 Kernel estimate of bivariate density function of blood fat data.

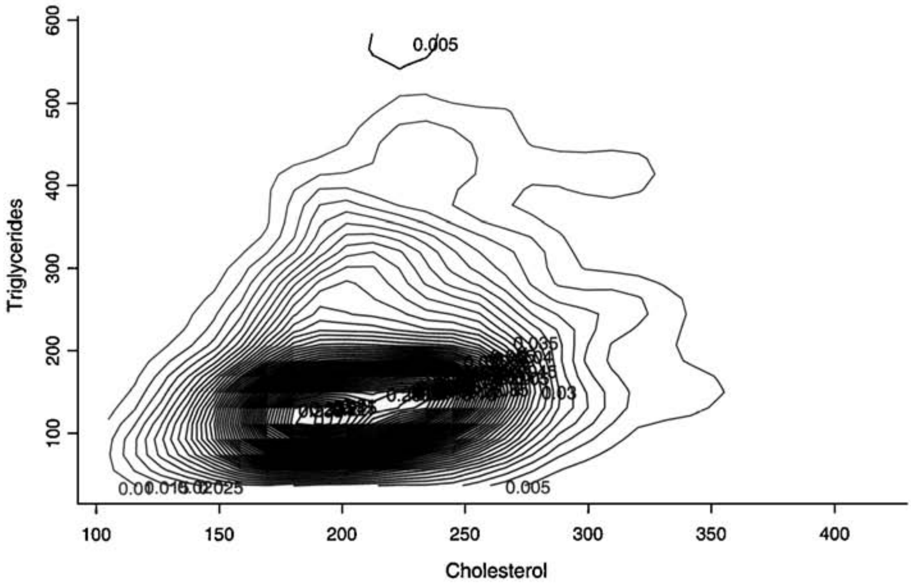


Figure 11.4 Contour plot of estimated bivariate density of blood fat data.

The density estimate might also be displayed as a contour plot using the S-PLUS contour function:

```
contour(den$seqx,den$seqy,den$den,xlab="Cholesterol",
ylab="Triglycerides",nlevels=50)
#the nlevels argument is used to increase
#the number of contours plotted
```

The contour plot is shown in Figure 11.4.

11.3.2 Discriminant Analysis

We begin this subsection by constructing the linear discriminant function for the no heart disease/heart disease groups first from principles using, in particular, the solve function in S-PLUS to invert a matrix:

```
#Calculate the discriminant function coefficients
#from first principles
#
#first calculate the covariance matrices in each group
```

```
#
#
bf <- bfc[-171, 2:3]
Group <- Group[-171]
v1 <- var(bf[Group=="No heart disease",])
v2 <- var(bf[Group=="Heart disease",])
#
#Calculate group mean vectors
#
m1 <- apply(bf[Group=="No heart disease",], 2, mean)
m2 <- apply(bf[Group=="Heart disease",], 2, mean)
#
#Find number of observations in each group
#
n1 <- length(Group[Group=="No heart disease"])
n2 <- length(Group[Group=="Heart disease"])
#
#Estimate assumed common covariance matrix
#
v <- ((n1 - 1) * v1 + (n2 - 1) * v2)/(n1 + n2 - 2)
#
#Calculate inverse of common covariance matrix and store
#as v
#
v <- solve(v)
#
#calculate discriminant function coefficients
#
a <- v %*% (m1 - m2)
#
#calculate threshold value for discriminant rule
#
z12 <- (m1 %*% a + m2 %*% a)/2
#
#plot the data labelling the members of the two groups
#and add the discriminant function line and an
#appropriate legend
#
```

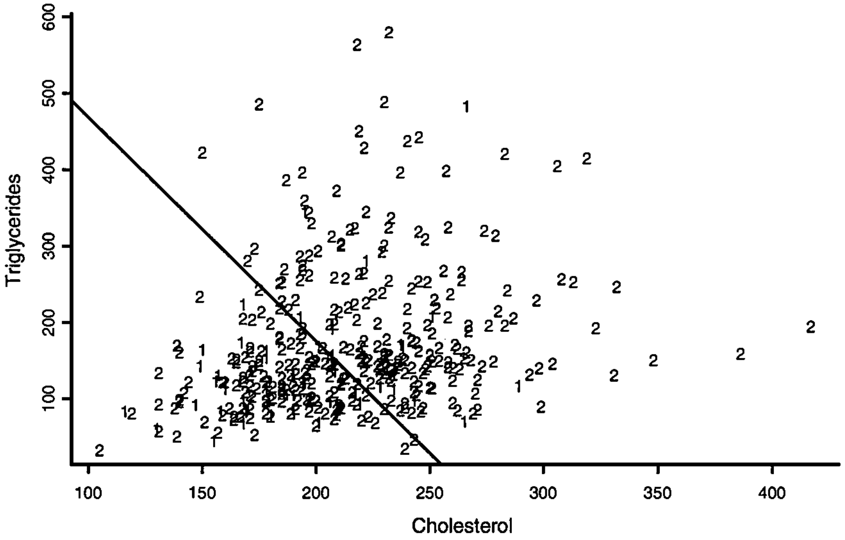


Figure 11.5 Plotted and discriminant function. 1 = No heart disease; 2 = heart disease.

```
plot(bf[, 1], bf[, 2], xlab=“Cholesterol”, ylab=
“Trygliceriides”, type=“n”)
text(bf[, 1], bf[, 2], labels=Group)
legend(locator(1), c(“No heart disease”, “Heart
disease”), pch=“12”)
#
#add estimated discriminant function to scatter plot
#
abline(z12/a[2], - a[1]/a[2], lwd=2, lty=1)
```

The estimated discriminant function is

$$z = -0.01007 \text{ Cholesterol } -0.00343 \text{ Triglycerides} \qquad (11.5)$$

and the threshold value is –2.62.

The plotted data and discriminant function are shown in Figure 11.5. Observations falling above the line would be classified as ‘heart disease’, those below the line as ‘no heart disease’.

We can also obtain the discriminant function along with information about its performance in terms of estimated misclassification rate by using the discrim function in S-PLUS.

```
bf.disc<-discrim(Group~Cholesterol+Triglycerides,data
=bf,prior="uniform")
summary(bf.disc)
```

The results are given in Table 11.3. The discriminant function coefficients given in (11.5) are obtained from this table by simply subtracting the appropriate linear coefficients for no heart disease and heart disease. The test for homogeneity of variance is not quite significant at the 5% level, and the tests for a difference in the bivariate means of the two groups all take the same *p*-value since there are only two groups. The difference is highly significant. Here, the estimated misclassification rates estimated from the original sample and from the leaving-out-one method are very similar.

The linear discriminant function derived above assumes that both groups have the same population covariance matrix. When this assumption is thought to be doubtful, a quadratic discriminant function can be derived (see Everitt and Dunn, 2001, for details). Largely as an exercise, we shall demonstrate how to find this function for the blood fat data by using the S-PLUS **Discriminant Analysis** dialog. For this analysis we shall use all the data, i.e., now including individual 171.

- Click on **Statistics**.
- Select **Multivariate**.
- Select **Discriminant Analysis**.

In the **Discriminant Analysis** dialog, which now appears, choose bf as the data set, and then Group as the **Dependent variable** and Cholesterol and Triglycerides as the **Independent**. Select **heteroscedastic** for **Covariance Struct** and set **Group Prior** to uniform. The dialog now appears as shown in Figure 11.6. Now check the **Results** tab and tick **Plot**. Finally, click on **OK**.

The results of the analysis are shown in Table 11.4 and the plotted quadratic discriminant function is shown in Figure 11.7. In Table 11.4, there are quadratic coefficients in addition to linear coefficients. The test for homogeneity of covariances differs from that in Table 11.3 because of the inclusion of individual 171 in this analysis. With this individual included, there is a significant difference between the covariance matrices of the two groups. The quadratic discriminant function classifies more of the no heart disease correctly than the linear function, but does less well on the heart disease group.

Table 11.3 Results from Using discrim Function on Blood Fat Data

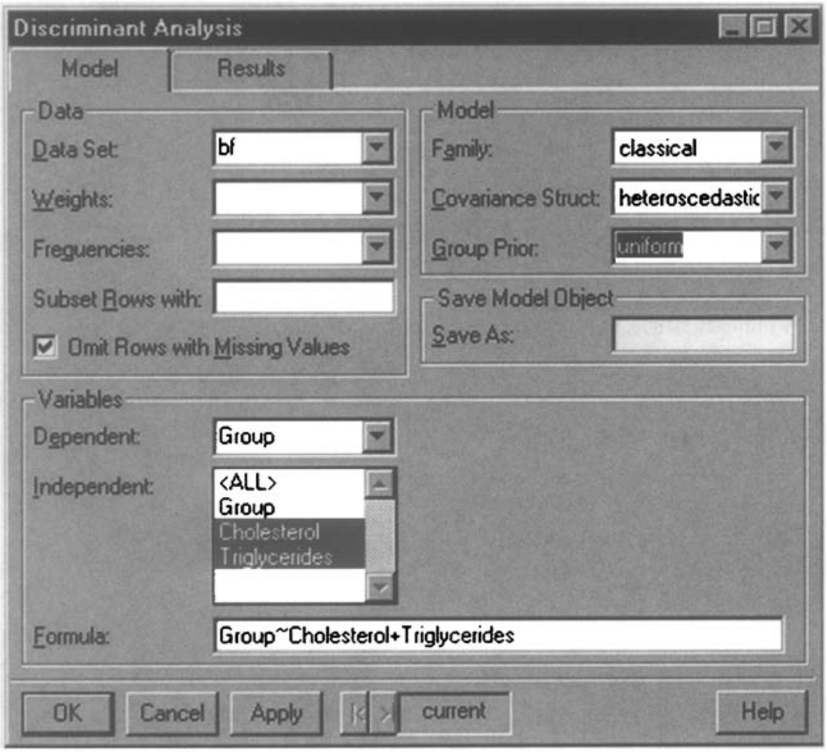
```
Call:
discrim(Group ~ Cholesterol + Triglycerides, data = bf, prior =
      "uniform")

Group means:
                    Cholesterol  Triglycerides   N   Priors
No heart disease            195            140  51      0.5
   Heart disease            216            177  31      0.5

Covariance Structure: homoscedastic
               Cholesterol  Triglycerides
 Cholesterol          1768            844
Triglycerides         8205

Constants:
No heart disease   Heart disease
           -11.6           -14.2

Linear Coefficients:
               No heart disease   Heart disease
 Cholesterol              0.108           0.118
Triglycerides             0.006           0.009

Tests for Homogeneity of Covariances:
          Statistic  df     Pr
 Box.M         7.73   3  0.052
  adj.M        7.62   3  0.055

Tests for the Equality of Means:
Group Variable: Group
                         Statistics     F  df1  df2        Pr
          Wilks Lambda       0.9616  7.33    2  367  0.000758
          Pillai Trace       0.0384  7.33    2  367  0.000758
Hoteling-Lawley Trace        0.0399  7.33    2  367  0.000758
    Roy Greatest Root        0.0399  7.33    2  367  0.000758
* Tests assume covariance homoscedasticity.
  F Statistic for Wilks' Lambda is exact.
  F Statistic for Roy's Greatest Root is an upper bound.
```

Table 11.3 (Continued) Results from Using discrim Function on Blood Fat Data

```
Hotelling's T Squared for Differences in Means Between Each Group:
                                     F  df1  df2       Pr
No heart disease-Heart disease    7.33    2  367  0.000758

95% Simultaneous Confidence Intervals Using the Dunnett Method:
                                     Estimate  Std.Error  Lower Bound
Nhrtdiss.Cholestr-Hrtdises.Cholestr     -20.7       6.34        -34.9
 Nhrtdiss.Trglycrd-Hrtdises.Trglycrd    -36.6      13.70        -67.3
                                          Upper Bound
Nhrtdiss.Cholestr-Hrtdises.Cholestr             -6.49  ****
 Nhrtdiss.Trglycrd-Hrtdises.Trglycrd            -6.03  ****
(critical point: 2.2411)
* Intervals excluding 0 are flagged by '****'

Mahalanobis Distance:
                  No heart disease  Heart disease
No heart disease             0.000          0.334
   Heart disease                            0.000

Kolmogorov-Smirnov Test for Normality:
              Statistic  Probability
 Cholesterol      0.057        0.180
Triglycerides     0.048        0.362

Plug-in classification table:
                  No heart disease  Heart disease  Error  Posterior.Error
No heart disease                35             16  0.314            0.461
   Heart disease               134            185  0.420            0.322
         Overall                            0.367  0.391
                  Stratified.Error
No heart disease             0.340
   Heart disease             0.451
         Overall             0.396
(from = rows,to = columns)

Optimal Error Rate:
 No heart disease  Heart disease  overall
            0.449          0.449    0.449
```

Table 11.3 (Continued) Results from Using discrim Function on Blood Fat Data

```
Rule Mean Square Error: 0.462
(conditioned on the training data)

Cross-validation table:
                  No heart disease  Heart disease  Error  Posterior.Error
No heart disease                34             17  0.333            0.458
   Heart disease               136            183  0.426            0.324
         Overall                            0.380  0.391
                  Stratified.Error
No heart disease             0.349
   Heart disease             0.441
         Overall             0.395

(from = rows,to = columns)
```



Discriminant Analysis

Data

Data Set: bf

Weights:

Frequencies:

Subset Rows with:

☑ Omit Rows with Missing Values

Model

Family: classical

Covariance Struct: heteroscedastic

Group Prior: uniform

Save Model Object

Save As:

Variables

Dependent: Group

Independent: <ALL> Group Cholesterol Triglycerides

Formula: Group~Cholesterol+Triglycerides

Figure 11.6 Completed Discriminant Analysis dialog.

Table 11.4 Quadratic Discriminant Function Results for Blood Fat Data

```
        *** Discriminant Analysis ***

Call:
discrim(Group ~ Cholesterol + Triglycerides, data = bf, family =
        Classical(cov.structure = "heteroscedastic"), na.action =
        na.omit, prior = "uniform")

Group means:
                    Cholesterol  Triglycerides   N Priors
 No heart disease           195            140   51   0.5
    Heart disease           216            179  320   0.5

Covariance Structure: heteroscedastic

Group: No heart disease
               Cholesterol  Triglycerides
  Cholesterol         1304            873
Triglycerides                        5519

Group: Heart disease
               Cholesterol  Triglycerides
  Cholesterol         1850            999
Triglycerides                       10373

Constants:
No heart disease   Heart disease
           -23.2           -21.9

Linear Coefficients:
               No heart disease   Heart disease
  Cholesterol             0.148           0.113
Triglycerides             0.002           0.006

Quadratic coefficents:

group: No heart disease
               Cholesterol  Triglycerides
  Cholesterol    -0.000429       0.000068
Triglycerides                   -0.000101
```

Table 11.4 (Continued) Quadratic Discriminant Function Results for Blood Fat Data

```
group: Heart disease
              Cholesterol  Triglycerides
 Cholesterol    –0.000285      0.0000274
Triglycerides                 –0.0000508

Tests for Homogeneity of Covariances:
        Statistic  df     Pr
Box.M        11.2   3  0.011
 adj.M       11.1   3  0.011

Hotelling's T Squared for Differences in Means between Each Group:
                                  F   df1   df2          Pr
No heart disease-Heart disease  9.4     2  74.8    0.000228
* df2 is Yao's approximation.

95% Simultaneous Confidence Intervals Using the Dunnett Method:
                                           Estimate  Std.Error  Lower Bound
Nhrtdiss.Cholestr-Hrtdises.Cholestr           –20.9        5.6        –33.6
 Nhrtdiss.Trglycrd-Hrtdises.Trglycrd          –39.0       11.9        –65.9
                                        Upper Bound
Nhrtdiss.Cholestr-Hrtdises.Cholestr            –8.2  ****
 Nhrtdiss.Trglycrd-Hrtdises.Trglycrd          –12.1  ****
(critical point: 2.272)
* Intervals excluding 0 are flagged by '****'

Pairwise Generalized Squared Distances:
                   No heart disease   Heart disease
No heart disease              0.000           0.315
    Heart disease             0.462           0.000

Kolmogorov-Smirnov Test for Normality:
              Statistic   Probability
 Cholesterol      0.062         0.111
Triglycerides     0.043         0.505
```

Table 11.4 (Continued) Quadratic Discriminant Function Results for Blood Fat Data

```
Plug-in classification table:
                   No heart disease  Heart disease  Error  Posterior.Error
No heart disease                 42              9  0.176            0.246
   Heart disease                177            143  0.553            0.407
         Overall                             0.365  0.326
                    Stratified.Error
No heart disease               0.111
   Heart disease               0.552
         Overall               0.331

(from = rows,to = columns)

Rule Mean Square Error: 0.522
(conditioned on the training data)

Cross-validation table:
                   No heart disease  Heart disease  Error  Posterior.Error
No heart disease                 40             11  0.216            0.252
   Heart disease                177            143  0.553            0.401
         Overall                             0.384  0.326
                    Stratified.Error
No heart disease               0.137
   Heart disease               0.526
         Overall               0.331
(from = rows, to = columns)
```

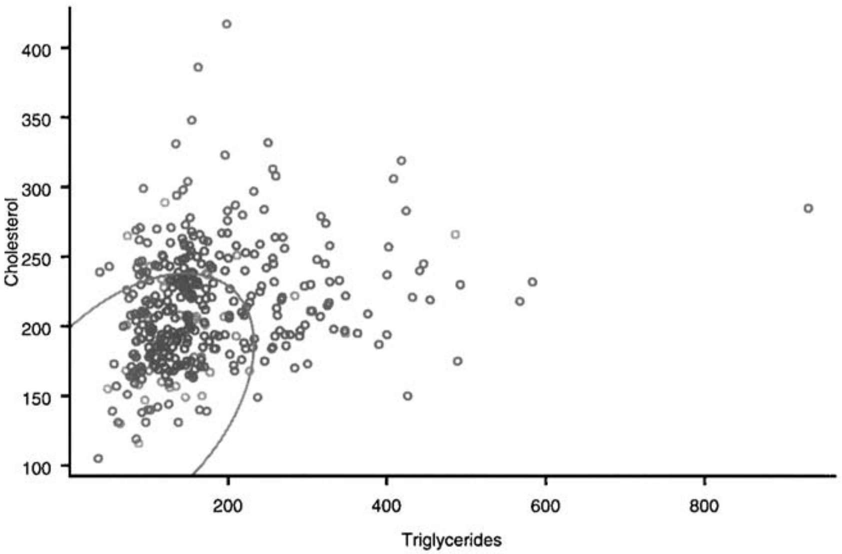


Figure 11.7 Plotted quadratic discriminant function.

Exercises

11.1. Investigate what happens when the discrim function is used on the blood fat data with other than uniform priors.

11.2. Investigate using the discrim function on the blood fat data when the assumption about the group covariance matrix is neither that they are equal nor that they are completely different.

Appendix A

The S-PLUS Language

A1 Vectors and Matrices

Vectors can be created using the concatenate function, c, which combines all values given as arguments to the function into a vector.

```
>x<-c(1,2,3,4)
>y<-c(5,6,7,8)
>xy<-c(x,y)
>xy
[1] 1 2 3 4 5 6 7 8
```

The number of elements in a vector can be determined using the length function

```
>length(xy)
[1] 8
```

Particular elements of vectors can be accessed using the square bracket nomenclature

```
>xy[2]
[1] 2
>xy[c(1,3,8)]
[1] 1 3 8
>xy[-c(1,3,8)]
[1] 2 4 5 6 7
```

The c function can also be used to combine strings denoted by enclosing them in " ". For example:

```
>names<-c("Brian","Rachel","Hywel","Dafydd")
>names
[1] "Brian", "Rachel", "Hywel", "Dafydd"
```

The c function also works with a mixture of numeric and string values, but in this case all elements in the resulting vector will be converted to strings:

```
>xnames<-c(x,names)
>xnames
[1] "1" "2" "3" "4" "Brian" "Rachel" "Hywel"
[8] "Dafydd"
```

Arithmetic operators (see Table A1) work element-wise on vectors; so, for example,

```
>x*y
[1] 5 1221 32
>x/x
[1] 1 1 1 1
>x-y
[1]-4 -4   -4   -4
>2*x
[1]2 4 6 8
```

Table A1 Arithmetic Operators

Operator	Meaning	Expression	Result
+	plus	2 + 3	5
–	minus	5 – 2	3
*	times	5 * 2	10
/	divided by	10/2	5
^	power	2^3	8

We can also apply mathematical functions to vectors, and they will be applied element by element. (The most common of these functions are listed in Table A2.) To restrict the number of decimal points printed, we first use the options function as follows:

Table A2 Common Functions

S-PLUS Function	Meaning
sqrt	square root
log	natural logarithm
log10	logarithm base 10
exp	exponential
abs	absolute value
round	round to nearest integer
ceiling	round up
floor	round down
sin, cos, tan	sine, cosine, tangent
asin, acos, atan	arc sine, arc cosine, arc tangent

```
options(digits=3)
>log(xy)
[1] 0.000 0.693 1.099 1.386 1.609 1.792 1.946 2.079
>exp(xy)
[1] 2.72 7.39 20.09 54.60 148.41 403.43 1096.63 2980.96
>sqrt(x*x+y*y)
[1] 5.10 6.32 7.62 8.94
```

Matrix objects are also frequently required when using S-PLUS and can be created by use of the matrix function. The general syntax is

```
matrix(data, nrow, ncol, byrow=F)
```

The last argument specifies whether the matrix is to be filled row by row or column by column, with the latter being the default. Some examples will help to clarify how the matrix function operates:

```
>X<-matrix(c(x,y),nrow=2)
>X
      [,1]  [,2]  [,3]  [,4]
[1,]     1     3     5     7
[2,]     2     4     6     8
```

Here, the number of columns is not specified and so is determined by simple division.

```
>X<-matrix(c(x,y),nrow=2,byrow=T)
>X
      [,1]  [,2]  [,3]  [,4]
[1,]     1     2     3     4
[2,]     5     6     7     8
```

Here, the matrix is filled row-wise instead of by columns since byrow is set to true.

Again, the square bracket convention can be used to refer to particular elements of matrices, or particular rows or columns, or particular subsets of rows and columns.

```
>X[1,1]
[1]  1
>X[2,]
[1]  5  6  7  8
>X[,3]
[1]  3  7
>X[,c(1, 4)]
      [,1]  [,2]
[1,]     1     4
[2,]     5     8
```

As with vectors, arithmetic operations operate element by element when applied to matrices:

```
>X+X
      [,1]  [,2]  [,3]  [,4]
[1,]     2     4     6     8
[2,]    10    12    14    16

>X/X
      [,1]  [,2]  [,3]  [,4]
[1,]     1     1     1     1
[2,]     1     1     1     1

>sqrt(X)
       [,1]   [,2]   [,3]   [,4]
[1,]   1.00   1.41   1.73   2.00
[2,]   2.24   2.45   2.65   2.83
```

Matrix multiplication is performed using the %*% operator

```
>X%*%t(X)
        [,1]  [,2]
[1,]     30    70
[2,]     70   174
```

Here, the matrix **X** is multiplied by its transpose which is found using the t function. Trying to multiply **X** by itself would lead to an error message:

```
>X%*%X
Error in "%*%.default" (X,X): Number of columns of x
should be the same as number of rows of y
```

A very powerful procedure in S-PLUS is the ability to subset matrices and vectors using logical expressions (the symbols used for logical operations are listed in Table A3). In addition to logical operations, there are also a number of logical functions, i.e., functions that return the values T or F.

```
>is.numeric(4)
[1]  T
>is.character(4)
[1]  F
>is.character("B")
[1]  T
```

Table A3 Logical Operators

Operator	Meaning
<	less than
>	greater than
< =	less than or equal to
> =	greater than or equal to
==	equal to
! =	not equal to
&	and
|	or
!	not

Of particular importance here is the function used for testing for missing values (NA in S-PLUS), is.na:

```
>is.na(c(10,20,NA,NA,3,NA))
[1]  F  F  T  T  F  T
>!is.na(c(10,20,NA,NA,3,NA))
[1]  T  T  F  F  T  F
```

Logical operators or functions operate on vectors and matrices in the same way as other operators, i.e., element by element:

```
>x<-c(1,2,3,4,5,6)
>x<4
[1]  T  T  T  F  F  F
```

A logical vector can be used to extract a subset of elements from another vector, for example,

```
>x[x<4]
[1]  1  2  3
>y<-c(2,8,10,12,16,18)
>y[x>=4]
[1]  12  16  18
>X<-matrix(c(1,2,-9,-9,7,-9,8,6),ncol=2)
>X[X==-9]<-NA
>X
       [,1]  [,2]
[1,]      1     7
[2,]      2    NA
[3,]     NA     8
[4,]     NA     6
```

A2 List Objects

List objects allow other S-PLUS objects to be linked together. For example,

```
>x<-c(1,2,3,4)
>X<-matrix(c(x,10,20,30,40),ncol=2)
>xXlist<-list(x,X)
>xXlist
```

```
[[1]]:
[1]  1  2  3  4
[[2]]:
      [,1] [,2]
[1,]    1   10
[2,]    2   20
[3,]    3   30
[4,]    4   40
```

Note that the elements of the list are referred to by a double square bracket notation. So,

```
>xXlist[[2]]
      [,1] [,2]
[1,]    1   10
[2,]    2   20
[3,]    3   30
[4,]    4   40
```

The components of a list can also be given names and can, of course, also include other list objects.

```
>newlist<-list(first=x,second=X,third=xXlist)
```

Now, the components of the list can also be referred to using the **list$name** notation

```
>newlist$first
[1]  1  2  3  4

>newlist$third
[[1]]:
[1]  1  2  3  4

[[2]]:
      [,1] [,2]
[1,]    1   10
[2,]    2   20
[3,]    3   30
[4,]    4   40
```

A list object can be used to give labels to the rows and/or columns of a matrix which is often very useful. For example:

```
>amatrix<-matrix(c(1,2,3,10,20,30,0,0,0),nrow=3,byrow=T)
>amatrix
       [,1]  [,2]  [,3]
[1,]     1     2     3
[2,]    10    20    30
[3,]     0     0     0
```

```
>dimnames(amatrix)<-list(c("R1","R2","R3"),c("C1","C2","C3"))
>amatrix
      C1   C2   C3
R1     1    2    3
R2    10   20   30
R3     0    0    0
```

If the matrix was large, say, 500 rows and 50 columns, then helpful row and column labels can be created easily using the paste function:

```
>dimnames(amatrix)<-list(paste("R", 1:500), paste("C", 1:50))
```

The row labels will be R1, R2, … R500, and the column labels C1, C2, … C50.

A3 Data Frames

Data sets in S-PLUS are usually stored as data frames, since these can bind together vectors of different types (for example, numeric and character), retaining the correct type for each vector. In many respects a data frame is similar to a matrix so that each vector should have the same number of elements. The syntax for creating data frame objects is data.frame(vector 1,vector 2,...); here is a small example:

```
>height<-c(50, 70, 45, 80, 100)
>weight<-c(120, 140, 100, 200, 190)
>age<-c(20, 40, 41, 31, 33)
>names<-c("Bob", "Ted", "Alice", "Mary", "Sue")
>sex<-c("Male", "Male", "Female", "Female", "Female")
>data<-data.frame (names, sex, height, weight, age)
```

```
>data
    names   sex      height  weight  age
1   Bob     Male       50     120    20
2   Ted     Male       70     140    40
3   Alice   Female     45     100    41
4   Mary    Female     80     200    31
5   Sue     Female    100     190    33
```

Particular parts of a data frame can be extracted in the same way as for matrices.

```
>data[,c(1, 2, 5)]
    names   sex      age
1   Bob     Male      20
2   Ted     Male      40
3   Alice   Female    41
4   Mary    Female    31
5   Sue     Female    33
```

Column names can also be used:

```
>data[,c("names","age")]
    names   age
1   Bob      20
2   Ted      40
3   Alice    41
4   Mary     31
5   Sue      33
```

Variables can also be accessed as with list objects:

```
>data$age
[1]  20  40  41  31  33
```

It is, however, more convenient to 'attach' a data frame object and then work with the column names directly. For example,

```
>attach(data)
>age
[1]  20  40  41  31  33
```

Note that the **attach** command places the data frame in the second position in the search path, so if, for example, we now assign a value to age

```
>age<-10
>age
[1]  10
```

a new object is created in the first position of the search path that 'masks' the age variable of the data data frame. Variables can be removed from the first position in the search path using the rm function.

```
>rm(age)
>age
1     2    3    4    5
20   40   41   31   33
```

To change the value of any or all elements of age in the data data frame, use the syntax

```
>data$age<-c(20,30,45,32,32)
```

A4 Reading Data into S-PLUS

S-PLUS can read data from a large number of different statistical packages and spreadsheet/database packages, including SPSS, Stata, SAS, Microsoft Excel, and Microsoft Access. To read a file from another package using the GUI, for example,

- Click on **File**.
- Select **Import Data**.
- Select **From File**.

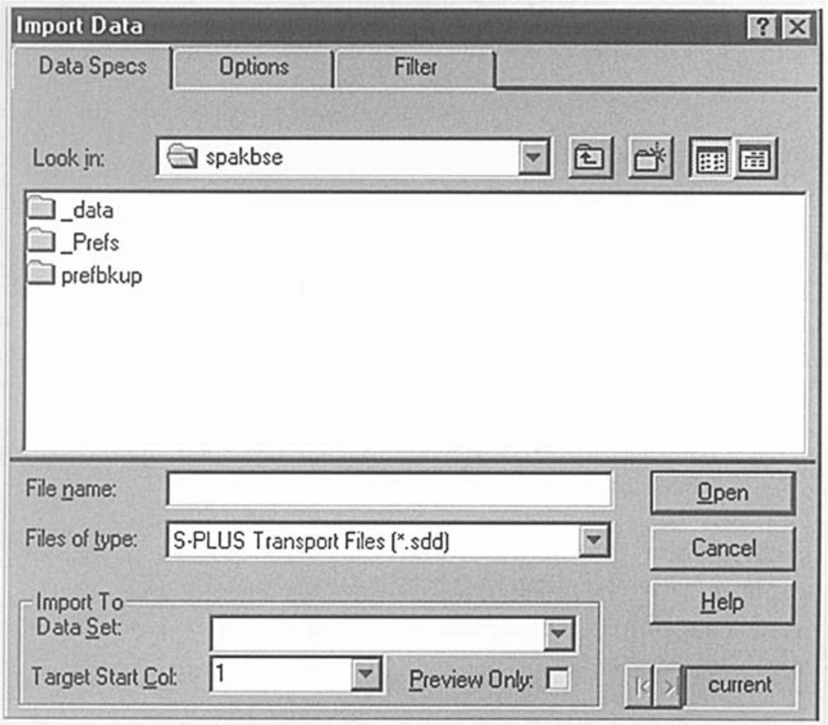
The **Import Data** dialog as shown in Figure A1 now appears.

In the **File name** window, enter the file name and then select the appropriate type in the Files type window, e.g., SPSS files (*sav).

ASCII data can be read using the scan function. For example, if the file data.dat in the directory C:\users\me contains the matrix data

```
123
456
321
```

they can be read into a vector using scan, and then converted into a matrix using the matrix function as usual.



Look in: spakbse

- _data
- _Prefs
- prefbkup

File name:

Files of type: S-PLUS Transport Files (*.sdd)

Import To

Data Set:

Target Start Col: 1

Preview Only: □

Figure A1 Import Data dialog.

```
>A<-matrix(scan(file=“c:\\users\\me\\data.dat”),nrow=3,
byrow=T)
```

Note that the scan function reads the data in lexicographical order (down the rows), so that the byrow=T option needs to be used in the matrix function.

Perhaps the most convenient way of reading-in ASCII data is by using the read.table function which is used in creating data frames. If the first row of the file contains the variable names, the header=T option causes these names to be used for the columns of the data frame. If, for example, the data in C:\users\me\children.dat contain

```
age   sex   y
11    boy   3.2
9     boy   5.8
13    girl  1.2
```

they can be read-in using

```
>child<-read.table("c:\\users\\me\\children.dat",header=T)
>child

   age  sex   y
1  11   boy   3.2
2  9    boy   5.8
3  13   girl  1.2
```

In many cases, all variables will be initially read into data in numeric form and then categorical variables designated as factor variables with their categories suitably labelled by use of the **factor** function. For example, the **rats** data frame used in Chapter 3 was initially constructed from an ASCII file in which the levels of poison were coded 1, 2, and 3, and the levels of treatment, 1, 2, 3, and 4. These were then altered to factor variables as follows;

```
>rats$Poison<-factor(rats$Poison,levels=1:3,
>labels=c("P1","P2","P3"))
>rats$Treatment<-factor(rats$Treatment,levels=1:4,
>labels=c("A","B","C","D"))
```

A5 S-PLUS Functions

S-PLUS has over 3000 in-line functions, a substantial minority of which have been used in this text. Information about these functions is available from the **help** function, for example,

```
>help(paste)
```

Here, we shall illustrate relatively briefly the use of just a small subset of perhaps the most widely used and most useful functions when analysing data. To begin we shall look at the two functions **seq** and **rep**, which are often used in the construction of vectors with a particular pattern of elements. For each function we include a summary of the material given by use of **help**(*function name*)

seq:

Description

Creates a vector of evenly spaced numbers. The beginning, end, spacing, and length of the sequence can be specified.

Usage

```
seq(...)

seq.default(from=<<see below>>, to=<<see below>>, by=<<see below>>,
  length=<<see below>>, along=NULL)
```

Optional Arguments

from: Starting value of the sequence. If *to*, *by*, and *length* are all given, the value for this is inferred; otherwise, the default is 1.

to: Ending value of sequence, a value less than from is allowed. If *from*, *by*, and *length* are all given, the value for this is inferred; otherwise, the default is 1.

by: Spacing between successive values in the sequence. If *from*, *to*, and *length* are all given, the value for this is inferred; otherwise, the default is 1.

length: Number of values in the result. If *from*, *to*, and *by* are all given, the value for this is inferred.

along: An object. The length of the object is used as the length of the returned value.

It is an error to specify all of the first four arguments.

Value

A numeric vector with values (from, from+by, from+2*by, ... to); *from* may be larger or smaller than *to*. If *by* is specified, it must have the appropriate sign to generate a finite sequence.

rep

Description

Replicates the input either a certain number of times or to a certain length.

Usage

```
rep(x, times=<<see below>>, length.out=<<see below>>,
 each=<<see below>>)
```

Required Arguments

x vector. Missing values (NAs) are allowed.
At least one of *times, length.out,* and *each* must be given.

Optional Arguments

times: How many times to replicate x. There are two ways to use *times*. If it is a single value, the whole of x is replicated that many times. If it is a vector that is the same length as x, the result is a vector with times[1] replications of x[1], times[2] of x[2], etc. Zero is allowed in both usages; if times=0, then the length of the result is 0. It is an error if the length of *times* is neither 1 nor the length of x.

length.out: The desired length of the result. This argument may be given instead of *times*, in which case x is replicated as much as needed to produce a result with *length.out* data values. If both *times* and *length.out* are given, *times* is ignored.

each: If *each* is supplied, each element of x is repeated each time. This vector is repeated again if *times* or *length.out* is also given.

Value

A vector of the same mode as x with the data values in x replicated according to the arguments *times*, *length.out*, and *each*. Any names are removed.

Details

Missing values (NAs) and Infs are treated just like other values.

Some examples of the use of both seq and rep are

```
> seq(0, 10, length=4)
[1] 0.000000 3.333333 6.666667 10.000000
> seq(0, 50, by=5)
[1] 0 5 10 15 20 25 30 35 40 45 50
> seq(0, 10, by=0.5)
[1] 0.0 0.5 1.0 1.5 2.0 2.5 3.0 3.5 4.0 4.5 5.0 5.5 6.0
[14] 6.5 7.0 7.5 8.0 8.5 9.0 9.5 10.0
```

```
> seq(5, 0, length=3)
[1] 5.0 2.5 0.0
> seq(5)
[1] 1 2 3 4 5
> seq(-5)
[1] 1 0 -1 -2 -3 -4 -5
> rep(10, 5)
[1] 10 10 10 10 10
> rep(c(10, 1), 3)
[1] 10 1 10 1 10 1
> rep(c(10, 1), c(3, 2))
[1] 10 10 10 1 1
> rep(rep(c(10, 1), c(3, 2)), 4)
[1] 10 10 10 1 1 10 10 10 1 1 10 10 10 1 1 10 10 10 1 1
> rep(1:5, 1:5)
[1] 1 2 2 3 3 3 4 4 4 4 5 5 5 5 5
```

Three functions of particular use in statistical work are mean, var, cor.

mean

Description

Returns a number that is the mean of the data. A fraction to be trimmed from each end of the ordered data can be specified.

Usage

mean(x, trim=0, na.rm=F)

Required Arguments

x: Numeric object. Missing values (NAs) are allowed.

Optional Arguments

trim: Fraction (between 0 and .5, inclusive) of values to be trimmed from each end of the ordered data. If *trim=.5*, the result is the median.

na.rm: Logical flag: should missing values be removed before computation?

Value

(trimmed) mean of x.

Details

If x contains any NAs, the result will be NA unless na.rm = TRUE.

var and cor

Description

Returns the variance of a vector, the variance–covariance (or correlation) matrix of a data matrix, or covariances between matrices or vectors. A trimming fraction may be specified for correlations.

Usage

```
var(x, y, na.method = "fail", unbiased = T, SumSquares = F)
cor(x, y, trim = 0, na.method = "fail", unbiased = T)
```

Required Arguments

x: Numeric matrix or vector, or data frame. May be complex. If a matrix, columns represent variables and rows represent observations. If a data frame, non-numeric variables result in missing values in the result.

Optional Arguments

y: Numeric matrix or vector, or data frame. May be complex. If a matrix, columns represent variables and rows represent observations. If a data frame, non-numeric variables result in missing values in the result. This must have the same number of observations as x.

trim: A number less than .5 giving the proportion trimmed in the internal calculations for cor. This should be a number larger than the suspected fraction of outliers.

na.method: A character string specifying how missing values are to be handled. Options are

“fail” (stop if any missing data are found),
“omit” (omit rows with any missing data),
“include” (missing values in the input result in missing values in the output)
“available” (use available observations, see below).
Only enough of the string to determine a unique match is required.

unbiased: If TRUE, then variances are sample variances, e.g.,

sum((x-mean(x))^2)/(N-1)

for a vector of length N, which is unbiased if the values in x are obtained by simple random sampling. If FALSE, the definition

sum((x-mean(x))^2)/N

is used instead.

SumSquares: If TRUE, then un-normalized sums of squares are returned, with no division by either N or (N-1) (and unbiased is ignored).

Value

cor() returns correlations, and var() returns variances and covariances or sums of squares.

If x is a matrix, the result is a matrix such that the [i,j] element is the covariance (correlation) of x[,i] and either y[,j] or x[,j]. If x is a vector, the result is a vector, with length equal to the number of columns of y (or length 1 if y is not supplied).

Some examples of the use of these three functions are

```
> x <- 1:10
> mean(x)
[1] 5.5
> var(x)
[1] 9.166667
> x <- c(x, NA)
> mean(x)
[1] NA
> mean(x, na.rm=T)
[1] 5.5
> var(x, na.method=“omit”)
[1] 9.166667
> X <- matrix(c(1, 4, 6, 3, 2, 1, 4, 5, 6), ncol=3)
> var(X)
          [,1] [,2] [,3]
[1,]  6.333333 -2.5  2.5
[2,] -2.500000  1.0 -1.0
[3,]  2.500000 -1.0  1.0
> cor(X)
           [,1]       [,2]       [,3]
[1,]  1.0000000 -0.9933993  0.9933993
[2,] -0.9933993  1.0000000 -1.0000000
[3,]  0.9933993 -1.0000000  1.0000000
```

Two very useful S-PLUS functions for applying a particular S-PLUS function to chosen parts of a matrix or vector are **apply** and **tapply**.

apply

Description

Returns a vector or array by applying a specified function to sections of an array.

Usage

apply(X, MARGIN, FUN, ...)

Required Arguments

X array. Missing values (NAs) are allowed if FUN accepts them.

MARGIN: The subscripts over which the function is to be applied. For example, if X is a matrix, 1 indicates rows, and 2 indicates columns. If the dimensions of X are named, as in the barley data sets, then those names can be used to specify the margin. For a more complex example of the use of MARGIN, see the examples below. Note that MARGIN tells which dimensions of X are retained in the result.

FUN: Function (or character string giving the name of the function) to be applied to the specified array sections. The character form is necessary only for functions with unusual names, e.g., %*%.

Optional Arguments

... any arguments to FUN; they are passed unchanged (including their names) to each call of FUN.

Value

If each call to FUN returns a vector of length N, and N > 1, apply returns an array of dimension

```
c(N,dim(X)[MARGIN])
```

If N==1 and MARGIN has length > 1, the value is an array of dimension dim(X)[MARGIN]; otherwise, it is a vector.

tapply

Description

Applies a function to each cell of a ragged array, that is, to the values corresponding to the same levels in all of several categories.

Usage

```
tapply(X, INDICES, FUN = <<see below>>, ..., simplify = T)
```

Required Arguments

X vector of data to be grouped by indices. Missing values (NAs) are allowed if FUN accepts them.

INDICES: List whose components are interpreted as categories, each of the same length as X. The elements of the categories define the position in a multiway array corresponding to each X observation. Missing values (NAs) are allowed. The names of INDICES are used as the names of the dimnames of the result. If a vector is given, it will be treated as a list with one component.

Optional Arguments

FUN: Function or character string giving the name of the function to be applied to each cell. If FUN is omitted, tapply returns a vector that can be used to subscript the multiway array that tapply normally produces. This vector is useful for computing residuals.

Details

Evaluates a function, FUN, on data values that correspond to each cell of a multiway array.

Some examples of the use of these two functions are

```
> apply(X, 2, mean)
[1] NA 1.75 NA
> apply(X, 2, max)
[1] NA 3 NA
> apply(X, 1, min)
[1] NA 2 1 NA
> X <- matrix(c(1, 4, 6, NA, 3, 2, 1, 1, NA, 4, 5, 6,),
ncol=3)
> apply(X, 2, mean)
[1] NA 1.75 NA
> apply(X, 2, mean, na.rm=T)
[1] 3.666667 1.750000 5.000000
> apply(is.na(X), 2, any)#
[1] T F T
> x <- 1:10
> y <- rep(c(“NO”, “YES”), c(5, 5))
> z <- rep(c(“C1”, “C2”, “C3”, “C4”, “C5”), 2)
> tapply(x, list(y), max)
NO   YES
5    10
> tapply(x, list(y, z), mean)
      C1   C2   C3   C4   C5
 NO    1    2    3    4    5
YES    6    7    8    9   10
```

A very useful set of functions in S-PLUS is those relating to probability distributions. For most common probability distributions, S-PLUS has four functions with prefixes d, p, q, and r to return the density (d), cumulative probability (p), quantile (q), or a random sample (r). The following illustrates the use of these functions for the normal distribution.

```
> rnorm(5, 3, 2)
[1] 3.287 3.273 0.132 3.617 2.638
> pnorm(c(-1.96, 0, 1.96))
[1] 0.025 0.500 0.975
> qnorm(c(0.025, 0.5, 0.975))
[1] -1.96 0.00 1.96
> dnorm(c(-1, 0, 1))
[1] 0.242 0.399 0.242
```

A6 Graphics

S-PLUS contains extensive graphical facilities for constructing a variety of plots and diagrams, from the simple to the not-so-simple.

To begin, a device on which to plot has to be specified. Usually this will be a Graphics window. In Windows 98/2000/NT, such a window can be created using the command:

```
>win.graph()
```

We can now create graphics using appropriate S-PLUS commands, with each new graph replacing the previous one. We can also create a postscript file of a plot by using the command:

```
>postscript(file="graph.ps")
```

After producing a postscript file we must close the file using the dev.off() command; otherwise, subsequent graphs will be superimposed on the first one.

A large number of graphics parameters control the appearance of a graph. Some of these are listed in Table A4. To find out about additional graphics parameters, use

```
>help(par)
```

Trellis graphics offer access to more-sophisticated diagrams such as coplots and dotplots. A trellis device can be specified for these by use of the command:

```
>trellis.device(win.graph)
```

or

```
>trellis.device(postscript,file = name)
```

Many examples of graphs produced by using the command language are given in the text.

A7 User Functions

S-PLUS commands can be used to write new functions for specific tasks. Although this is a very powerful feature of the software, we give only a few simple examples in this section, merely to illustrate the possibilities.

Table A.4 Commands to Add to Existing Graphs and Plotting Parameters

To add to existing graphs:

Function	Description
points (x, y)	Points at coordinates *x* and *y*
text (x, y, text)	Text at specified coordinates
lines (x, y)	Lines to connect the points given by *x* and *y*
segments (*x*1, *y*1, *x*2, *y*2)	Line segments from (*x*1, *y*1) to (*x*2 to *y*2)
arrows (*x*1, *y*1, *x*2, *y*2)	Arrows segments from (*x*1, *y*1) to (*x*2 to *y*2)
abline (a, b)	Line with intercept *a* and slope *b*
legend (x, y, legend)	Legend
title (“title”, “subtitle”)	Title at top of figure

Plotting parameters:

Parameter	Purpose
type = “p”/“l”/“h”/“s”/“n”, etc	Points/lines/vertical bars/steps/nothing
axes = T/F	With/without axes
main	Main title
sub	Subtitle
xlab, ylab	x/y Axis label
xlim, ylim = c(min, max)	x/y Axis range
pch = 1/2/3, etc. or pch = “+”/“.”, etc	Plot character
lty = 1/2/3, etc	Line style
lwd	Line width (1 default)

(More complex examples are described at various places in the text.) A detailed account of writing functions in S-PLUS is given in Venables and Ripley (2000).

As a first illustration we shall create a function **mysum**, which calculates the power of the sum of arguments supplied and returns the result:

```
>mysum<-function(a,b,p=1){
  (a+b)^p
{
```

Now **mysum** can be used to take the power of the sum of two numbers:

```
>mysum(1,2)
[1]  3
>mysum(1,2,p=2)
[1]  9
```

The function can also be applied to numerical vectors of the same length:

```
>a<-c(1,2,3,4)
>b<-c(5,6,7,8)
>mysum(a,b,p=3)
[1]  216  512  1000  1728

>mysum(a/2,b/10,p=5)
[1]  1  10  52  172
```

And the function can also be applied to two matrices with the same number of rows and the same number of columns.

```
>a<-matrix(c(1,2,3,4),ncol=2)
>b<-matrix(c(5,6,7,8),ncol=2)
>mysum(a,b,p=3)
       [,1]   [,2]
[1,]   216   1000
[2,]   512   1728
```

The general syntax of a function is

```
function-name<-function (arguments)
{
function body (S-PLUS expressions)
return (output arguments)
}
```

The output arguments are often stored as a list, for example,

```
meanvar<-function(x)
{
m<-mean(x,na.rm=T)
v<-var(x,na.method=omit")
result<-list(mean=m,variance=v)
}

>meanvar(1:10)
$mean:
[1] 5.5

$variance:
[1] 9.2
```

When writing functions users should try to avoid duplicating the names of existing S-PLUS functions.

Appendix B

Answers to Selected Exercises

Chapter 1

```
#
#
#Exercise 1.1
#
apply(jets[,2:6],2,mean)
#
#Exercise 1.3
#
par(mfrow=c(2,3))
box plot(FFD,ylab="FFD")
box plot(SPR,ylab="SPR")
box plot(RGF,ylab="RGF")
box plot(PLF,ylab="PLF")
box plot(SLF,ylab="SLF")
#
#Exercise 1.4
#
par(mfrow=c(l ,1))
```

```
hist(FFD,probability=T)
lines(density(FFD))
```

Chapter 2

```
#
#
#Exercise 2.1
#
plot(husbage,wifeage)
rug(jitter(husbage[!is.na(husbage)]),side=1)
rug(jitter(wifeage[!is.na(wifeage)]),side=2)
#
#
#Exercise 2.5
#
persp(hist2d(husbage,wifeage),xlab="Husband's
age",ylab="Wife's age",zlab="Frequency")
#
#
#Exercise 2.6
#
```

Access Scatter Plot Matrix dialog from Graphics 2D; click on Line/Histogram tab and tick **draw histogram**

```
#
#
```

Chapter 3

```
#
#
#Exercise 3.1
#
#Here simply use the ANOVA dialog as in the test but use
log(Time)
#as the dependent variable.
#
#
```

```
#Exercise 3.4
#
summary(aov(Response~Status:Condition+Status+Condition))
#
#This gives exactly the same result as
#
summary(aov(Response~Status+Condition+Status:Condition))
#
#S-PLUS does not adjust main effects for the interaction
#composed
#of the main effect factors.
#
#
```

Chapter 5

```
#
#
#Exercise 5.2
#
#
ses<-predict(fit.log,se.fit=T)
#
predict.val<-exp(ses$fit)/(1+exp(ses$fit))
ul<-
exp(ses$fit+1.96*ses$se.fit)/(1+exp(ses$fit+1.96*ses$se.fit)
)
ll<-exp(ses$fit-1.96*ses$se.fit)/(1+exp(ses$fit-1.96*ses$se.fit))
#
ylim<-range(ul,ll)
plot(0:10,predict.val[1:11],xlab="GHQ",ylab="Predicted value
of probability of caseness",
type="l",ylim=ylim)
lines(0:10,ul[1:11],lty=2)
lines(0:10,ll[1:11],lty=2)
legend(locator(1),c("Predicted","95%CI"),lty=1:2)
#
#
```

Chapter 6

```
#
#
#Exercise 6.1
#
t.test(depress.sm[group=="TAU"],depress.sm[group=="BtB"],var
.equal=F)
#
#
#Exercise 6.3
#
#function for filling in missing values in rows of a matrix
by LOCF
#assumes that subject drops out so that a missing value is
not followed
#by any genuine observations
#
locf<-function(X) {
    n<-length(X[,1])
    p<-length(X[1,])
    for(i in 1:n) {
        x<-X[i,]
        y<-x[!is.na(x)]
        N<-length(y)
        if(N!=p) y<-c(y,rep(y[N],p-N))
            X[i,]<-y
    }
    X
}
#
depress.locf<-apply(locf(depress[,4:7]),1,mean)
t.test(depress.locf[group=="TAU"],depress.locf[group=="BtB"]
)
#
#
```

Chapter 7

```
#
#
#Exercise 7.3
#
#
#### function returning - log-likelihood for a mixture of
#two normal distributions
#with both component distributions having the same variance
#
LL<-function(params,data) {
     t1<-dnorm(data,params[2],params[3])
     t2<-dnorm(data,params[4],params[3])
     f<-params[1]*t1+(1-params[1])*t2
     ll<-sum(log(f))
     -ll
}
### fit mixture to geyser data
geyser.res<-
nlminb(c(0.5,50,10,80),LL,data=geyser,lower=c(0.001,-
Inf,0.001,-Inf)
,upper=c(0.999,Inf,Inf,Inf))
#
same<-geyser.res$parameters
#
#assume parameter estimates for different component
variances are in the vector diff
#
x<-seq(40,120,length=100)
#
f1s<-dnorm(x,same[2],same[3])
f2s<-dnorm(x,same[4],same[3])
fs<-same[1]*f1s+(1-same[1])*f2s
#
f1d<-dnorm(x,diff[2],diff[3])
f2d<-dnorm(x,diff[4],diff[5])
fd<-diff[1]*f1d+(1-diff[1])*f2d
```

```
hist(geyser,probability=T,col=0,ylab="Density",ylim=c(0,0.05
),
xlab="Eruption times")
lines(x,fs,lty=1)
lines(x,fd,lty=2)
legend(locator(1),c("Equal variances","Different
variances"),lty=1:2)
#
#
```

Chapter 9

```
#
#
#Exercise 9.3
#
#
skulls.pc<-princomp(skulls[,-1],cor=T)
#
skulls.pc$loadings
#
#
skulls.pcx<-skulls.pc$scores[,1]
skulls.pcy<-skulls.pc$scores[,2]
par(pty="s")
xlim<-range(skulls.pcx)
plot(skulls.pcx,skulls.pcy,xlim=xlim,ylim=xlim,xlab="PC1",yl
ab="PC2",type="n")
labs<-rep(1:5,rep(30,5))
text(skulls.pcx,skulls.pcy,labels=labs)
#
#convex hull
#
for(i in 1:5) {
X<-skulls.pcx[labs==i]
Y<-skulls.pcy[labs==i]
hull<-chull(X,Y)
hull
polygon(X[hull],Y[hull],density=15,angle=30)
}
#
#
```

Chapter 10

```
#
#
#Exercise 10.1
#
#
n<-length(lowest[,1])
#
#get within group sum of squares regarding data as a single
 cluster
#
wss1<-(n-1)*(var(lowest[,2])+var(lowest[,3])+var(lowest[,4])+
var(lowest[,5]))
#
#apply kmeans for 2 to 6 groups and get within cluster ss
#
wss<-numeric(0)
#
for(i in 2:6) {W<-
sum(kmeans(as.matrix(lowest[,2:5]),i)$withinss)
                   wss<-c(wss,W)
                  }
wss<-c(wss1,wss)
win.graph()
plot(1:6,wss,xlab="Number of clusters",ylab="Within cluster
sum of squares",type="l")
#
#
Exercise 10.3
#
#
#need to look at the eigenvalues in a similar way as for PCA
```

```
#
coords<-cmdscale(congress,k=6,eig=T)
#
plot(1:6,coords$eig,type="l")
#
#
###################################################
######################
```

References

Aitkin, M. (1978). The analysis of unbalanced cross-classifications (with discussion). *Journal of the Royal Statistical Society, A*, 41, 195–223.

Atkinson, A.C. (1987). *Plots, Transformations and Regression*, Oxford Science Publications, Oxford, U.K.

Becker, R.A., Chambers, J.M., and Wilks, A.R. (1988*). New S Language.* Wadsworth and Brook/Cole, Pacific Grove, California.

Burns, K.C. (1984). Motion sickness incidence distribution of time to first emesis and comparison of some complex motion conditions, *Aviation Space and Environmental Medicine*, 56, 521–527.

Chambers, J.M. and Hastie, T.J. (1992). *Statistical Models in S.* Wadsworth and Brook/Cole, Pacific Grove, California.

Chatterjee, S. and Chatterjee, S. (1982). New lamps for old: An exploratory analysis of running times in Olympic Games, *Applied Statistics*, 30, 14–22.

Cleveland, W.S. (1993). *Visualizing Data*, Hobart Press, Summit, New Jersey.

Collett, D. (1991). *Modelling Binary Data.* CRC/Chapman & Hall, London.

Collett, D. (1994). *Modelling Survival Data in Medical Research.* CRC/Chapman & Hall, London.

Cook, R.D. and Weisberg, S. (1982). *Residuals and Influence in Regression.* CRC/Chapman & Hall, London.

Diggle, P.J., Liang, K., and Zeger, S.L. (1994). *Analysis of Longitudinal Data,* Oxford Science Publications, Oxford, U.K.

Efron, B. and Tibshirani, R.J. (1993). *An Introduction to the Bootstrap.* CRC/Chapman & Hall, New York.

Everitt, B.S. (2001). *Statistics for Psychologists.* Lawrence Erlbaum Associates, Mahwah, New Jersey.

Everitt, B.S. (2002). An evaluation of the gap statistic for estimating the number of clusters in a data set. In preparation.

Everitt, B.S. and Dunn, G. (2001). *Applied Multivariate Data Analysis,* 2nd ed. Arnold, London.

Everitt, B.S. and Hand, D.J. (1981). *Finite Mixture Distributions.* CRC/Chapman & Hall, London.

Everitt, B.S. and Pickles, A. (2000). *Statistical Aspects of the Design and Analysis of Clinical Trials.* ICP, London.

Everitt, B.S. and Rabe-Hesketh, S. (1997). *The Analysis of Proximity Data.* Arnold, London.

Everitt, B.S., Landau, S., and Leese, M. (2001). *Cluster Analysis,* 4th ed. Arnold, London.

Goldberg, D. (1972). *The Detection of Psychiatric Illness by Questionnaire.* Oxford University Press, Oxford, U.K.

Hand, D.J. (1998). Discriminant analysis linear. In *Encyclopedia of Biostatistics,* Vol. 2, P. Armitage and T. Colton, Eds., Wiley, Chichester, U.K.

Hand, D.J., Daly, F., Lunn, A.D., McConway, K.J., and Ostrowski, E. (1994). *A Handbook of Small Data Sets.* CRC/Chapman & Hall, London.

Krause, A. and Olson, M. (2000). *The Basics of S and S-PLUS,* 2nd ed. Springer, New York.

McCullagh, P. and Nelder, J.A. (1989). *Generalized Linear Models.* Chapman and Hall, London.

Nelder, J.A., (1977). A reformulation of linear models. *Journal of the Royal Statistical Society, A*, 140, 48–63.

Pinheiro, J.C. and Bates, D.M (2000). *Mixed-Effects Models in S and S-PLUS.* Springer, New York.

Pollock, K.H., Winterstein, S.R., and Conroy, M.J. (1989). Estimation and analysis of survival distributions for radio-tagged animals. *Biometrics*, 45, 99–109.

Rawlings, J.O. (1988). *Applied Regression Analysis.* Wadsworth Books, Pacific Grove, California.

Silverman, B.W. (1986). *Density Estimation for Statistics and Data Analysis.* CRC/Chapman & Hall, London.

Stanley, W. and Miller, M. (1979). Measuring technological change in jet fighter aircraft. Report no. R-2249-AF, Rand Corp., Santa Monica, California.

Therneau, T.M. and Grambach, P.M. (2000). *Modelling Survival Data.* Springer, New York.

Tibshirani, R., Walther, G., and Hastie, T. (2001). Estimating the number of clusters in a data set via the gap statistic. *Journal of the Royal Statistical Society, Series B,* 63, 411–423.

Venables, W.N. and Ripley B.D. (1997). *Modern Applied Statistics with S-PLUS.* Springer, New York.