Using R for Data Analysis and Graphics

Introduction, Code and Commentary

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Languages shape the way we think, and determine what we can think about (Benjamin Whorf.).

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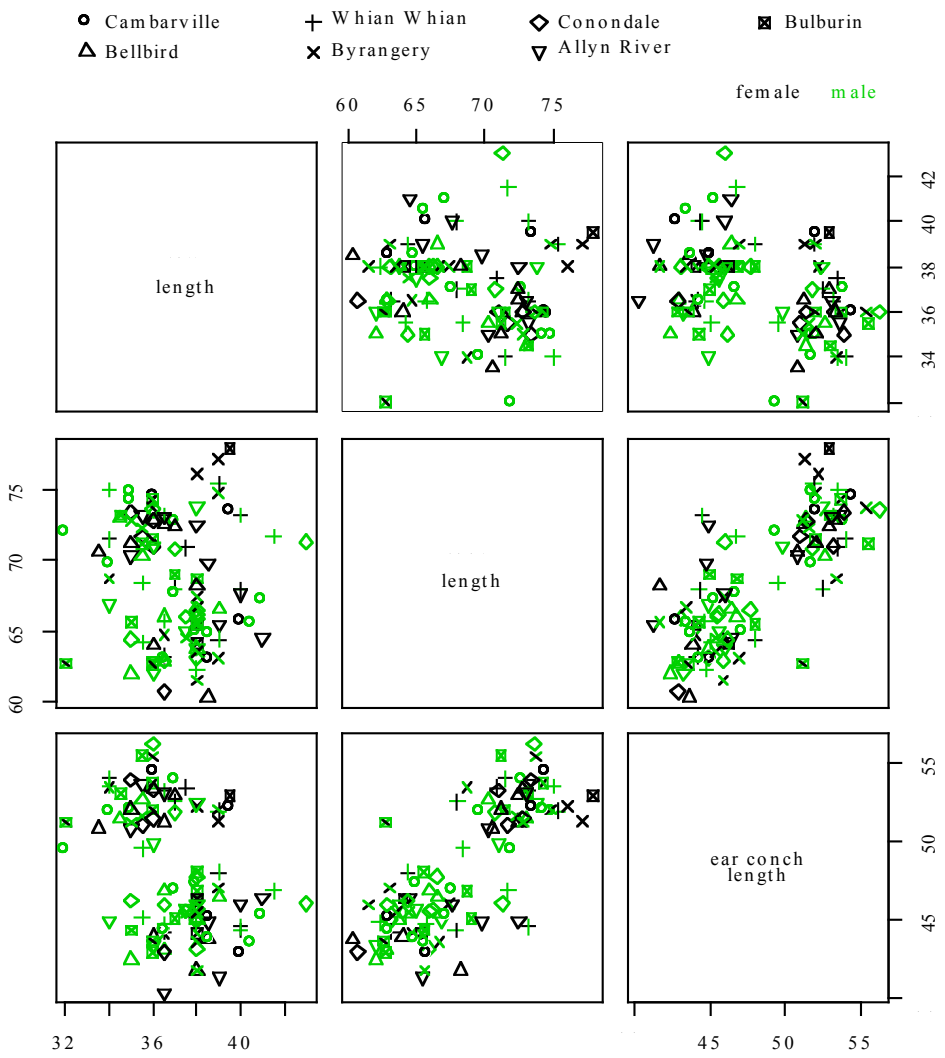

Lindenmayer, D. B., Viggers, K. L., Cunningham, R. B., and Donnelly, C. F. : Morphological variation among populations of the mountain brushtail possum, *trichosurus caninus* Ogibly (Phalangeridae:Marsupialia). Australian Journal of Zoology 43: 449-459, 1995.

possum *n*. **1** Any of many chiefly herbivorous, long-tailed, tree-dwelling, mainly Australian marsupials, some of which are gliding animals (e.g. *brush-tailed possum*, *flying possum*). **2** a mildly scornful term for a person. **3** an affectionate mode of address.

From the Australian Oxford Paperback Dictionary, 2nd ed, 1996.

Introduction

These notes are designed to allow individuals who have a basic grounding in statistical methodology to work through examples that demonstrate the use of R for a range of types of data manipulation, graphical presentation and statistical analysis. Books that provide a more extended commentary on the methods illustrated in these examples include Maindonald and Braun (2003).

The R System

R implements a dialect of the S language that was developed at AT&T Bell Laboratories by Rick Becker, John Chambers and Allan Wilks. Versions of R are available, at no cost, for 32-bit versions of Microsoft Windows for Linux, for Unix and for Macintosh OS X. (There are are older versions of R that support 8.6 and 9.) It is available through the Comprehensive R Archive Network (CRAN). Web addresses are given below.

The citation for John Chambers' 1998 Association for Computing Machinery Software award stated that S has "forever altered how people analyze, visualize and manipulate data." The R project enlarges on the ideas and insights that generated the S language.

Here are points relating to the use of R that potential users might note:

R has extensive and powerful graphics abilities, that are tightly linked with its analytic abilities.

The R system is developing rapidly. New features and abilities appear every few months.

Simple calculations and analyses can be handled straightforwardly, albeit (in the current version) using a command line interface. Chapters 1 and 2 indicate the range of abilities that are immediately available to novice users. If simple methods prove inadequate, there can be recourse to the huge range of more advanced abilities that R offers. Adaptation of available abilities allows even greater flexibility.

The R community is widely drawn, from application area specialists as well as statistical specialists. It is a community that is sensitive to the potential for misuse of statistical techniques and suspicious of what might appear to be mindless use. Expect scepticism of the use of models that are not susceptible to some minimal form of data-based validation.

Because R is free, users have no right to expect attention, on the R-help list or elsewhere, to queries. Be grateful for whatever help is given.

Point and click interfaces are at an early stage of development.

While R is as reliable as any statistical software that is available, and exposed to higher standards of scrutiny than most other systems, there are traps that call for special care. Many of the model fitting routines are leading edge. There is a limited tradition of experience of the limitations and pitfalls of some of the newer abilities. Whatever the statistical system, and especially when there is some element of complication, check each step with care.

There is no substitute for experience and expert knowledge, even when the statistical analysis task may seem straightforward. Neither R nor any other statistical system will give the statistical expertise that is needed to use sophisticated abilities, or to know when naïve methods are not enough. Experience with the use of R is however, more than with most systems, likely to be an educational experience.

Hurrah for the R development team!

The Look and Feel of R

R is a functional language.[1] There is a language core that uses standard forms of algebraic notation, allowing the calculations such as **2+3**, or **3^11**. Beyond this, most computation is handled using functions. The action of quitting from an R session uses the function call **q()**.

It is often possible and desirable to operate on objects – vectors, arrays, lists and so on – as a whole. This largely avoids the need for explicit loops, leading to clearer code. Section 2.1.5 has an example.

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[1] The structure of an R program has similarities with programs that are written in C or in its successors C++ and Java. Important differences are that R has no header files, most declarations are implicit, there are no pointers, and vectors of text strings can be defined and manipulated directly. The implementation of R uses a computing model that is based on the Scheme dialect of the LISP language.

The Use of these Notes

The notes are designed so that users can run the examples in the script files (*ch1-2.R, ch3-4.R*, etc.) using the notes as commentary. Under Windows an alternative to typing the commands at the console is, as demonstrated in Section 1.2, to open a display file window and transfer the commands across from the that window.

Readers of these notes may find it helpful to have available for reference the document: "An Introduction to R", written by the R Development Core Team, supplied with R distributions and available from CRAN sites.

The R Project

The initial version of R was developed by Ross Ihaka and Robert Gentleman, both from the University of Auckland. Development of R is now overseen by a `core team' of about a dozen people, widely drawn from different institutions worldwide. The development model is similar to that of the Linux operating system.

Like Linux, R is an "open source" system. Source-code is available for inspection or for adaptation to other systems. In principle, if it is unclear what a routine does, one can check the source code. Exposing code to the critical scrutiny of highly expert users has proved an extremely effective way to identify bugs and other inadequacies, and to elicit ideas for enhancement. Reported bugs are commonly fixed in the next minor-minor release, which will usually appear within a matter of weeks.

Novice users will notice small but occasionally important differences between the S dialect that R implements and the commercial S-PLUS implementation of S. Those who write their own substantial functions and (more importantly) packages will find large differences. Packages that have been written for R offer abilities that are broadly comparable with, or in some instances go beyond, those in S-PLUS libraries. These give access to up-to-date methodology from leading statistical researchers. R has strong graphics abilities. The *lattice* graphics package gives many of the abilities that are in the S-PLUS trellis library.

R provides a language environment that is attractive for the development of new scientific computational tools. Computer-intensive components can, if computational efficiency demands, be handled by a call to a function that is written in the C language.

The R system may struggle to handle very large data sets. Depending on available computer memory, the processing of a data set containing one hundred thousand observations and perhaps twenty variables may press the limits of what R can easily handle.

Web Pages and Email Lists

For a variety of official and contributed documentation, for copies of various versions of R, and for other information, go to http://cran.r-project.org and find the nearest CRAN (Comprehensive R Archive Network) mirror site. Australian users may wish to go directly to http://mirror.aarnet.edu.au/pub/CRAN

There is no official support for R. The r-help email list gives access to an informal support network that can be highly effective. Details of the R-help list, and of other lists that serve the R community, are available from the web site for the R project at http://www.R-project.org/

Be sure to check the available documentation before posting to the email lists. Email archives can be searched for questions that may have been previously answered.

Datasets that relate to these notes

Copy down the R image file usingR.RData from http://wwwmaths.anu.edu.au/~johnm/r/dsets/
Section 1.6 explains how to access the datasets. Datasets are also available individually; go to
http://wwwmaths.anu.edu.au/~johnm/r/dsets/individual-dsets/

Jeff Wood (CMIS, CSIRO), Andreas Ruckstuhl (Technikum Winterthur Ingenieurschule, Switzerland) and John Braun (University of Western Ontario) gave me exemplary help in getting the earlier S-PLUS version of this document somewhere near shipshape form. John Braun gave valuable help with proofreading, and provided several of the data sets and a number of the exercises. I take full responsibility for the errors that remain. I am grateful, also, to various scientists named in the notes who have allowed me to use their data.

1. Starting Up

R must be installed on your system! If it is not, follow the installation instructions appropriate to the operating system. Installation is now especially straightforward for Windows users. Copy down the latest *SetupR.exe* from the relevant *base* directory on the nearest CRAN site, click on its icon to start installation, and follow instructions. Packages that do not come with the base distribution must be downloaded and installed separately.

It pays to have a separate working directory for each major project. For more details. see the README file that is included with the R distribution. Users of Microsoft Windows may wish to create a separate icon for each such working directory. First create the directory. Then right click|copy[2] to copy an existing R icon, it, right click|paste to place a copy on the desktop, right click|rename on the copy to rename it[3], and then finally go to right click|properties to set the **Start in** directory to be the working directory that was set up earlier.

1.1 Getting started under Windows

Click on the R icon. Or if there is more than one icon, choose the icon that corresponds to the project that is in hand. For this demonstration I will click on my *r-notes* icon.

In interactive use under Microsoft Windows there are several ways to input commands to R. Figures 1 and 2 demonstrate two of the possibilities. Either or both of the following may be used at the user's discretion.

This document mostly assumes that users will type commands into the *command window*, at the command line prompt. Figure 1 shows the command window as it appears when version 2.0.0 of R has just been started.

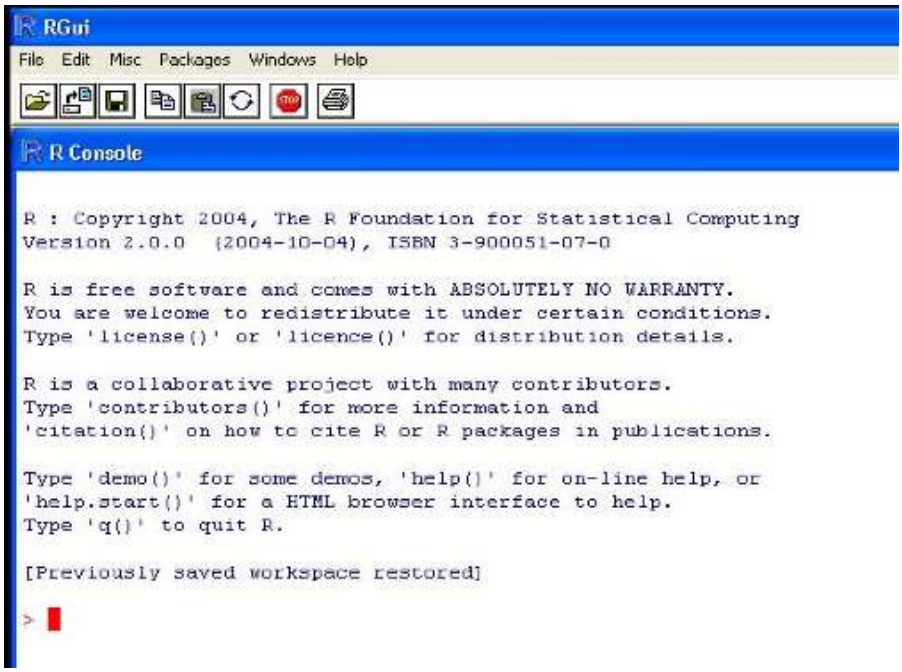


Fig. 1: The upper left portion of the R console (command line) window, for version 2.0.0 of R, immediately after starting up.

The command line prompt, i.e. the `>`, is an invitation to start typing in your commands. For example, type **`2+2`** and press the **Enter** key. Here is what appears on the screen:

```
> 2+2
[1] 4
>
```

Here the result is 4. The **`[1]`** says, a little strangely, "first requested element will follow". Here, there is just one element. The `>` indicates that R is ready for another command.

---

[2] This is a shortcut for "right click, then left click on the copy menu item".

[3] Enter the name of your choice into the name field. For ease of remembering, choose a name that closely matches the name of the workspace directory, perhaps the name itself.

For later reference, note that the exit or quit command is

```
> q()
```

Alternatives to the use of **q()** are to click on the **File** menu and then on **Exit**, or to click on the □ in the top right hand corner of the R window. There will be a message asking whether to save the workspace image. Clicking **Yes** (the safe option) will save all the objects that remain in the workspace – any that were there at the start of the session and any that have been added since.

1.2 Use of an Editor Script Window

The screen snapshot in Figure2 shows a *script file* window. This allows input to R of statements from a file that has been set up in advance, or that have been typed or copied into the window. To get a script file window, go to the **File** menu. If a new blank window is required, click on **New script**. To load an existing file, click on **Open script…**; you will be asked for the name of a file whose contents are then displayed in the window. In Figure 2 the file was **firstSteps.R**.

Highlight the commands that are intended for input to R. Click on the `Run line or selection' icon, which is the middle icon of the script file editor toolbar in Figs. 2 and 3, to send commands to R.

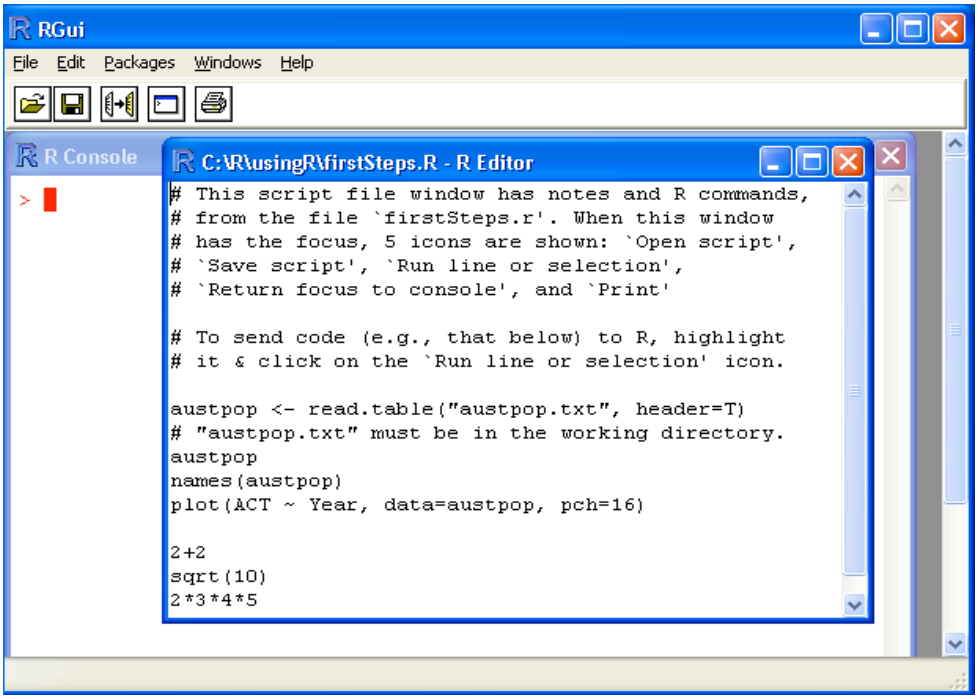


Fig. 2: The focus is on an R display file window, with the console window in the background.

Fig. 3: This shows the five icons that appear when the focus is on a script file window. The icons are, starting from the left:
Open script, Save script, Run line or selection, Return focus to console, and Print. The text in a script file window can be edited, or new text added. Display file windows, which have a somewhat similar set of icons but do not allow editing, are another possibility.

Under Unix, the standard form of input is the command line interface. Under both Microsoft Windows and Linux (or Unix), a further possibility is to run R from within the emacs editor[4]. Under Microsoft Windows, an attractive option is to use the R-WinEdt utility that is designed for use with the shareware WinEdt editor[5].

[4] This requires emacs, and ESS which runs under emacs. Both are free. Look under Software|Other on the CRAN page.

1.3 A Short R Session

We will read into R a file that holds population figures for Australian states and territories, and total population, at various times since 1917, then using this file to create a graph. The data in the file are:

```
Year  NSW Vic.  Qld   SA   WA Tas.  NT ACT Aust.
1917 1904 1409  683  440  306  193   5   3  4941
1927 2402 1727  873  565  392  211   4   8  6182
1937 2693 1853  993  589  457  233   6  11  6836
1947 2985 2055 1106  646  502  257  11  17  7579
1957 3625 2656 1413  873  688  326  21  38  9640
1967 4295 3274 1700 1110  879  375  62 103 11799
1977 5002 3837 2130 1286 1204  415 104 214 14192
1987 5617 4210 2675 1393 1496  449 158 265 16264
1997 6274 4605 3401 1480 1798  474 187 310 18532
```

The following reads in the data from the file **austpop.txt** on a disk in drive **a:**

```
> austpop <- read.table("a:/austpop.txt", header=T)
```

The **<-** is a left diamond bracket (**<**) followed by a minus sign (**-**). It means "is assigned to". Use of **header=T** causes R to use= the first line to get header information for the columns. If column headings are not included in the file, the argument can be omitted.

Now type in **austpop** at the command line prompt, displaying the object on the screen:

```
> austpop
  Year  NSW Vic.  Qld   SA   WA Tas.  NT ACT Aust.
1 1917 1904 1409  683  440  306  193   5   3  4941
2 1927 2402 1727  873  565  392  211   4   8  6182
. . .
```

The object **austpop** is, in R parlance, a *data frame*. Data frames that consist entirely of numeric data have the same form of rectangular layout as numeric matrices. Here is a plot of the ACT population between 1917 and 1997 (Figure 4).

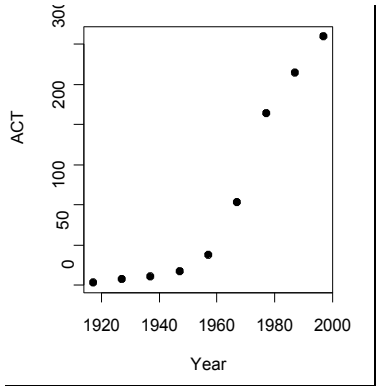


Figure 4: ACT population, at various times between 1917 and 1997.

We first of all remind ourselves of the column names:

```
> names(austpop)
 [1] "Year"  "NSW"   "Vic."  "Qld"   "SA"    "WA"    "Tas."  "NT"
 [9] "ACT"   "Aust."
```

---

[5] The R-WinEdt utility, which is free, is a "plugin" for WinEdt. For links to the relevant web pages, for WinEdt R-WinEdt and various other editors that work with R, look under Software|Other on the CRAN web page.

A simple way to get the plot is:

```
> plot(ACT ~ Year, data=austpop, pch=16)
```

The option **pch=16** sets the plotting character to solid black dots. Figure 4 shows the graph:This plot can be improved greatly. We can specify more informative axis labels, change size of the text and of the plotting symbol, and so on.

1.3.1 Entry of Data at the Command Line

A data frame is a rectangular array of columns of data. Here we will have two columns, and both columns will be numeric. The following data gives, for each amount by which an elastic band is stretched over the end of a ruler, the distance that the band moved when released:

stretch	46	54	48	50	44	42	52
distance	148	182	173	166	109	141	166

The function **data.frame()** can be used to input these (or other) data directly at the command line. We will give the data frame the name **elasticband**:

```
elasticband <- data.frame(stretch=c(46,54,48,50,44,42,52),
    distance=c(148,182,173,166,109,141,166))
```

1.3.2 Entry and/or editing of data in an editor window

To edit the file elasticband in a spreadsheet-like format, type

```
elasticband <- edit(elasticband)
```

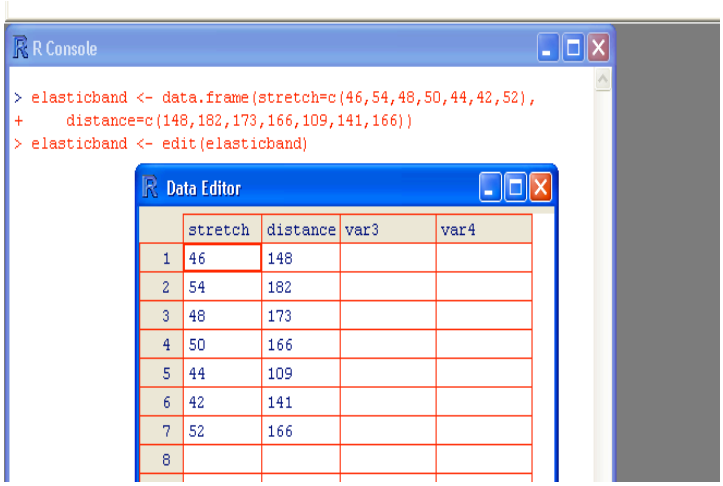


Figure 5: Editor window, showing the data frame **elasticband**.

1.3.3 Options for read.table()

The function **read.table()** takes, optionally various parameters additional to the file name that holds the data. Specify **header=TRUE** if there is an initial row of header names. The default is **header=FALSE**. In addition users can specify the separator character or characters. Command alternatives to the default use of a space are **sep=","** and **sep="\t"**. This last choice makes tabs separators. Similarly, users can control over the choice of missing value character or characters, which by default is **NA**. If the missing value character is a period (“.”), specify **na.strings="."**.

There are several variants of **read.table()** that differ only in having different default parameter settings. Note in particular **read.csv()**, which has settings that are suitable for comma delimited (csv) files that have been generated from Excel spreadsheets.

If **read.table()** detects that lines in the input file have different numbers of fields, data input will fail, with an error message that draws attention to the discrepancy. It is then often useful to use the function **count.fields()** to report the number of fields that were identified on each separate line of the file.

1.3.4 Options for plot() and allied functions

The function plot() and related functions accept parameters that control the plotting symbol, and the size and colour of the plotting symbol. Details will be given in section 3.3.

1.4 Further Notational Details

As noted earlier, the command line prompt is

```
>
```

R commands (expressions) are typed following this prompt[6].

There is also a continuation prompt, used when, following a carriage return, the command is still not complete. By default, the continuation prompt is

```
+
```

In these notes, we often continue commands over more than one line, but omit the + that will appear on the commands window if the command is typed in as we show it.

For the names of R objects or commands, case is significant. Thus **`Austpop`** is different from **`austpop`**. For file names however, the Microsoft Windows conventions apply, and case does not distinguish file names. On Unix systems letters that have a different case are treated as different.

Anything that follows a **`#`** on the command line is taken as comment and ignored by R.

Note: Recall that, in order to quit from the R session we had to type **`q()`**. This is because **`q`** is a function. Typing **`q`** on its own, without the parentheses, displays the text of the function on the screen. Try it!

1.5 On-line Help

To get a help window (under R for Windows) with a list of help topics, type:

```
> help()
```

In R for Windows, an alternative is to click on the help menu item, and then use key words to do a search. To get help on a specific R function, e.g. **`plot()`**, type in

```
> help(plot)
```

The two search functions **`help.search()`** and **`apropos()`** can be a huge help in finding what one wants. Examples of their use are:

```
> help.search("matrix")
(This lists all functions whose help pages have a title or alias in which the text string
“matrix” appears.)
> apropos(“matrix”)
```

(This lists all function names that include the text “matrix”.)

The function **help.start()** opens a browser window that gives access to the full range of documentation for syntax, packages and functions.

Experimentation often helps clarify the precise action of an R function.

1.6 The Loading or Attaching of Datasets

The recommended way to access datasets that are supplied for use with these notes is to attach the file **`usingR.RData`**., available from the author's web page. Place this file in the working directory and, from within the R session, type:

```
> attach("usingR.RData")
```

Files that are mentioned in these notes, and that are not supplied with R (e.g., from the *datasets* or *MASS* packages) should then be available without need for any further action.

---

[6] Multiple commands may appear on the one line, with the semicolon (**`;`**) as the separator.

Users can also load (use **load()**) or attach (use **attach()**) specific files. These have a similar effect, the difference being that with **attach()** datasets are loaded into memory only when required for use.

Distinguish between the attaching of image files and the attaching of data frames. The attaching of data frames will be discussed later in these notes.

1.7 Exercises

1. In the data frame **elasticband** from section 1.3.1, plot **distance** against **stretch**.

2. The following ten observations, taken during the years 1970-79, are on October snow cover for Eurasia. (Snow cover is in millions of square kilometers):

```
year snow.cover
1970 6.5
1971 12.0
1972 14.9
1973 10.0
1974 10.7
1975 7.9
1976 21.9
1977 12.5
1978 14.5
1979 9.2
```

i. Enter the data into R. [Section 1.3.1 showed one way to do this. To save keystrokes, enter the successive years as **1970:1979**]

ii. Plot **snow.cover** versus **year**.

iii Use the **hist()** command to plot a histogram of the snow cover values.

iv. Repeat ii and iii after taking logarithms of snow cover.

3. Input the following data, on damage that had occurred in space shuttle launches prior to the disastrous launch of Jan 28 1986. These are the data, for 6 launches out of 24, that were included in the pre-launch charts that were used in deciding whether to proceed with the launch. (Data for the 23 launches where information is available is in the data set **orings** that accompanies these notes.)

Temperature (F)	Erosion incidents	Blowby incidents	Total incidents
53	3	2	5
57	1	0	1
63	1	0	1
70	1	0	1
70	1	0	1
75	0	2	1

Enter these data into a data frame, with (for example) column names **temperature**, **erosion**, **blowby** and **total**. (Refer back to Section 1.3.1). Plot total incidents against temperature.

2. An Overview of R

2.1 The Uses of R

2.1.1 R may be used as a calculator.

R evaluates and prints out the result of any expression that one types in at the command line in the console window. Expressions are typed following the prompt (**>**) on the screen. The result, if any, appears on subsequent lines

```
> 2+2
[1] 4
> sqrt(10)
[1] 3.162278
> 2*3*4*5
[1] 120
> 1000*(1+0.075)^5 - 1000 # Interest on $1000, compounded annually
[1] 435.6293
>                         # at 7.5% p.a. for five years
> pi  # R knows about pi
[1] 3.141593
> 2*pi*6378 #Circumference of Earth at Equator, in km; radius is 6378 km
[1] 40074.16
> sin(c(30,60,90)*pi/180) # Convert angles to radians, then take sin()
[1] 0.5000000 0.8660254 1.0000000
```

2.1.2 R will provide numerical or graphical summaries of data

A special class of object, called a *data frame*, stores rectangular arrays in which the columns may be vectors of numbers or factors or text strings. Data frames are central to the way that all the more recent R routines process data. For now, think of data frames as matrices, where the rows are observations and the columns are variables.

As a first example, consider the data frame **`hills`** that accompanies these notes[7]. This has three columns (variables), with the names **`distance`**, **`climb`**, and **`time`**. Typing in **`summary(hills)`** gives summary information on these variables. There is one column for each variable**`,`** thus:

```
> load("hills.Rdata")   # Assumes hills.Rdata is in the working directory
> summary(hills)
     distance          climb           time
   Min.: 2.000      Min.: 300      Min.: 15.95
 1st Qu.: 4.500   1st Qu.: 725   1st Qu.: 28.00
  Median: 6.000    Median:1000    Median: 39.75
    Mean: 7.529      Mean:1815      Mean: 57.88
 3rd Qu.: 8.000   3rd Qu.:2200   3rd Qu.: 68.62
   Max.:28.000      Max.:7500      Max.:204.60
```

We may for example require information on ranges of variables. Thus the range of distances (first column) is from 2 miles to 28 miles, while the range of times (third column) is from 15.95 (minutes) to 204.6 minutes.

We will discuss graphical summaries in the next section.

---

[7] There is also a version in the Venables and Ripley MASS library.

2.1.3 R has extensive graphical abilities

The main R graphics function is **plot()**. In addition to **plot()** there are functions for adding points and lines to existing graphs, for placing text at specified positions, for specifying tick marks and tick labels, for labelling axes, and so on.

There are various other alternative helpful forms of graphical summary. A helpful graphical summary for the **hills** data frame is the scatterplot matrix, shown in Figure 6. For this, type:

```
> pairs(hills)
```

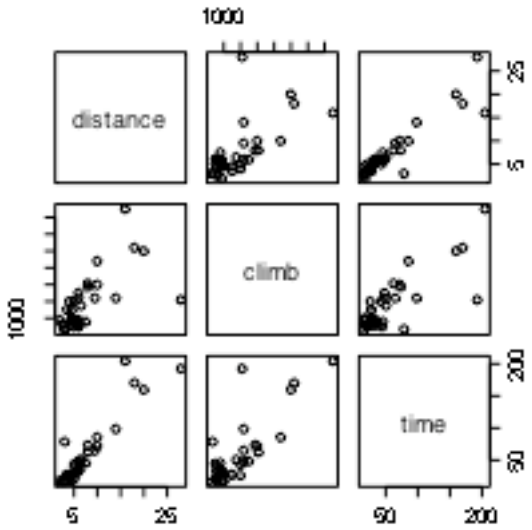


Figure 6: Scatterplot matrix for the Scottish hill race data

2.1.4 R will handle a variety of specific analyses

The examples that will be given are correlation and regression.

Correlation:

We calculate the correlation matrix for the **hills** data:

```
> options(digits=3)
> cor(hills)
         distance climb  time
distance    1.000 0.652 0.920
   climb    0.652 1.000 0.805
    time    0.920 0.805 1.000
```

Suppose we wish to calculate logarithms, and then calculate correlations. We can do all this in one step, thus:

```
> cor(log(hills))
         distance climb  time
distance     1.00 0.700 0.890
   climb     0.70 1.000 0.724
    time     0.89 0.724 1.000
```

Unfortunately R was not clever enough to relabel distance as log(distance), climb as log(climb), and time as log(time). Notice that the correlations between time and distance, and between time and climb, have reduced. Why has this happened?

Straight Line Regression:

Here is a straight line regression calculation. The data are stored in the data frame **elasticband** that accompanies these notes. The variable names are the names of columns in that data frame. The formula that is

supplied to the **lm()** command asks for the regression of distance travelled by the elastic band (**distance**) on the amount by which it is stretched (**stretch**).

```
> plot(distance ~ stretch,data=elasticband, pch=16)
> elastic.lm <- lm(distance~stretch,data=elasticband)
> lm(distance ~stretch,data=elasticband)

Call:
lm(formula = distance ~ stretch, data = elasticband)

Coefficients:
(Intercept)      stretch
    -63.571        4.554
```

More complete information is available by typing

```
> summary(lm(distance~stretch,data=elasticband))
```

Try it!

2.1.5 R is an Interactive Programming Language

We calculate the Fahrenheit temperatures that correspond to Celsius temperatures 25, 26, …, 30:

```
> celsius <- 25:30
> fahrenheit <- 9/5*celsius+32
> conversion <- data.frame(Celsius=celsius, Fahrenheit=fahrenheit)
> print(conversion)
  Celsius Fahrenheit
1      25       77.0
2      26       78.8
3      27       80.6
4      28       82.4
5      29       84.2
6      30       86.0
```

2.2 R Objects

All R entities, including functions and data structures, exist as objects. They can all be operated on as data. Type in **ls()** to see the names of all objects in your workspace. An alternative to **ls()** is **objects()**. In both cases there is provision to specify a particular pattern, e.g. starting with the letter `p'[8].

Typing the name of an object causes the printing of its contents. Try typing **q**, **mean**, etc.

In a long session, it makes sense to save the contents of the working directory from time to time. It is also possible to save individual objects, or collections of objects into a named image file. Some possibilities are:

```
save.image()                  # Save contents of workspace, into the file .RData
save.image(file="archive.RData")      # Save into the file archive.RData
save(celsius, fahrenheit, file="tempscales.RData")
```

Image files, from the working directory or (with the path specified) from another directory, can be attached, thus making objects in the file available on request. For example

```
attach("tempscales.RData")
ls(pos=2)   # Check the contents of the file that has been attached
```

The parameter **pos** gives the position on the search list. (The search list is discussed later in this chapter, in Section 2.9.)

---

[8] Type in **help(ls)** and **help(grep)** to get details. The pattern matching conventions are those used for **grep()**, which is modelled on the Unix grep command.

Important: On quitting, R offers the option of saving the workspace image, by default in the file **.RData** in the working directory. This allows the retention, for use in the next session in the same workspace, any objects that were created in the current session. Careful housekeeping may be needed to distinguish between objects that are to be kept and objects that will not be used again. Before typing **q()** to quit, use **rm()** to remove objects that are no longer required. Saving the workspace image will then save everything remains. The workspace image will be automatically loaded upon starting another session in that directory.

*[9]2.3 Looping

A simple example of a **for** loop is[10]

```
for (i in 1:10) print(i)
```

Here is another example of a **for** loop, to do in a complicated way what we did very simply in section 2.1.5:

```
> # Celsius to Fahrenheit
> for (celsius in 25:30)
+     print(c(celsius, 9/5*celsius + 32))
[1] 25 77
[1] 26.0 78.8
[1] 27.0 80.6
[1] 28.0 82.4
[1] 29.0 84.2
[1] 30 86
```

2.3.1 More on looping

Here is a long-winded way to sum the three numbers 31, 51 and 91:

```
> answer <- 0
> for (j in c(31,51,91)){answer <- j+answer}
> answer
[1] 173
```

The calculation iteratively builds up the object answer, using the successive values of **j** listed in the vector (31,51,91). i.e. Initially, **j**=31, and **answer** is assigned the value 31 + 0 = 31. Then **j**=51, and **answer** is assigned the value 51 + 31 = 82. Finally, **j**=91, and answer is assigned the value 91 + 81 = 173. Then the procedure ends, and the contents of **answer** can be examined by typing in answer and pressing the **Enter** key.

There is a more straightforward way to do this calculation:

```
> sum(c(31,51,91))
[1] 173
```

Skilled R users have limited recourse to loops. There are often, as in this and earlier examples, better alternatives.

2.4 Vectors

Examples of vectors are

```
c(2,3,5,2,7,1)
3:10   # The numbers 3, 4, .., 10
c(T,F,F,F,T,T,F)
c("Canberra","Sydney","Newcastle","Darwin")
```

---

[9] Asterisks (*) identify sections that are more technical and might be omitted at a first reading

[10] Other looping constructs are:

repeat <expression> ## break must appear somewhere inside the loop

while (x>0) <expression>

Here <expression> is an R statement, or a sequence of statements that are enclosed within braces

Vectors may have mode logical, numeric or character[11]. The first two vectors above are numeric, the third is logical (i.e. a vector with elements of mode logical), and the fourth is a string vector (i.e. a vector with elements of mode character).

The missing value symbol, which is **NA**, can be included as an element of a vector.

2.4.1 Joining (concatenating) vectors

The **c** in **c(2, 3, 5, 7, 1)** above is an acronym for "concatenate", i.e. the meaning is: "Join these numbers together in to a vector. Existing vectors may be included among the elements that are to be concatenated. In the following we form vectors **x** and **y**, which we then concatenate to form a vector **z**:

```
> x <- c(2,3,5,2,7,1)
> x
[1] 2 3 5 2 7 1
> y <- c(10,15,12)
> y
[1] 10 15 12

> z <- c(x, y)
> z
[1]  2  3  5  2  7  1 10 15 12
```

The concatenate function **c()** may also be used to join lists.

2.4.2 Subsets of Vectors

There are two common ways to extract subsets of vectors[12].

1. Specify the numbers of the elements that are to be extracted, e.g.

```
> x <- c(3,11,8,15,12)  # Assign to x the values 3, 11, 8, 15, 12
> x[c(2,4)]   # Extract elements (rows) 2 and 4
[1] 11 15
```

One can use negative numbers to omit elements:

```
> x <- c(3,11,8,15,12)
> x[-c(2,3)]
[1]  3 15 12
```

2. Specify a vector of logical values. The elements that are extracted are those for which the logical value is **T**. Thus suppose we want to extract values of **x** that are greater than 10.

```
> x>10  # This generates a vector of logical (T or F)
[1] F T F T T
> x[x>10]
[1] 11 15 12
```

Arithmetic relations that may be used in the extraction of subsets of vectors are **<**, **<=**, **>**, >=, **==**, and **!=**. The first four compare magnitudes, **==** tests for equality, and **!=** tests for inequality.

---

[11] It will, later in these notes, be important to know the "class" of such objects. This determines how the method used by such generic functions as **print()**, **plot()** and **summary()**. Use the function **class()** to determine the class of an object.

[12] A third more subtle method is available when vectors have named elements. One can then use a vector of names to extract the elements, thus:

```
> c(Andreas=178, John=185, Jeff=183)[c("John","Jeff")]
 John Jeff
  185  183
```

2.4.3 The Use of NA in Vector Subscripts

Note that any arithmetic operation or relation that involves **NA** generates an **NA**. Set

```
y <- c(1, NA, 3, 0, NA)
```

Be warned that **y[y==NA] <- 0** leaves **y** unchanged. The reason is that all elements of **y==NA** evaluate to **NA**. This does not select an element of **y**, and there is no assignment.

To replace all **NA**s by 0, use

```
y[is.na(y)] <- 0
```

2.4.4 Factors

A factor is a special type of vector, stored internally as a numeric vector with values 1, 2, 3, *k*. The value *k* is the number of levels. An attributes table gives the 'level' for each integer value[13]. Factors provide a compact way to store character strings. They are crucial in the representation of categorical effects in model and graphics formulae. The class attribute of a factor has, not surprisingly, the value "factor".

Consider a survey that has data on 691 females and 692 males. If the first 691 are females and the next 692 males, we can create a vector of strings that that holds the values thus:

```
gender <- c(rep("female",691), rep("male",692))
```

(The usage is that **rep("female", 691)** creates 691 copies of the character string "female", and similarly for the creation of 692 copies of "male".)

We can change the vector to a factor, by entering:

```
gender <- factor(gender)
```

Internally the factor **gender** is stored as 691 1's, followed by 692 2's. It has stored with it the table:

1	female
2	male

Once stored as a factor, the space required for storage is reduced.

In most cases where the context seems to demand a character string, the 1 is translated into "female" and the 2 into "male". The values "female" and "male" are the *levels* of the factor. By default, the levels are in alphanumeric order, so that "female" precedes "male". Hence:

```
> levels(gender)  # Assumes gender is a factor, created as above
[1] "female" "male"
```

The order of the levels in a factor determines the order in which the levels appear in graphs that use this information, and in tables. To cause "male" to come before "female", use

```
gender <- relevel(gender, ref="male")
```

An alternative is

```
gender <- factor(gender, levels=c("male", "female"))
```

This last syntax is available both when the factor is first created, or later when one wishes to change the order of levels in an existing factor. Incorrect spelling of the level names will generate an error message. Try

```
gender <- factor(c(rep("female",691), rep("male",692)))
table(gender)
gender <- factor(gender, levels=c("male", "female"))
table(gender)
gender <- factor(gender, levels=c("Male", "female"))
                  # Erroneous - "male" rows now hold missing values
table(gender)
rm(gender)          # Remove gender
```

---

[13] The attributes() function makes it possible to inspect attributes. For example

```
attributes(factor(1:3))
```

The function **levels()** gives a better way to inspect factor levels.

2.5 Data Frames

Data frames are fundamental to the use of the R modelling and graphics functions. A data frame is a generalisation of a matrix, in which different columns may have different modes. All elements of any column must however have the same mode, i.e. all numeric or all factor, or all character.

Among the data sets that are supplied to accompany these notes is one called **Cars93.summary**, created from information in the **Cars93** data set in the Venables and Ripley *MASS* package. Here it is:

```
> Cars93.summary
        Min.passengers Max.passengers No.of.cars abbrev
Compact              4              6         16      C
Large                6              6         11      L
Midsize              4              6         22      M
Small                4              5         21     Sm
Sporty               2              4         14     Sp
Van                  7              8          9      V
```

The data frame has row labels (access with **row.names(Cars93.summary)**) Compact, Large, . . . The column names (access with **names(Cars93.summary)**) are **Min.passengers** (i.e. the minimum number of passengers for cars in this category), **Max.passengers, No.of.cars**., and **abbrev**. The first three columns have mode numeric, and the fourth has mode character. Columns can be vectors of any mode. The column **abbrev** could equally well be stored as a factor.

Any of the following[14] will pick out the fourth column of the data frame **Cars93.summary**, then storing it in the vector **type**.

```
type <- Cars93.summary$abbrev
type <- Cars93.summary[,4]
type <- Cars93.summary[,"abbrev"]
type <- Cars93.summary[[4]]       # Take the object that is stored
# in the fourth list element.
```

2.5.1 Data frames as lists

A data frame is a list[15] of column vectors, all of equal length. Just as with any other list, subscripting extracts a list. Thus **Cars93.summary[4]** is a data frame with a single column, which is the fourth column vector of **Cars93.summary**. As noted above, use **Cars93.summary[[4]]** or **Cars93.summary[,4]** to extract the column vector.

The use of matrix-like subscripting, e.g. **Cars93.summary[,4]** or **Cars93.summary[1, 4]**, takes advantage of the rectangular structure of data frames.

2.5.2 Inclusion of character string vectors in data frames

When data are input using **read.table()**, or when the **data.frame()** function is used to create data frames, vectors of character strings are by default turned into factors. The parameter setting **as.is=T, available both with read.table() and with data.frame(),** will if needed ensure that character strings are input without such conversion**.**

2.5.3 Built-in data sets

We will often use data sets that accompany one of the R packages, usually stored as data frames. One such data frame, in the *datasets* package, is **trees**, which gives girth, height and volume for 31 Black Cherry Trees.

```
> data(trees)      # Load data set (not needed for versions of R >= 2.0.0)
```

Here is summary information on this data frame

```
> summary(trees)
```

---

[14] Also legal is **Cars93.summary[2]**. This gives a data frame with the single column **Type**.

[15] In general forms of list, elements that are of arbitrary type. They may be any mixture of scalars, vectors, functions, etc.

```
     Girth           Height       Volume
 Min.   : 8.30   Min.   :63   Min.   :10.20
 1st Qu.:11.05   1st Qu.:72   1st Qu.:19.40
 Median :12.90   Median :76   Median :24.20
 Mean   :13.25   Mean   :76   Mean   :30.17
 3rd Qu.:15.25   3rd Qu.:80   3rd Qu.:37.30
 Max.   :20.60   Max.   :87   Max.   :77.00
```

Type **data()** to get a list of built-in data sets in the packages that have been loaded[16].

2.6 Common Useful Functions

```
print()     # Prints a single R object
cat()       # Prints multiple objects, one after the other
length()    # Number of elements in a vector or of a list
mean()
median()
range()
unique()    # Gives the vector of distinct values
diff()      # Replace a vector by the vector of first differences
              # N. B. diff(x) has one less element than x
sort()      # Sort elements into order, but omitting NAs
order()     # x[order(x)] orders elements of x, with NAs last
cumsum()
cumprod()
rev()       # reverse the order of vector elements
```

The functions **mean()**, **median()**, **range(),** and a number of other functions, take the argument **na.rm=T;** i.e. remove NAs, then proceed with the calculation.

By default, **sort()** omits any NAs. The function **order()** places NAs last. Hence:

```
> x <- c(1, 20,  2, NA, 22)
> order(x)
[1] 1 3 2 5 4
> x[order(x)]
[1]  1  2 20 22 NA
> sort(x)
[1]  1  2 20 22
```

2.6.1 Applying a function to all columns of a data frame

The function **sapply()** takes as arguments the the data frame, and the function that is to be applied. The following applies the function **is.factor()** to all columns of the supplied data frame **rainforest**[17].

```
> sapply(rainforest, is.factor)
    dbh    wood    bark    root  rootsk  branch species
  FALSE   FALSE   FALSE   FALSE   FALSE   FALSE    TRUE
> sapply(rainforest[,-7], range)   # The final column (7) is a factor
     dbh wood bark root rootsk branch
[1,]   4   NA   NA   NA     NA     NA
[2,]  56   NA   NA   NA     NA     NA
```

---

[16] The list include all packages that are in the current environment.

[17] Source: Ash, J. and Southern, W. 1982: Forest biomass at Butler's Creek, Edith & Joy London Foundation, New South Wales, Unpublished manuscript. See also Ash, J. and Helman, C. 1990: Floristics and vegetation biomass of a forest catchment, Kioloa, south coastal N.S.W. Cunninghamia, 2(2): 167-182.

The functions **mean()** and **range()**, and a number of other functions, take the parameter **na.rm**. For example

```
> range(rainforest$branch, na.rm=T)  # Omit NAs, then determine the range
[1]   4 120
```

One can specify **na.rm=T** as a third argument to the function **sapply**. This argument is then automatically passed to the function that is specified in the second argument position. For example:

```
> sapply(rainforest[,-7], range, na.rm=T)
     dbh wood bark root rootsk branch
[1,]   4    3    8    2    0.3      4
[2,]  56 1530  105  135   24.0    120
```

Chapter 8 has further details on the use of **sapply()**. There is an example that shows how to use it to count the number of missing values in each column of data.

2.7 Making Tables

table() makes a table of counts. Specify one vector of values (often a factor) for each table margin that is required. For example:

```
> library(lattice)  # The data frame barley accompanies lattice
> table(barley$year, barley$site)

     Grand Rapids Duluth University Farm Morris Crookston Waseca
1932 10           10     10              10     10        10
1931 10           10     10              10     10        10
```

WARNING: **NA**s are by default ignored. The action needed to get **NA**s tabulated under a separate **NA** category depends, annoyingly, on whether or not the vector is a factor. If the vector is not a factor, specify **exclude=NULL**. If the vector is a factor then it is necessary to generate a new factor that includes **"NA"** as a level. Specify **x <- factor(x,exclude=NULL)**

```
> x_c(1,5,NA,8)
> x <- factor(x)
> x
[1] 1  5  NA 8
Levels:  1 5 8
> factor(x,exclude=NULL)
[1] 1  5  NA 8
Levels:  1 5 8 NA
```

2.7.1 Numbers of NAs in subgroups of the data

The following gives information on the number of NAs in subgroups of the data:

```
> table(rainforest$species, !is.na(rainforest$branch))

                FALSE TRUE
Acacia mabellae     6   10
C. fraseri          0   12
Acmena smithii     15   11
B. myrtifolia       1   10
```

Thus for Acacia mabellae there are 6 NAs for the variable branch (i.e. number of branches over 2cm in diameter), out of a total of 16 data values.

2.8 The Search List

R has a search list where it looks for objects. This can be changed in the course of a session. To get a full list of these directories, called *databases*, type:

```
> search()
[1] ".GlobalEnv"        "package:methods"   "package:stats"
```

```
[4] "package:graphics"  "package:grDevices" "package:utils"
[7] "package:datasets"  "Autoloads"         "package:base"
```

Notice that the loading of a new package extends the search list.

```
> library(MASS)
> search()
 [1] ".GlobalEnv"        "package:MASS"      "package:methods"
 [4] "package:stats"     "package:graphics"  "package:grDevices"
 [7] "package:utils"     "package:datasets"  "Autoloads"
[10] "package:base"
```

Use of **attach()** likewise extends the search list. This function can be used to attach data frames or lists (use the name, without quotes) or image (**.RData**) files (the file name is placed in quotes).

The following demonstrates the attaching of the data frame **primates**:

```
> names(primates)
[1] "Bodywt"  "Brainwt"
> Bodywt
Error: Object "Bodywt" not found
> attach(primates)     # R will now know where to find Bodywt
> Bodywt
[1]  10.0 207.0  62.0   6.8  52.2
```

Once the data frame **primates** has been attached, its columns can be accessed by giving their names, without further reference to the name of the data frame. In technical terms, the data frame becomes a *database*, which is searched as required for objects that the user may specify.

2.9 Functions in R

We give two simple examples of R functions.

2.9.1 An Approximate Miles to Kilometers Conversion

```
miles.to.km <- function(miles)miles*8/5
```

The return value is the value of the final (and in this instance only) expression that appears in the function body[18]. Use the function thus

```
> miles.to.km(175)  # Approximate distance to Sydney, in miles
[1] 280
```

The function will do the conversion for several distances all at once. To convert a vector of the three distances 100, 200 and 300 miles to distances in kilometers, specify:

```
> miles.to.km(c(100,200,300))
[1] 160 320 480
```

2.9.2 A Plotting function

The data set **florida** has the votes in the 2000 election for the various US Presidential candidates, county by county in the state of Florida. The following plots the vote for Buchanan against the vote for Bush.

```
attach(florida)
plot(BUSH, BUCHANAN, xlab="Bush", ylab="Buchanan")
detach(florida)   # In S-PLUS, specify detach("florida")
```

Here is a function that makes it possible to plot the figures for any pair of candidates.

```
plot.florida <- function(xvar="BUSH", yvar="BUCHANAN"){
    x <- florida[,xvar]
    y <- florida[,yvar]
```

[18] Alternatively a return value may be given using an explicit **return()** statement. This is however an uncommon construction

```
    plot(x, y, xlab=xvar,ylab=yvar)
    mtext(side=3, line=1.75,
     "Votes in Florida, by county, in \nthe 2000 US Presidential election")
}
```

Note that the function body is enclosed in braces ({ }).

Figure 7 shows the graph produced by **`plot.florida()`**, i.e. parameter settings are left at their defaults.

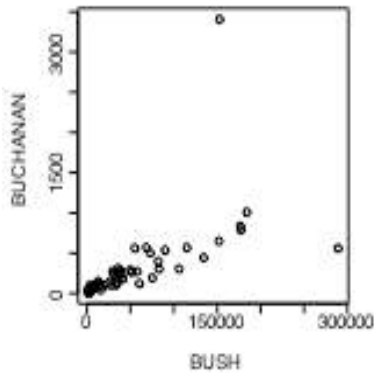


Figure 7: Election night count of votes received, by county, in the US 2000 Presidential election.

As well as **`plot.florida()`**, the function allows, e.g.

```
plot.florida(yvar="NADER")  # yvar="NADER" over-rides the default
plot.florida(xvar="GORE", yvar="NADER")
```

2.10 More Detailed Information

Chapters 7 and 8 have a more detailed coverage of the topics in this chapter. It may pay, at this point, to glance through chapters 7 and 8. Remember also to use R's help pages and functions.

Topics from chapter 7, additional to those covered above, that may be important for relatively elementary uses of R include:

The entry of patterned data (7.1.3)

The handling of missing values in subscripts when vectors are assigned (7.2)

Unexpected consequences (e.g. conversion of columns of numeric data into factors) from errors in data (7.4.1).

2.11 Exercises

1. For each of the following code sequences, predict the result. Then do the computation:

a)
```
answer <- 0
for (j in 3:5){ answer <- j+answer }
```

b)
```
answer<- 10
for (j in 3:5){ answer <- j+answer }
```

c)
```
answer <- 10
for (j in 3:5){ answer <- j*answer }
```

2. Look up the help for the function **`prod()`**, and use **`prod()`** to do the calculation in 1(c) above. Alternatively, how would you expect **`prod()`** to work? Try it!

3. Add up all the numbers from 1 to 100 in two different ways: using **`for`** and using **`sum`**. Now apply the function to the sequence 1:100. What is its action?

4. Multiply all the numbers from 1 to 50 in two different ways: using **`for`** and using **`prod`**.

5. The volume of a sphere of radius r is given by $4\pi r^3/3$. For spheres having radii 3, 4, 5, …, 20 find the corresponding volumes and print the results out in a table. Use the technique of section 2.1.5 to construct a data frame with columns **`radius`** and **`volume`**.

6. Use **`sapply()`** to apply the function **`is.factor`** to each column of the supplied data frame **`tinting`**. For each of the columns that are identified as factors, determine the levels. Which columns are ordered factors? [Use **`is.ordered()`**].

3. Plotting

The functions **plot()**, **points()**, **lines()**, **text()**, **mtext(), axis(), identify()** etc. form a suite that plots points, lines and text. To see some of the possibilities that R offers, enter

```
demo(graphics)
```

Press the Enter key to move to each new graph.

3.1 plot () and allied functions

The following both plot **y** against **x**:

```
plot(y ~ x)  # Use a formula to specify the graph
plot(x, y)   #
```

Obviously **x** and **y** must be the same length.

Try

```
plot((0:20)*pi/10, sin((0:20)*pi/10))
plot((1:30)*0.92, sin((1:30)*0.92))
```

Comment on the appearance that these graphs present. Is it obvious that these points lie on a sine curve? How can one make it obvious? (Place the cursor over the lower border of the graph sheet, until it becomes a double-sided arror. Drag the border in towards the top border, making the graph sheet short and wide.)

Here are two further examples.

```
attach(elasticband)   # R now knows where to find distance & stretch
plot(distance ~ stretch)
plot(ACT ~ Year, data=austpop, type="l")
plot(ACT ~ Year, data=austpop, type="b")
```

The **points()** function adds points to a plot. The **lines()** function adds lines to a plot[19]. The **text()** function adds text at specified locations. The **mtext()** function places text in one of the margins. The **axis()** function gives fine control over axis ticks and labels.

Here is a further possibility

```
attach(austpop)
plot(spline(Year, ACT), type="l")  # Fit smooth curve through points
detach(austpop)   # In S-PLUS, specify detach("austpop")
```

3.1.1 Newer plot methods

Above, I described the default plot method. The plot function is a generic function that has special methods for "plotting" various different classes of object. For example, plotting a data frame gives, for each numeric variable, a normal probability plot. Plotting the **lm** object that is created by the use of the **lm()** modelling function gives diagnostic and other information that is intended to help in the interpretation of regression results.

Try

```
plot(hills)  # Has the same effect as pairs(hills)
```

3.2 Fine control – Parameter settings

The default settings of parameters, such as character size, are often adequate. When it is necessary to change parameter settings for a subsequent plot, the **par()** function does this. For example,

```
par(cex=1.25, mex=1.25)   # character (cex) & margin (mex) expansion
```

---

[19] Actually these functions differ only in the default setting for the parameter **type.** The default setting for **points()** is **type = "p"**, and for **lines()** is **type = "l"**. **Explicitly** setting **type = "p"** causes either function to plot points, **type = "l" gives lines**.

increases the text and plot symbol size 25% above the default. The addition of **mex=1.25** makes room in the margin to accommodate the increased text size.

On the first use of **par()** to make changes to the current device, it is often useful to store existing settings, so that they can be restored later. For this, specify

```
oldpar <- par(cex=1.25, mex=1.25)
```

This stores the existing settings in **oldpar**, then changes parameters (here **cex** and **mex**) as requested. To restore the original parameter settings at some later time, enter **par(oldpar)**. Here is an example:

```
attach(elasticband)
oldpar <- par(cex=1.5, mex=1.5)
plot(distance ~ stretch)
par(oldpar)         # Restores the earlier settings
detach(elasticband)
```

Inside a function specify, e.g.

```
oldpar <- par(cex=1.25, mex=1.25)
on.exit(par(oldpar))
```

Type in **help(par)** to get details of all the parameter settings that are available with **par()**.

3.2.1 Multiple plots on the one page

The parameter **mfrow** can be used to configure the graphics sheet so that subsequent plots appear row by row, one after the other in a rectangular layout, on the one page. For a column by column layout, use **mfcol instead**. In the example below we present four different transformations of the primates data, in a two by two layout:

```
par(mfrow=c(2,2), pch=16)
data(Animals)     # Needed if Animals (MASS package) is not already loaded
attach(Animals)
plot(body, brain)
plot(sqrt(body), sqrt(brain))
plot((body)^0.1, (brain)^0.1)
plot(log(body),log(brain))
detach(Animals)
par(mfrow=c(1,1), pch=1)      # Restore to 1 figure per page
```

3.2.2 The shape of the graph sheet

Often it is desirable to exercise control over the shape of the graph page, e.g. so that the individual plots are rectangular rather than square. The R for Windows functions **win.graph()** or **x11()** that set up the Windows screen take the parameters **width** (in inches), **height** (in inches) and **pointsize** (in 1/72 of an inch). The setting of **pointsize** (default =12) determines character heights. It is the relative sizes of these parameters that matter for screen display or for incorporation into Word and similar programs. Graphs can be enlarged or shrunk by pointing at one corner, holding down the left mouse button, and pulling.

3.3 Adding points, lines and text

Here is a simple example that shows how to use the function **text()** to add text labels to the points on a plot.

```
> primates
               Bodywt Brainwt
 Potar monkey    10.0     115
      Gorilla   207.0     406
        Human    62.0    1320
Rhesus monkey     6.8     179
        Chimp    52.2     440
```

Observe that the row names store labels for each row[20].

```
attach(primates)  # Needed if primates is not already attached.
plot(Bodywt, Brainwt)
text(x=Bodywt, y=Brainwt, labels=row.names(primates), adj=0)
   # adj=0 implies left adjusted text
```

Figure 8A shows the result.

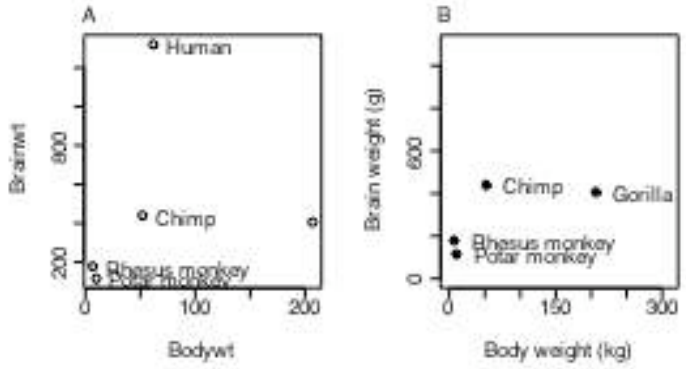


Figure 8: Plot of the primates data, with labels on points. Figure 8B is an improved version of Figure 8A.

Figure 8A would be adequate for identifying points, but is not a presentation quality graph. We now show how to improve it.

Figure 8B uses the **xlab** (x-axis) and **ylab** (y-axis) parameters to specify meaningful axis titles. It uses the parameter setting **pos=4** to move the labelling to the right of the points. It sets **pch=16** to make the plot character a heavy black dot. This helps make the points stand out against the labelling.

Here is the R code for Figure 8B:

```
plot(x=Bodywt, y=Brainwt, pch=16,
       xlab="Body weight (kg)", ylab="Brain weight (g)",
       xlim=c(0,310), ylim=c(0,1100))
# Specify xlim so that there is room for the labels
text(x=Bodywt y=Brainwt, labels=row.names(primates), pos=4)
detach(primates)
```

To place the text to the left of the points, specify

```
text(x=Bodywt, y=Brainwt, labels=row.names(primates), pos=2)
```

3.3.1 Size, colour and choice of plotting symbol

For **plot()** and **points()** the parameter **cex** ("character expansion") controls the size, while **col** ("colour") controls the colour of the plotting symbol. The parameter **pch** controls the choice of plotting symbol.

The parameters **cex** and **col** may be used in a similar way with **text()**. Try

```
plot(1, 1, xlim=c(1, 7.5), ylim=c(0,5), type="n")   # Do not plot points
points(1:7, rep(4.5, 7), cex=1:7, col=1:7, pch=0:6)
text(1:7,rep(3.5, 7), labels=paste(0:6), cex=1:7, col=1:7)
```

The following, added to the plot that results from the above three statements, demonstrates other choices of pch.

```
points(1:7,rep(2,7), pch=(0:6)+7)         # Plot symbols 7 to 13
```

---

[20] Row names can be created in several different ways. They can be assigned directly, e.g.

```
row.names(primates) <- c("Potar monkey","Gorilla","Human", "Rhesus monkey","Chimp")
```

When using **read.table()** to input data, the parameter **row.names** is available to specify, by number or name, a column that holds the row names.

```
text((1:7)+0.25, rep(2,7), paste((0:6)+7))  # Label with symbol number
points(1:7,rep(1,7), pch=(0:6)+14)        # Plot symbols 14 to 20
text((1:7)+0.25, rep(1,7), paste((0:6)+14)) # Labels with symbol number
```

Here (Figure 9) is the plot:

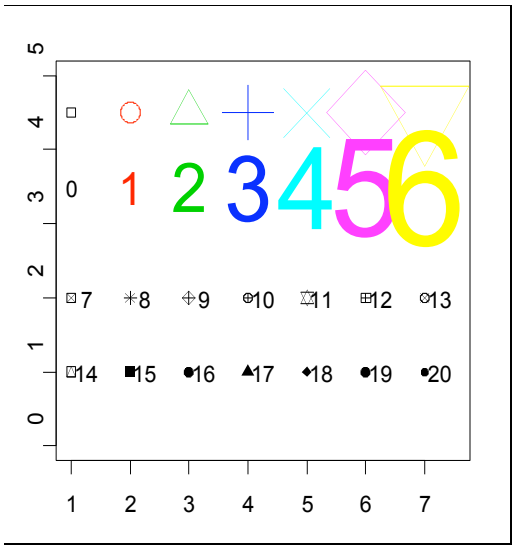


Figure 9: Different plot symbols, colours and sizes

A variety of color palettes are available. Here is a function that displays some of the possibilities:

```
view.colours <- function(){
     plot(1, 1, xlim=c(0,14), ylim=c(0,3), type="n", axes=F,
          xlab="",ylab="")
     text(1:6, rep(2.5,6), paste(1:6), col=palette()[1:6], cex=2.5)
     text(10, 2.5, "Default palette", adj=0)
     rainchars <- c("R","O","Y","G","B","I","V")
     text(1:7, rep(1.5,7), rainchars, col=rainbow(7), cex=2.5)
     text(10, 1.5, "rainbow(7)", adj=0)
     cmtxt <- substring("cm.colors", 1:9,1:9)
        # Split "cm.colors" into its 9 characters
     text(1:9, rep(0.5,9), cmtxt, col=cm.colors(9), cex=3)
     text(10, 0.5, "cm.colors(9)", adj=0)
}
```

To run the function, enter

```
view.colours()
```

3.3.2 Adding Text in the Margin

`mtext(side, line, text, ..)` adds text in the margin of the current plot. The sides are numbered 1(x-axis), 2(y-axis), 3(top) and 4.

3.4 Identification and Location on the Figure Region

Two functions are available for this purpose. Draw the graph first, then call one or other of these functions.

identify() labels points. One positions the cursor near the point that is to be identified, and clicks the left mouse button.

locator() prints out the co-ordinates of points. One positions the cursor at the location for which coordinates are required, and clicks the left mouse button.

A click with the right mouse button signifies that the identification or location task is complete, unless the setting of the parameter **n** is reached first. For **identify()** the default setting of **n** is the number of data points, while for **locator()** the default setting is **n** = 500.

3.4.1 identify()

This function requires specification of a vector **x**, a vector **y**, and a vector of text strings that are available for use a labels. The data set **florida** has the votes for the various Presidential candidates, county by county in the state of Florida. We plot the vote for Buchanan against the vote for Bush, then invoking **identify()** so that we can label selected points on the plot.

```
attach(florida)
plot(BUSH, BUCHANAN, xlab="Bush", ylab="Buchanan")
identify(BUSH, BUCHANAN, County)
detach(florida)
```

Click to the left or right, and slightly above or below a point, depending on the preferred positioning of the label. When labelling is terminated (click with the right mouse button), the row numbers of the observations that have been labelled are printed on the screen, in order.

3.4.2 locator()

Left click at the locations whose coordinates are required

```
attach(florida)  # if not already attached
plot(BUSH, BUCHANAN, xlab="Bush", ylab="Buchanan")
locator()
detach(florida)
```

The function can be used to mark new points (specify **type="p"**) or lines (specify **type="l"**) or both points and lines (specify **type="b"**).

3.5 Plots that show the distribution of data values

We discuss histograms, density plots, boxplots and normal probability plots.

3.5.1 Histograms

The shapes of histograms depend on the placement of the breaks, as Figure 10 illustrates:

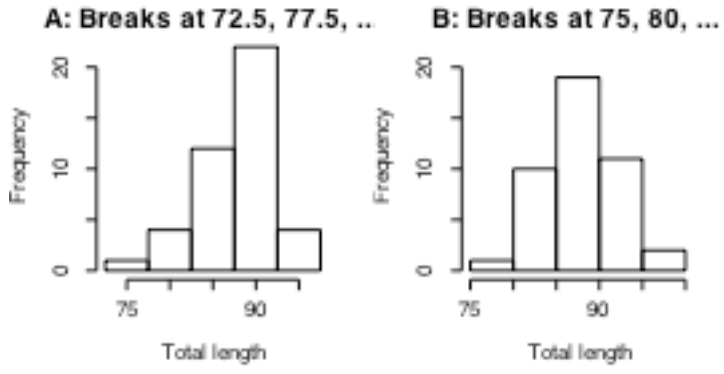


Figure 10: The two graphs show the same data, but with a different choice of breakpoints.

Here is the code used to plot the histograms:

```
par(mfrow = c(1, 2))
attach(possum)
here <- sex == "f"
hist(totlngth[here], breaks = 72.5 + (0:5) * 5, ylim = c(0, 22),
```

```
          xlab="Total length", main ="A: Breaks at 72.5, 77.5, ...")
hist(totlngth[here], breaks = 75 + (0:5) * 5, ylim = c(0, 22),
          xlab="Total length", main="B: Breaks at 75, 80, ...")
par(mfrow=c(1,1))
detach(possum)
```

3.5.2 Density Plots

Density plots, now that they are available, are often a preferred alternative to a histogram. In Figure 11 the histograms from Figure 10 are overlaid with a density plot.

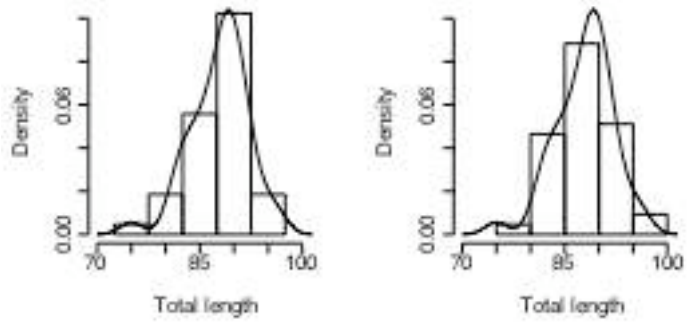


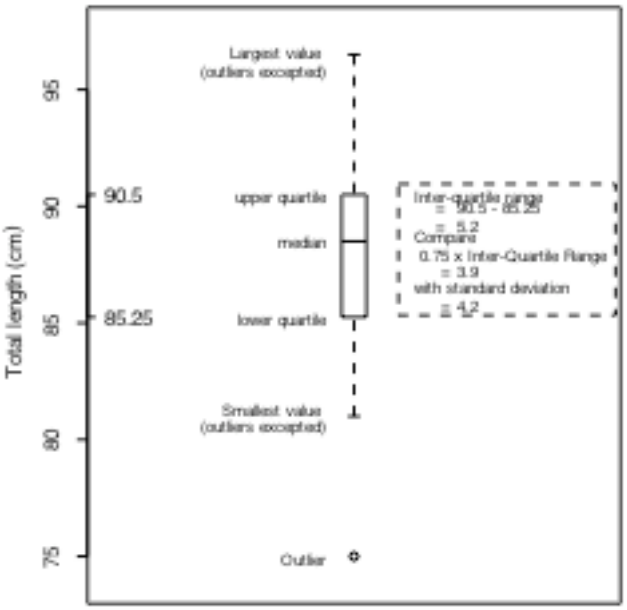
Figure 11: On each of the histograms from Figure 10 a density plot has been overlaid.

Density plots do not depend on a choice of breakpoints. The choice of width and type of window, controlling the nature and amount of smoothing, does affect the appearance of the plot. The main effect is to make it more or less smooth.

The following will give a density plot:

```
attach(possum)
plot(density(totlngth[here]),type="l")
detach(possum)
```

Note that in Fig. 12 the y-axis for the histogram is labelled so that the area of a rectangle is the frequency for that




```
obability = T,
 main="")
```

3.5

We

Fig n of boxplots.

Figure 12: Boxplot of female possum lengths, with additional labelling information.

3.5.4 Normal probability plots

qqnorm(y) gives a normal probability plot of the elements of **y**. The points of this plot will lie approximately on a straight line if the distribution is Normal. In order to calibrate the eye to recognise plots that indicate non-normal variation, it is helpful to do several normal probability plots for random samples of the relevant size from a normal distribution.

```
x11(width=8, height=6)  # This is a better shape for this plot
attach(possum)
here <- sex == "f"
par(mfrow=c(3,4))             # A 3 by 4 layout of plots
y <- totlngth[here]
qqnorm(y,xlab="", ylab="Length", main="Possums")
for(i in 1:11)qqnorm(rnorm(43),xlab="", ylab="Simulated lengths",
                     main="Simulated")
detach(possum)
# Before continuing, type dev.off()
```

Figure 13 shows the plots. There is one unusually small value. Otherwise the points for the female possum lengths are as close to a straight line as in many of the plots for random normal data.

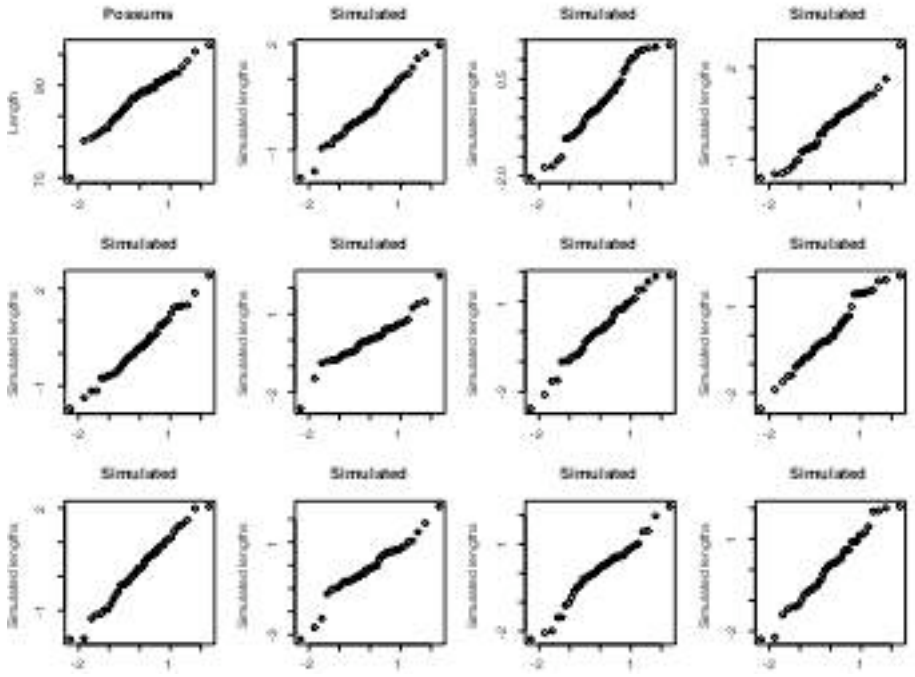


Figure 13: Normal probability plots. If data are from a normal distribution then points should fall, approximately, along a line. The plot in the top left hand corner shows the 43 lengths of female possums. The other plots are for independent normal random samples of size 43.

The idea is an important one. In order to judge whether data are normally distributed, examine a number of randomly generated samples of the same size from a normal distribution. It is a way to train the eye.

By default, **rnorm()** generates random samples from a distribution with mean 0 and standard deviation 1.

3.6 Other Useful Plotting Functions

For the functions demonstrated here, we use data on the heights of 100 female athletes[21].

[21] Data relate to the paper: Telford, R.D. and Cunningham, R.B. 1991: Sex, sport and body-size dependency of hematology in highly trained athletes. *Medicine and Science in Sports and Exercise* 23: 788-794.

3.6.1 Scatterplot smoothing

panel.smooth() plots points, then adds a smooth curve through the points. For example:

```
attach(ais)
here<- sex=="f"
plot(pcBfat[here]~ht[here], xlab = "Height", ylab = "% Body fat")
panel.smooth(ht[here],pcBfat[here])
detach(ais)
```

3.6.2 Adding lines to plots

Use the function **abline()** for this. The parameters may be an intercept and slope, or a vector that holds the intercept and slope, or an lm object. Alternatively it is possible to draw a horizontal line (h = <height>), or a vertical line (v = <ordinate>).

```
attach(ais)
here<- sex=="f"
plot(pcBfat[here] ~ ht[here], xlab = "Height", ylab = "% Body fat")
abline(lm(pcBfat[here] ~ ht[here]))
detach(ais)
```

3.6.3 Rugplots

By default **rug(x)** adds, along the x-axis of the current plot, vertical bars showing the distribution of values of **x**. It can however be particularly useful for showing the actual values along the side of a boxplot. Figure 14 shows a boxplot of the distribution of height of female athletes, with a rugplot added on the y-axis.

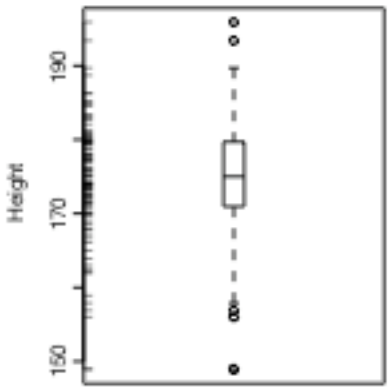


Figure 14: Distribution of heights of female athletes.
The bars on the left plot show actual data values.

Here is the code

```
attach(ais)
here <- sex == "f"
boxplot(ht[here], boxwex = 0.15, ylab = "Height")
rug(ht[here], side = 2)
detach(ais)
```

The parameter **boxwex** controls the width of the boxplot.

3.6.4 Scatterplot matrices

Section 2.1.3 demonstrated the use of the **pairs()** function.

3.6.5 Dotcharts

These can be a good alternative to barcharts. They have a much higher information to ink ratio! Try

```
data(islands)      # Use for versions <=1.9.1; base package
dotchart(islands)  # vector of named numeric values
```

Unfortunately there are many names, and there is substantial overlap. The following is better, but shrinks the sizes of the points so that they almost disappear:

```
dotchart(islands, cex=0.5)
```

3.7 Plotting Mathematical Symbols

Both **`text()`** and **`mtext()`** will take an expression rather than a text string. **`In plot()`**, either or both of **`xlab`** and **`ylab`** can be an expression. Figure 15 was produced with

```
plot(x, y, xlab="Radius", ylab=expression(Area == pi*r^2))
```

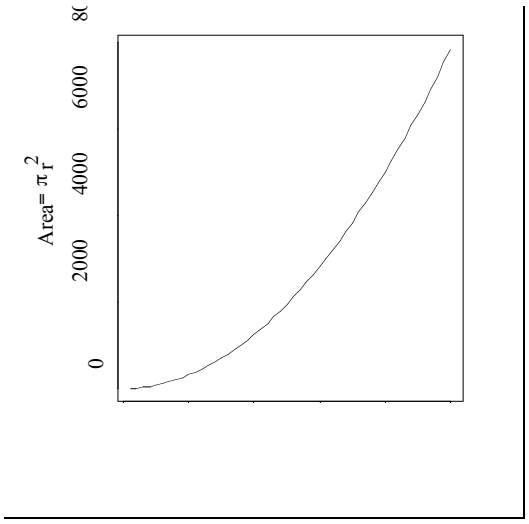


Figure 15: The y-axis label is a mathematical expression.

Notice that in **`expression(Area == pi*r^2)`**, there is a double equals sign ("**==**"), although what will appear on the plot is **`Area = pi*r^2, with a single equals sign. The reason for this is that Area == pi*r^2 is a valid mathematical expression, while Area = pi*r^2 is not.`**

`See help(plotmath) for detailed information on the plotting of mathematical expressions. There is a further example in chapter 12.`

The final plot from

```
demo(graphics)
```

shows some of the possibilities for plotting mathematical symbols.

3.8 Guidelines for Graphs

Design graphs to make their point tersely and clearly, with a minimum waste of ink. Label as necessary to identify important features. In scatterplots the graph should attract the eye's attention to the points that are plotted, and to important grouping in the data. Use solid points, large enough to stand out relative to other features, when there is little or no overlap.

When there is extensive overlap of plotting symbols, use open plotting symbols. Where points are dense, overlapping points will give a high ink density, which is exactly what one wants.

Use scatterplots in preference to bar or related graphs whenever the horizontal axis represents a quantitative effect.

Use graphs from which information can be read directly and easily in preference to those that rely on visual impression and perspective. Thus in scientific papers contour plots are much preferable to surface plots or two-dimensional bar graphs.

Draw graphs so that reduction and reproduction will not interfere with visual clarity.

Explain clearly how error bars should be interpreted — □ SE limits, □ 95% confidence interval, □ SD limits, or whatever. Explain what source of `error(s)' is represented. It is pointless to present information on a source of error that is of little or no interest, for example analytical error when the relevant source of `error' for comparison of treatments is between fruit.

Use colour or different plotting symbols to distinguish different groups. Take care to use colours that contrast.

The list of references at the end of this chapter has further comments on graphical and other presentation issues.

3.9 Exercises

1. Plot the graph of brain weight (**brain**) versus body weight (**body**) for the data set **Animals from the MASS package**. Label the axes appropriately.
[To access this data frame, specify **library(MASS); data(Animals)**]

2. Repeat the plot 1, but this time plotting log(brain weight) versus log(body weight). Use the row labels to label the points with the three largest body weight values. Label the axes in untransformed units.

3. Repeat the plots 1 and 2, but this time place the plots side by side on the one page.

4. The data set **huron** that accompanies these notes has mean July average water surface elevations, in feet, IGLD (1955) for Harbor Beach, Michigan, on Lake Huron, Station 5014, for 1860-1986[22]. (Alternatively you can work with the vector **LakeHuron** from the *datasets* package, that has mean heights for 1875-1772 only.)

a) Plot **mean.height** against year.

b) Use the identify function to determine which years correspond to the lowest and highest mean levels. That is, type

```
identify(huron$year,huron$mean.height,labels=huron$year)
```

and use the left mouse button to click on the lowest point and highest point on the plot. To quit, press both mouse buttons simultaneously.

c) As in the case of many time series, the mean levels are correlated from year to year. To see how each year's mean level is related to the previous year's mean level, use

```
lag.plot(huron$mean.height)
```

This plots the mean level at year i against the mean level at year i-1.

5. Check the distributions of head lengths (**hdlngth**) in the **possum**[23] data set that accompanies these notes. Compare the following forms of display:

a) a histogram (**hist(possum$hdlngth)**);

b) a stem and leaf plot (**stem(qqnorm(possum$hdlngth))**;

c) a normal probability plot (**qqnorm(possum$hdlngth)**); and

d) a density plot (**plot(density(possum$hdlngth)).**

What are the advantages and disadvantages of these different forms of display?

6. Try **x <- rnorm(10)**. Print out the numbers that you get. Look up the help for **rnorm**. Now generate a sample of size 10 from a normal distribution with mean 170 and standard deviation 4.

7. Use **mfrow()** to set up the layout for a 3 by 4 array of plots. In the top 4 rows, show normal probability plots (section 3.4.2) for four separate `random' samples of size 10, all from a normal distribution. In the middle 4

---

[22] Source: Great Lakes Water Levels, 1860-1986. U.S. Dept. of Commerce, National Oceanic and AtmosphericAdministration, National Ocean Survey.

[23] Data relate to the paper: Lindenmayer, D. B., Viggers, K. L., Cunningham, R. B., and Donnelly, C. F. 1995. Morphological variation among populations of the mountain brush tail possum, *Trichosurus caninus* Ogilby (Phalangeridae: Marsupialia). Australian Journal of Zoology 43: 449-458.

rows, display plots for samples of size 100. In the bottom four rows, display plots for samples of size 1000. Comment on how the appearance of the plots changes as the sample size changes.

8. The function **`runif()`** can be used to generate a sample from a uniform distribution, by default on the interval 0 to 1. Try **`x <- runif(10)`**, and print out the numbers you get. Then repeat exercise 6 above, but taking samples from a uniform distribution rather than from a normal distribution. What shape do the points follow?

*9. If you find exercise 8 interesting, you might like to try it for some further distributions. For example **`x <- rchisq(10,1)`** will generate 10 random values from a chi-squared distribution with degrees of freedom 1. The statement **`x <- rt(10,1)`** will generate 10 random values from a t distribution with degrees of freedom one. Make normal probability plots for samples of various sizes from these distributions.

10. For the first two columns of the data frame **`hills`**, examine the distribution using:

(a) histograms

(b) density plots

(c) normal probability plots.

Repeat (a), (b) and (c), now working with the logarithms of the data values.

3.10 References

Bell Lab's Trellis Page: http://cm.bell-labs.com/cm/ms/departments/sia/project/trellis/

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4. Lattice graphics

Lattice plots allow the use of the layout on the page to reflect meaningful aspects of data structure. They offer abilities similar to those in the S-PLUS *trellis* library.

The *lattice* package sits on top of the *grid* package. To use lattice graphics, both these packages must be installed. Providing it is installed, the grid package will be loaded automatically when lattice is loaded.

The older **`coplot()`** function that is in the *base* package has some of same abilities as **`xyplot( )`**, but with a limitation to two conditioning factors or variables only.

4.1 Examples that Present Panels of Scatterplots – Using `xyplot()`

The basic function for drawing panels of scatterplots is **`xyplot()`**. We will use the data frame **`tinting`** (supplied) to demonstrate the use of **`xyplot()`**. These data are from an experiment that investigated the effects of tinting of car windows on visual performance[24]. The authors were mainly interested in visual recognition tasks that would be performed when looking through side windows.

In this data frame, **`csoa`** (critical stimulus onset asynchrony, i.e. the time in milliseconds required to recognise an alphanumeric target), **`it`** (inspection time, i. e. the time required for a simple discrimination task) and **`age`** are variables, **`tint`** (level of tinting: no, lo, hi) and **`target`** (contrast: locon, hicon) are ordered factors, **`sex`** (1 = male, 2 = female) and **`agegp`** (1 = young, in the early 20s; 2 = an older participant, in the early 70s) are factors. Figure 16 shows the style of graph that one can get from xyplot(). The different symbols are different contrasts.

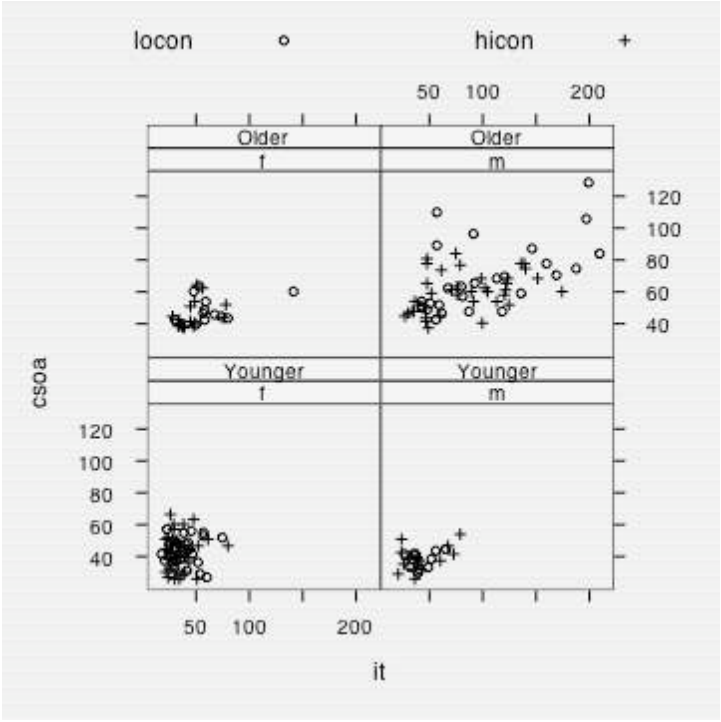

Figure 16: csoa versus it, for each combination of females/males and elderly/young. The two targets (low, + = high contrast) are shown with different symbols.

In a simplified version of Figure 16 above, we might plot **`csoa`** against **`it`** for each combination of **`sex`** and **`agegp`**. For this simplified version, it would be enough to type:

```
xyplot(csoa ~ it | sex * agegp, data=tinting) # Simple use of xyplot()
```

[24] Data relate to the paper: Burns, N. R., Nettlebeck, T., White, M. and Willson, J. 1999. Effects of car window tinting on visual performance: a comparison of elderly and young drivers. Ergonomics 42: 428-443.

Here is the statement used to get Figure 16. The two different symbols distinguish between low contrast and high contrast targets.

```
xyplot(csoa~it|sex*agegp, data=tinting, panel=panel.superpose,
     groups=target, auto.key=list(columns=2))
```

If colour is available, different colours will be used for the different groups.

A striking feature is that the very high values, for both **csoa** and **it**, occur only for elderly males. It is apparent that the long response times for some of the elderly males occur, as we might have expected, with the low contrast target. The following puts smooth curves through the data, separately for the two target types:

```
xyplot(csoa~it|sex*agegp, data=tinting, panel=panel.superpose,
     groups=target, type=c("p","smooth")
```

The relationship between **csoa** and **it** seems much the same for both levels of contrast.

Finally, we do a plot (Figure 17) that uses different symbols (in black and white) for different levels of tinting. The longest times are for the high level of tinting.

```
xyplot(csoa~it|sex*agegp, data=tinting, groups=tint,
     auto.key=list(columns=3))
```

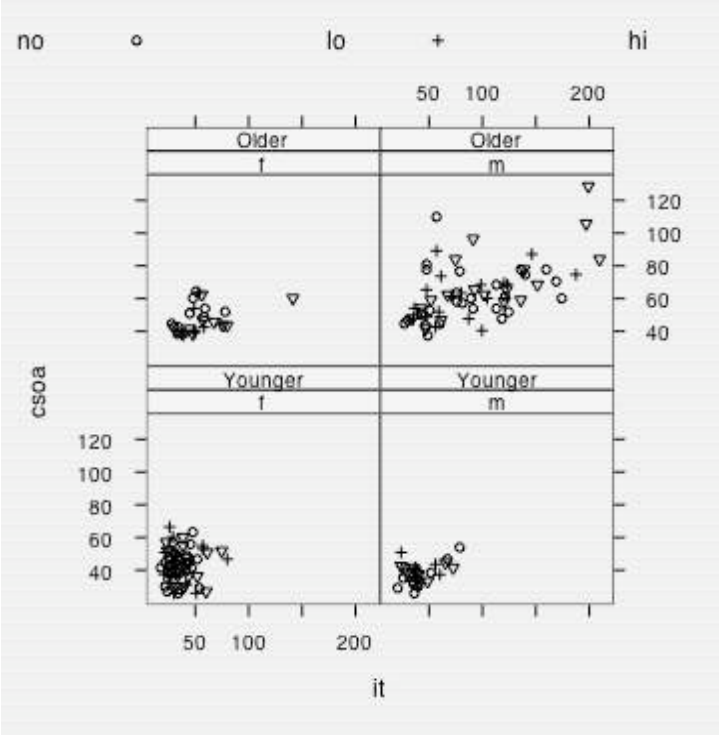

Figure 17: csoa versus it, for each combination of females/males and elderly/young. The different levels of tinting (no, +=low, >=high) are shown with different symbols.

4.2 An incomplete list of lattice Functions

```
splom( ~ data.frame)                    # Scatterplot matrix
bwplot(factor ~ numeric , . .)          # Box and whisker plot
qqnorm(numeric , . .)                   # normal probability plots
dotplot(factor ~ numeric , . .)         # 1-dim. Display
stripplot(factor ~ numeric , . .)       # 1-dim. Display
barchart(character ~ numeric , . .)
histogram( ~ numeric , . .)
densityplot( ~ numeric , . .)           # Smoothed version of histogram
qqmath(numeric ~ numeric , . .)    # QQ plot
splom( ~ dataframe, . .)                # Scatterplot matrix
parallel( ~ dataframe, . .)             # Parallel coordinate plots
```

In each instance, conditioning variables can be added.

4.3 Exercises

1. The following data gives milk volume (g/day) for smoking and nonsmoking mothers[25]:
Smoking Mothers: 621, 793, 593, 545, 753, 655, 895, 767, 714, 598, 693
Nonsmoking Mothers: 947, 945, 1086, 1202, 973, 981, 930, 745, 903, 899, 961
Present the data (i) in side by side boxplots; (ii) using a dotplot form of display.

2. Repeat the plot as in exercise 1, but this time including a scatterplot smooth on each panel.

3. For the possum data set, generate the following plots:

a) histograms of **`hdlngth`** – use **`hist()`**;

b) normal probability plots of **`hdlngth`** – use **`qqnorm()`**;

c) density plots of **`hdlngth`** – use **`plot(density())`**. Investigate the effect of varying the density bandwidth (**`bw`**).

4. The following exercises relate to the data frame **`possum`** that accompanies these notes:

(a) Using the **`coplot`** function, explore the relation between **`hdlngth`** and **`totlngth`**, taking into account **`sex`** and **`Pop`**.

(b) Construct a contour plot of **`chest`** versus **`belly`** and **`totlngth`**.

(c) Construct box and whisker plots for **`hdlngth`**, using **`site`** as a factor.

(d) Construct normal probability plots for **`hdlgth`**, for each separate level of **`sex`** and **`Pop`**. Is there evidence that the distribution of **`hdlgth`** varies with the level of these other factors.

6. The frame **`airquality`** that is in the *datasets* package has columns **`Ozone`**, **`Solar.R`**, **`Wind`**, **`Temp`**, **`Month`** and **`Day`**. Plot **`Ozone`** against **`Solar.R`** for each of three temperature ranges, and each of three wind ranges.

[25] Data are from the paper ``Smoking During Pregnancy and Lactation and Its Effects on Breast Milk Volume'' (Amer. J. of Clinical Nutrition).

5. Linear (Multiple Regression) Models and Analysis of Variance

5.1 The Model Formula in Straight Line Regression

We begin with the straight line regression example that appeared earlier, in section 2.1.4. First we plot the data:

```
plot(distance ~ stretch, data=elasticband)
```

The code for the regression calculation is:

```
elastic.lm <- lm(distance ~ stretch, data=elasticband)
```

Here **`distance ~ stretch`** is a model formula. Other model formulae will appear in the course of this chapter. Figure 18 shows the plot:

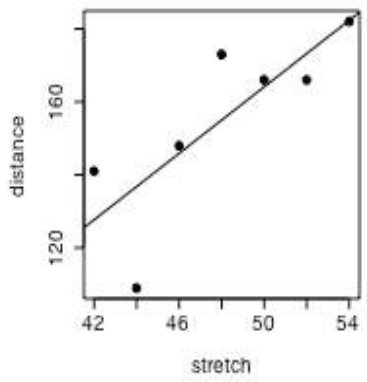

Figure 18: Plot of distance versus stretch for the elastic band data, with fitted least squares line

The output from the regression is an **`lm`** object, which we have called **`elastic.lm`** . Now examine a summary of the regression results. Notice that the output documents the model formula that was used:

```
> options(digits=4)
> summary(elastic.lm)
Call:
lm(formula = distance ~ stretch, data = elasticband)

Residuals:
      1       2       3       4       5       6       7
  2.107  -0.321  18.000   1.893 -27.786  13.321  -7.214

Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept)   -63.57      74.33   -0.86    0.431
stretch         4.55       1.54    2.95    0.032

Residual standard error: 16.3 on 5 degrees of freedom
Multiple R-Squared: 0.635,      Adjusted R-squared: 0.562
F-statistic: 8.71 on 1 and 5 degrees of freedom,        p-value: 0.0319
```

5.2 Regression Objects

An **`lm`** object is a list of named elements. Above, we created the object **`elastic.lm`** . Here are the names of its elements:

```
> names(elastic.lm)
 [1] "coefficients"  "residuals"     "effects"       "rank"
```

```
[5] "fitted.values" "assign"        "qr"            "df.residual"
[9] "xlevels"       "call"          "terms"         "model"
```

Various functions are available for extracting information that you might want from the list. This is better than manipulating the list directly. Examples are:

```
> coef(elastic.lm)
(Intercept)     stretch
    -63.571       4.554
> resid(elastic.lm)
       1        2        3        4        5        6        7
 2.1071  -0.3214  18.0000   1.8929 -27.7857  13.3214  -7.2143
```

The function most often used to inspect regression output is **`summary()`**. It extracts the information that users are most likely to want. For example, in section 5.1, we had

```
summary(elastic.lm)
```

There is a plot method for **`lm`** objects that gives the diagnostic information shown in Figure 19.

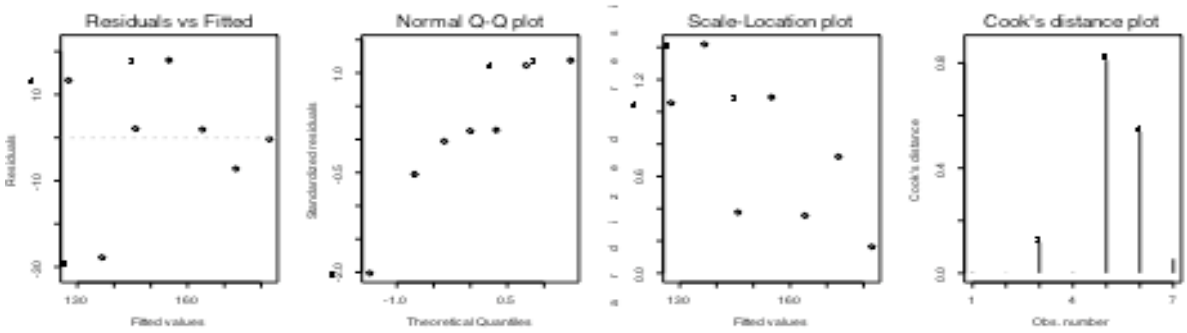

Figure 19: Diagnostic plot of lm object, obtained by **`plot(elastic.lm)`**.

To get Figure 19, type:

```
x11(width=7, height=2, pointsize=10)
par(mfrow = c(1, 4), par()$mar=c(5.1,4.1,2.1,1.1))
plot(elastic.lm)
par(mfrow=c(1,1))
```

By default the first, second and fourth plot use the row names to identify the three most extreme residuals. [If explicit row names are not given for the data frame, then the row numbers are used.]

5.3 Model Formulae, and the X Matrix

The model formula for the elastic band example was **`distance ~ stretch`**. The model formula is a recipe for setting up the calculations. All the calculations described in this chapter require the use of an model matrix or X matrix, and a vector y of values of the dependent variable. For some of the examples we discuss later, it helps to know what the X matrix looks like. Details for the elastic band example follow.

The X matrix, with the y-vector alongside, is:

X		y
	Stretch (mm)	Distance (cm)
1	46	148
1	54	182
1	48	173
1	50	166
1	44	109
1	42	141
1	52	166

The model matrix relates to the part of the model that appears to the right of the equals sign. The straight line model is

$$y = a + b\,x + \text{residual}$$

which we write as

$$y = 1 \times a + x \times b + \text{residual}$$

The parameters that are to be estimated are *a* and *b*. *Fitted* values are given by multiplying each column of the model matrix by its corresponding parameter, i.e. the first column by *a* and the second column by *b*, and adding. Another name is *predicted* values. The aim is to reproduce, as closely as possible, the values in the y-column. The *residuals* are the differences between the values in the y-column and the fitted values. Least squares regression, which is the form of regression that we describe in this course, chooses *a* and *b* so that the sum of squares of the residuals is as small as possible.

The function **`model.matrix()`** prints out the model matrix. Thus:

```
> model.matrix(distance ~ stretch, data=elasticband)
(Intercept) stretch
1           1      46
2           1      54
3           1      48
4           1      50
5           1      44
6           1      42
7           1      52
attr(,"assign")
[1] 0 1
```

Another possibility, with **`elastic.lm`** as in section 5.1, is:

```
model.matrix(elastic.lm)
```

The following are the fitted values and residuals that we get with the estimates of *a* (= -63.6) and *b* (= 4.55) that result from least squares regression

X		$\hat{y}$	*y*	$y - \hat{y}$
	Stretch (mm)	*(Fitted)*	*(Observed)*	*(Residual)*
1 × -63.6	× 4.55	1 × -63.6 + 4.55 × Stretch	Distance (mm)	Observed - Fitted
1	46	-63.6 + 4.55 × 46 = 145.7	148	148-145.7 = 2.3
1	54	-63.6 + 4.55 × 54 = 182.1	182	182-182.1 = -0.1
1	48	-63.6 + 4.55 × 48 = 154.8	173	173-154.8 = 18.2
1	50	-63.6 + 4.55 × 50 = 163.9	166	166-163.9 = 2.1
1	44	-63.6 + 4.55 × 44 = 136.6	109	109-136.6 = -27.6
1	42	-63.6 + 4.55 × 42 = 127.5	141	141-127.5 = 13.5
1	52	-63.6 + 4.55 × 52 = 173.0	166	166-173.0 = -7.0

Note the use of the symbol $\hat{y}$ [pronounced y-hat] for predicted values.

We might alternatively fit the simpler (no intercept) model. For this we have

$$y = x \times b + e$$

where *e* is a random variable with mean 0. The X matrix then consists of a single column, the x's.

5.3.1 Model Formulae in General

Model formulae take a form such as:

y~x+z : lm, glm,, etc.

y~x + fac + fac:x : lm, glm, aov, etc. (If **fac** is a factor and **x** is a variable, **fac:x** allows a different slope for each different level of **fac**.)

Model formulae are widely used to set up most of the model calculations in R.

Notice the similarity between model formulae and the formulae that are used for specifying coplots. Thus, recall that the graph formula for a coplot that gives a plot of **y** against **x** for each different combination of levels of **fac1** (across the page) and **fac2** (up the page) is:

```
y ~ x | fac1+fac2
```

*5.3.2 Manipulating Model Formulae

Model formulae can be assigned, e.g.

```
formyxz <- formula(y~x+z)
```

or

```
formyxz <- formula("y~x+z")
```

The argument to **formula()** can, as just demonstrated, be a text string. This makes it straightforward to paste the argument together from components that are stored in text strings. For example

```
> names(elasticband)
[1] "stretch"  "distance"
> nam <- names(elasticband)
> formds <- formula(paste(nam[1],"~",nam[2]))
> lm(formds, data=elasticband)

Call:
lm(formula = formds, data = elasticband)

Coefficients:
(Intercept)     distance
    26.3780       0.1395
```

Note that graphics formulae can be manipulated in exactly the same way as model formulae.

5.4 Multiple Linear Regression Models

5.4.1 The data frame Rubber

The data set **Rubber** from the *MASS* package is from the accelerated testing of tyre rubber[26]. The variables are **loss** (the abrasion loss in gm/hr), **hard** (hardness in `Shore' units), and **tens** (tensile strength in kg/sq m).

We obtain a scatterplot matrix (Figure 20) thus:

```
library(MASS)  # if needed
data(Rubber)   # not needed for versions 1.9.1 and later
pairs(Rubber)
```

[26] The original source is O.L. Davies (1947) Statistical Methods in Research and Production. Oliver and Boyd, Table 6.1 p. 119.

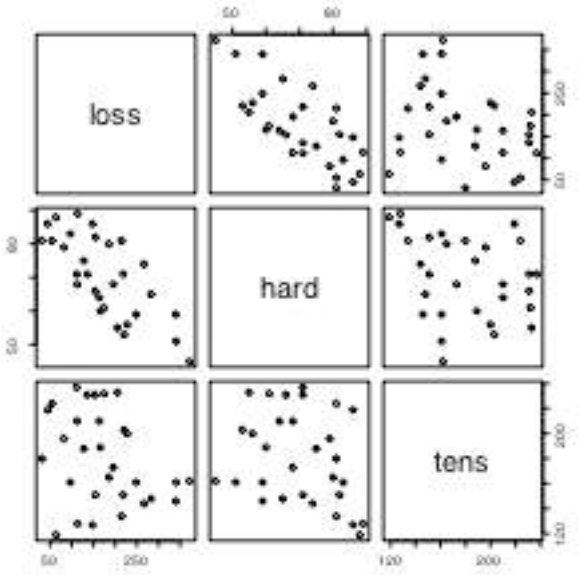

Figure 20: Scatterplot matrix for the Rubber data frame from the *MASS* package.

There is a negative correlation between loss and hardness. We proceed to regress loss on **hard** and **tens**.

```
Rubber.lm <- lm(loss~hard+tens, data=Rubber)
> options(digits=3)
> summary(Rubber.lm)

Call:
lm(formula = loss ~ hard + tens, data = Rubber)

Residuals:
   Min     1Q Median     3Q    Max
-79.38 -14.61   3.82  19.75  65.98

Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept)  885.161     61.752   14.33  3.8e-14
hard          -6.571      0.583  -11.27  1.0e-11
tens          -1.374      0.194   -7.07  1.3e-07

Residual standard error: 36.5 on 27 degrees of freedom
Multiple R-Squared: 0.84,       Adjusted R-squared: 0.828
F-statistic:   71 on 2 and 27 degrees of freedom,       p-value: 1.77e-011
```

In addition to the use of **plot.lm()**, note the use of **termplot()**. Figure 21) used the following code:

```
par(mfrow=c(1,2))
termplot(Rubber.lm, partial=TRUE, smooth=panel.smooth)
par(mfrow=c(1,1))
```

This plot raises interesting questions.

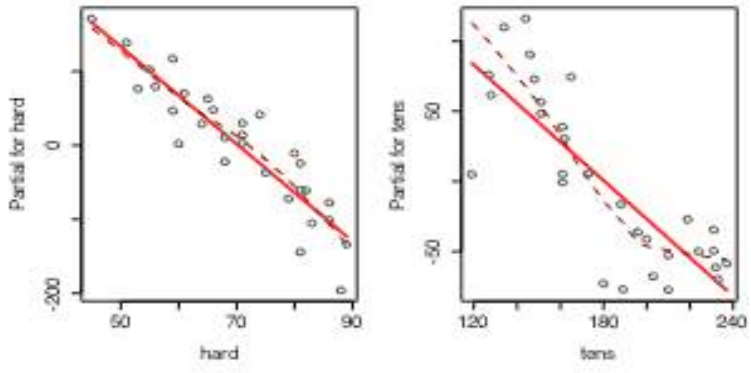

Figure 21: Plot, obtained with termplot(), showing the contribution of each of the two terms in the model, at the mean of the contributions for the other term. A smooth curve has, in each panel, been fitted through the partial residuals. There is a clear suggestion that, at the upper end of the range, the response is not linear with tensile strength.

5.4.2 Weights of Books

The books to which the data in the data set **oddbooks** (accompanying these notes) refer were chosen to cover a wide range of weight to height ratios. Here are the data:

```
> oddbooks
   thick height width weight
1     14   30.5  23.0   1075
2     15   29.1  20.5    940
3     18   27.5  18.5    625
4     23   23.2  15.2    400
5     24   21.6  14.0    550
6     25   23.5  15.5    600
7     28   19.7  12.6    450
8     28   19.8  12.6    450
9     29   17.3  10.5    300
10    30   22.8  15.4    690
11    36   17.8  11.0    400
12    44   13.5   9.2    250
```

Notice that as thickness increases, weight reduces.

```
> logbooks <- log(oddbooks) # We might expect weight to be
>                           # proportional to thick * height * width
> logbooks.lm1<-lm(weight~thick,data=logbooks)
> summary(logbooks.lm1)$coef
            Estimate Std. Error t value Pr(>|t|)
(Intercept)     9.69      0.708    13.7 8.35e-08
thick          -1.07      0.219    -4.9 6.26e-04

> logbooks.lm2<-lm(weight~thick+height,data=logbooks)
> summary(logbooks.lm2)$coef
            Estimate Std. Error t value Pr(>|t|)
(Intercept)   -1.263      3.552  -0.356   0.7303
thick          0.313      0.472   0.662   0.5243
height         2.114      0.678   3.117   0.0124

> logbooks.lm3<-lm(weight~thick+height+width,data=logbooks)
> summary(logbooks.lm3)$coef
```

```
             Estimate Std. Error t value Pr(>|t|)
(Intercept)    -0.719      3.216  -0.224    0.829
thick           0.465      0.434   1.070    0.316
height          0.154      1.273   0.121    0.907
width           1.877      1.070   1.755    0.117
```

So is **weight** proportional to **thick * height * width**?

The correlations between **thick, height** and **width** are so strong that if one tries to use more than one of them as a explanatory variables, the coefficients are ill-determined. They contain very similar information, as is evident from the scatterplot matrix. The regressions on **height** and **width** give plausible results, while the coefficient of the regression on **thick** is entirely an artefact of the way that the books were selected.

The design of the data collection really is important for the interpretation of coefficients from a regression equation. Even though regression equations from observational data may work quite well for predictive purposes, the individual coefficients may be misleading. This is more than an academic issue, as the analyses in Lalonde (1986) demonstrate. They had data from experimental "treatment" and "control" groups, and also from two comparable non-experimental "controls". The regression estimate of the treatment effect, when comparison was with one of the non-experimental controls, was statistically significant but with the wrong sign! The regression should be fitted only to that part of the data where values of the covariates overlap substantially. Dehejia and Wahba demonstrate the use of scores ("propensities") to identify subsets that are defensibly comparable. The propensity is then the only covariate in the equation that estimates the treatment effect. It is impossible to be sure that any method is giving the right answer.

5.5 Polynomial and Spline Regression

Calculations that have the same structure as multiple linear regression are able to model a curvilinear response. Curves are constructed from linear combinations of transformed values. Note that polynomial curves of high degree are in general unsatisfactory. Spline curves, constructed by joining low order polynomial curves (typically cubics) in such a way that the slope changes smoothly, are in general preferable.

5.5.1 Polynomial Terms in Linear Models

The data frame **seedrates**[27] that accompanies these notes gives, for each of a number of different seeding rates, the number of barley grain per head.

```
plot(grain ~ rate, data=seedrates)   # Plot the data
```

Figure 22 shows the data, with fitted quadratic curve:

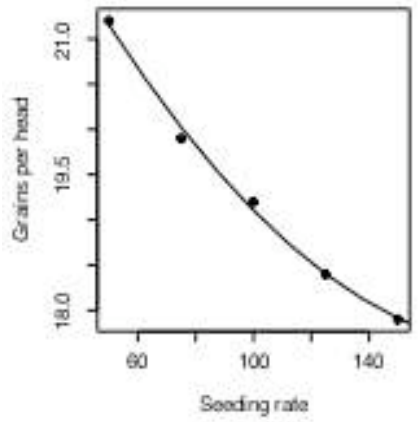

Figure 22: Number of grain per head versus seeding rate, for the barley seeding rate data, with fitted quadratic curve.

[27] Data are from McLeod, C. C. (1982) Effect of rates of seeding on barley grown for grain. New Zealand Journal of Agriculture 10: 133-136. Summary details are in Maindonald, J. H. (1992).

We will need an X-matrix with a column of ones, a column of values of **rate**, and a column of values of **rate**^{2}. For this, both **rate** and **I(rate^2)** must be included in the model formula.

```
> seedrates.lm2 <- lm(grain ~ rate+I(rate^2), data=seedrates)
> summary(seedrates.lm2)

Call:
lm(formula = grain ~ rate + I(rate^2), data = seedrates)

Residuals:
       1        2        3        4        5
 0.04571 -0.12286  0.09429 -0.00286 -0.01429

Coefficients:
             Estimate Std. Error t value Pr(>|t|)
(Intercept) 24.060000   0.455694   52.80  0.00036
rate        -0.066686   0.009911   -6.73  0.02138
I(rate^2)    0.000171   0.000049    3.50  0.07294

Residual standard error: 0.115 on 2 degrees of freedom
Multiple R-Squared: 0.996,      Adjusted R-squared: 0.992
F-statistic:  256 on 2 and 2 degrees of freedom,        p-value: 0.0039
> hat <- predict(seedrates.lm2)
> lines(spline(seedrates$rate, hat))
> # Placing the spline fit through the fitted points allows a smooth curve.
> # For this to work the values of seedrates$rate must be ordered.
```

Again, check the form of the model matrix. Type:

```
> model.matrix(grain~rate+I(rate^2),data=seedrates)
  (Intercept) rate I(rate^2)
1           1   50      2500
2           1   75      5625
3           1  100     10000
4           1  125     15625
5           1  150     22500
attr(,"assign")
[1] 0 1 2
```

This was a (small) extension of linear models, to handle a specific form of non-linear relationship. Any transformation can be used to form columns of the model matrix. Thus, an x^3 column might be added.

Once the model matrix has been formed, we are limited to taking linear combinations of columns.

5.5.2 What order of polynomial?

A polynomial of degree 2, i.e. a quadratic curve, looked about right for the above data. How does one check?

One way is to fit polynomials, e.g. of each of degrees 1 and 2, and compare them thus:

```
> seedrates.lm1<-lm(grain~rate,data=seedrates)
> seedrates.lm2<-lm(grain~rate+I(rate^2),data=seedrates)
> anova(seedrates.lm2,seedrates.lm1)
Analysis of Variance Table

Model 1: grain ~ rate + I(rate^2)
Model 2: grain ~ rate
  Res.Df Res.Sum Sq Df    Sum Sq F value  Pr(>F)
1      2   0.026286
2      3   0.187000 -1 -0.160714  12.228 0.07294
```

The F-value is large, but on this evidence there are too few degrees of freedom to make a totally convincing case for preferring a quadratic to a line. However the paper from which these data come gives an independent estimate of the error mean square (0.17 on 35 d.f.) based on 8 replicate results that were averaged to give each value for number of grains per head. If we compare the change in the sum of squares (0.1607, on 1 df) with a mean square of 0.17^2 (35 df), the F-value is now 5.4 on 1 and 35 degrees of freedom, and we have p=0.024 . The increase in the number of degrees of freedom more than compensates for the reduction in the F-statistic.

```
> # However we have an independent estimate of the error mean
> # square. The estimate is 0.17^2, on 35 df.
> 1-pf(0.16/0.17^2, 1, 35)
[1] 0.0244
```

Finally note that R^2 was 0.972 for the straight line model. This may seem good, but given the accuracy of these data it was not good enough! The statistic is an inadequate guide to whether a model is adequate. Even for any one context, R^2 will in general increase as the range of the values of the dependent variable increases. (R^2 is larger when there is more variation to be explained.) A predictive model is adequate when the standard errors of predicted values are acceptably small, not when R^2 achieves some magic threshold.

5.5.3 Pointwise confidence bounds for the fitted curve

Here is code that gives pointwise 95% confidence bounds. Note that these do not combine to give a confidence region for the total curve! The construction of such a region is a much more complicated task!

```
plot(grain ~ rate, data = seedrates, pch = 16, xlim = c(50, 175), ylim
                = c(15.5, 22),xlab="Seeding rate",ylab="Grains per head")
new.df <- data.frame(rate = c((4:14) * 12.5))
seedrates.lm2 <- lm(grain ~ rate + I(rate^2), data = seedrates)
pred2 <- predict(seedrates.lm2, newdata = new.df, interval="confidence")
hat2 <- data.frame(fit=pred2[,"fit"],lower=pred2[,"lwr"], upper=pred2[,"upr"])
attach(new.df)
lines(rate, hat2$fit)
lines(rate,hat2$lower,lty=2)
lines(rate, hat2$upper,lty=2)
detach(new.df)
```

The extrapolation has deliberately been taken beyond the range of the data, in order to show how the confidence bounds spread out. Confidence bounds for a fitted line spread out more slowly, but are even less believable!

5.5.4 Spline Terms in Linear Models

By now, readers of this document will be used to the idea that it is possible to use linear models to fit terms that may be highly nonlinear functions of one or more of the variables. The fitting of polynomial functions was a simple example of this. Spline functions variables extend this idea further. The splines that I demonstrate are constructed by joining together cubic curves, in such a way the joins are smooth. The places where the cubics join are known as `knots'. It turns out that, once the knots are fixed, and depending on the class of spline curves that are used, spline functions of a variable can be constructed as a linear combination of basis functions, where each basis function is a transformation of the variable.

The data frame **cars** is in the *datasets* package.

```
> data(cars)
> plot(dist~speed,data=cars)
> library(splines)
> cars.lm<-lm(dist~bs(speed),data=cars)  # By default, there are no knots
> hat<-predict(cars.lm)
> lines(cars$speed,hat,lty=3)  # NB assumes values of speed are sorted
> cars.lm5 <- lm(dist~bs(speed,5),data=cars)  # try for a closer fit (1 knot)
> ci5<-predict(cars.lm5,interval="confidence",se.fit=T)
> names(ci5)
```

```
[1] "fit"            "se.fit"         "df"             "residual.scale"
> lines(cars$speed,ci5$fit[,"fit"])
> lines(cars$speed,ci5$fit[,"lwr"],lty=2)
> lines(cars$speed,ci5$fit[,"upr"],lty=2)
```

5.6 Using Factors in R Models

Factors are crucial for specifying R models that include categorical or "factor" variables,. Consider data from an experiment that compared houses with and without cavity insulation[28]. While one would not usually handle these calculations using an **lm** model, it makes a simple example to illustrate the choice of a baseline level, and a set of contrasts. Different choices, although they fit equivalent models, give output in which some of the numbers are different and must be interpreted differently.

We begin by entering the data from the command line:

```
insulation <- factor(c(rep("without", 8), rep("with", 7)))
# 8 without, then 7 with
    # `with' precedes `without' in alphanumeric order, & is the baseline
kWh <- c(10225, 10689, 14683, 6584, 8541, 12086, 12467,
    12669, 9708, 6700, 4307, 10315, 8017, 8162, 8022)
```

To formulate this as a regression model, we take kWh as the dependent variable, and the factor insulation as the explanatory variable.

```
> insulation <- factor(c(rep("without", 8), rep("with", 7)))
> # 8 without, then 7 with
> kWh <- c(10225, 10689, 14683, 6584, 8541, 12086, 12467,
+ 12669, 9708, 6700, 4307, 10315, 8017, 8162, 8022)
> insulation.lm <- lm(kWh ~ insulation)
> summary(insulation.lm, corr=F)

Call:
lm(formula = kWh ~ insulation)
Residuals:
   Min     1Q Median     3Q    Max
 -4409   -979    132   1575   3690

Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept)     7890        874    9.03  5.8e-07
insulation      3103       1196    2.59    0.022

Residual standard error: 2310 on 13 degrees of freedom
Multiple R-Squared: 0.341,      Adjusted R-squared: 0.29
F-statistic: 6.73 on 1 and 13 degrees of freedom,       p-value: 0.0223
```

The p-value is 0.022, which may be taken to indicate ($p < 0.05$) that we can distinguish between the two types of houses. But what does the "intercept" of 7890 mean, and what does the value for "insulation" of 3103 mean? To interpret this, we need to know that the factor levels are, by default, taken in alphabetical order, and that the initial level is taken as the baseline. So **with** comes before **without**, and **with** is the baseline. Hence:

Average for Insulated Houses = 7980

To get the estimate for uninsulated houses take 7980 + 3103 = 10993.

The standard error of the difference is 1196.

---

[28] Data are from Hand, D. J.; Daly, F.; Lunn, A. D.; Ostrowski, E., eds. (1994). A Handbook of Small Data Sets. Chapman and Hall.

5.6.1 The Model Matrix

It often helps to keep in mind the model matrix or X matrix. Here are the X and the y that are used for the calculations. Note that the first eight data values were all **without**s:

Contrast			kWh	
□ 7980	□ 3103	Add to get	Compare with	Residual
1	1	7980+3103=10993	10225	10225-10993
1	1	7980+3103=10993	10689	10689-10993
. . . .	. . . .		. . . .	. . . .
1	0	7980+0	9708	9708-7980
1	0	7980+0	6700	6700-7980
. . . .	. . . .		. . . .	. . . .

Type

```
model.matrix(kWh~insulation)
```

and check that it gives the above model matrix.

*5.6.2 Other Choices of Contrasts

There are other ways to set up the X matrix. In technical jargon, there are other choices of *contrasts*. One obvious alternative is to make **without** the first factor level, so that it becomes the baseline. For this, specify:

```
insulation <- relevel(insulation, baseline="without")
  # Make `without' the baseline
```

Another possibility is to use what are called the "sum" contrasts. With the "sum" contrasts the baseline is the mean over all factor levels. The effect for the first level is omitted; the user has to calculate it as minus the sum of the remaining effects. Here is the output from use of the `sum' contrasts[29]:

```
> options(contrasts = c("contr.sum", "contr.poly"), digits = 2)
   #  Try the `sum' contrasts
> insulation <- factor(insulation, levels=c("without", "with"))
   # Make `without' the baseline
> insulation.lm <- lm(kWh ~ insulation)
> summary(insulation.lm, corr=F)

Call:
lm(formula = kWh ~ insulation)

Residuals:
   Min     1Q Median     3Q    Max
 -4409   -979    132   1575   3690

Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept)     9442        598   15.78  7.4e-10
insulation      1551        598    2.59    0.022

Residual standard error: 2310 on 13 degrees of freedom
Multiple R-Squared: 0.341,      Adjusted R-squared: 0.29
```

[29] The second string element, i.e. **"contr.poly"**, is the default setting for factors with ordered levels. [Use the function ordered() to create ordered factors.]

```
F-statistic: 6.73 on 1 and 13 degrees of freedom,   p-value: 0.0223
```

Here is the interpretation:

average of (mean for "without", "mean for with") = 9442

To get the estimate for uninsulated houses (the first level), take 9442 + 1551 = 10993

The `effects' sum to one. So the effect for the second level (`with') is -1551. Thus

to get the estimate for insulated houses (the first level), take 9442 - 1551 = 7980.

The sum contrasts are sometimes called "analysis of variance" contrasts.

```
It is possible to set the choice of contrasts for each factor separately, with a statement
such as:
insulation <- C(insulation, contr=treatment)
```

Also available are the helmert contrasts. These are not at all intuitive and rarely helpful, even though S-PLUS uses them as the default. Novices should avoid them[30].

5.7 Multiple Lines – Different Regression Lines for Different Species

The terms that appear on the right of the model formula may be variables or factors, or interactions between variables and factors, or interactions between factors. Here we take advantage of this to fit different lines to different subsets of the data.

In the example that follows, we had weights for a porpoise species (*Stellena styx*) and for a dolphin species (*Delphinus delphis*). We take x_1 to be a variable that has the value 0 for *Delphinus delphis*, and 1 for *Stellena styx*. We take x_2 to be body weight. Then possibilities we may want to consider are:

A: A single line: $y = a + b\,x_2$

B: Two parallel lines: $y = a_1 + a_2\,x_1 + b\,x_2$
[For the first group (*Stellena styx;* $x_1 = 0$) the constant term is a_1, while for the second group (*Delphinus delphis;* $x_1 = 1$) the constant term is $a_1 + a_2$.]

C: Two separate lines: $y = a_1 + a_2\,x_1 + b_1\,x_2 + b_2\,x_1\,x_2$
[For the first group (*Delphinus delphis;* $x_1 = 0$) the constant term is a_1 and the slope is b_1. For the second group (*Stellena styx;* $x_1 = 1$) the constant term is $a_1 + a_2$, and the slope is $b_1 + b_2$.]

We show results from fitting the first two of these models, i.e. A and B:

```
> plot(logheart ~ logweight, data=dolphins)  # Plot the data
> options(digits=4)
> cet.lm1 <- lm(logheart ~ logweight, data = dolphins)
> summary(cet.lm1, corr=F)

Call:
lm(formula = logheart ~ logweight, data = dolphins)

Residuals:
     Min       1Q   Median       3Q      Max
-0.15874 -0.08249  0.00274  0.04981  0.21858

Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept)    1.325      0.522    2.54    0.024
logweight      1.133      0.133    8.52  6.5e-07

Residual standard error: 0.111 on 14 degrees of freedom
Multiple R-Squared: 0.838,      Adjusted R-squared: 0.827
```

[30] In general, use either the treatment contrasts or the sum contrasts. With the sum contrasts the baseline is the overall mean.

```
F-statistic: 72.6 on 1 and 14 degrees of freedom,   p-value: 6.51e-007
```

For model B (parallel lines) we have

```
> cet.lm2 <- lm(logheart ~ factor(species) + logweight, data=dolphins)
```

Check the model matrix:

```
> model.matrix(cet.lm2)
   (Intercept) factor(species) logweight
1            1               1     3.555
2            1               1     3.738
. . . .
8            1               0     3.989
. . . .
16           1               0     3.951
attr(,"assign")
[1] 0 1 2
attr(,"contrasts")
[1] "contr.treatment"
```

Enter **summary(cet.lm2)** to get an output summary, and **plot(cet.lm2)** to plot diagnostic information for this model.

For model C, the statement is:

```
> cet.lm3 <- lm(logheart ~ factor(species) + logweight +
    factor(species):logweight, data=dolphins)
```

Check what the model matrix looks like:

```
> model.matrix(cet.lm3)
   (Intercept) factor(species) logweight factor(species).logweight
1            1               1     3.555                     3.555
. . . .
8            1               0     3.989                     0.000
. . . .
16           1               0     3.951                     0.000
attr(,"assign")
[1] 0 1 2 3
attr(,"contrasts")$"factor(species)"
[1] "contr.treatment"
```

Now see why one should not waste time on model C.

```
> anova(cet.lm1,cet.lm2,cet.lm3)
Analysis of Variance Table

Model 1: logheart ~ logweight
Model 2: logheart ~ factor(species) + logweight
Model 3: logheart ~ factor(species) + logweight + factor(species):logweight
  Res.Df Res.Sum Sq Df Sum Sq F value Pr(>F)
1     14     0.1717
2     13     0.0959  1 0.0758   10.28 0.0069
3     12     0.0949  1 0.0010    0.12 0.7346
```

5.8 aov models (Analysis of Variance)

The class of models that can be directly fitted as **aov** models is quite limited. In essence, **aov** provides, for data where all combinations of factor levels have the same number of observations, another view of an **lm** model. One can however specify the error term that is to be used in testing for treatment effects. See section 5.8.2 below.

By default, R uses the treatment contrasts for factors, i.e. the first level is taken as the baseline or reference level. A useful function is **relevel()**. The parameter **ref** can be used to set the level that you want as the reference level.

5.8.1 Plant Growth Example

Here is a simple randomised block design:

```
> data(PlantGrowth)
> attach(PlantGrowth)
> boxplot(split(weight,group))    # Looks OK
> data()
> PlantGrowth.aov <- aov(weight~group)
> summary(PlantGrowth.aov)
            Df  Sum Sq Mean Sq F value  Pr(>F)
group        2  3.7663  1.8832  4.8461 0.01591
Residuals   27 10.4921  0.3886
> summary.lm(PlantGrowth.aov)

Call:
aov(formula = weight ~ group)

Residuals:
    Min      1Q  Median      3Q     Max
-1.0710 -0.4180 -0.0060  0.2627  1.3690

Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept)   5.0320     0.1971  25.527   <2e-16
grouptrt1    -0.3710     0.2788  -1.331   0.1944
grouptrt2     0.4940     0.2788   1.772   0.0877

Residual standard error: 0.6234 on 27 degrees of freedom
Multiple R-Squared: 0.2641,     Adjusted R-squared: 0.2096
F-statistic: 4.846 on 2 and 27 degrees of freedom,      p-value: 0.01591

> help(cabbages)
> data(cabbages)                  # From the MASS package
> names(cabbages)
[1] "Cult"   "Date"   "HeadWt" "VitC"
> coplot(HeadWt~VitC|Cult+Date,data=cabbages)
```

Examination of the plot suggests that cultivars differ greatly in the variability in head weight. Variation in the vitamin C levels seems relatively consistent between cultivars.

```
> VitC.aov<-aov(VitC~Cult+Date,data=cabbages)
> summary(VitC.aov)
            Df  Sum Sq Mean Sq F value    Pr(>F)
Cult         1 2496.15 2496.15 53.0411 1.179e-09
Date         2  909.30  454.65  9.6609 0.0002486
Residuals   56 2635.40   47.06
```

*5.8.2 Shading of Kiwifruit Vines

These data (yields in kilograms) are in the data frame **kiwishade** that accompanies these notes. They are from an experiment[31] where there were four treatments - no shading, shading from August to December, shading from December to February, and shading from February to May. Each treatment appeared once in each of the three blocks. The northernmost plots were grouped in one block because they were similarly affected by shading from the sun. For the remaining two blocks shelter effects, in one case from the east and in the other case from the west, were thought more important. Results are given for each of the four vines in each plot. In experimental design parlance, the four vines within a plot constitute subplots.

The **block:shade** mean square (sum of squares divided by degrees of freedom) provides the error term. (If this is not specified, one still gets a correct analysis of variance breakdown. But the F-statistics and p-values will be wrong.)

```
> kiwishade$shade <- relevel(kiwishade$shade, ref="none")
> ## Make sure that the level "none" (no shade) is used as reference
> kiwishade.aov<-aov(yield~block+shade+Error(block:shade),data=kiwishade)
> summary(kiwishade.aov)

Error: block:shade
          Df  Sum Sq Mean Sq F value   Pr(>F)
block      2  172.35   86.17  4.1176 0.074879
shade      3 1394.51  464.84 22.2112 0.001194
Residuals  6  125.57   20.93
Error: Within
          Df Sum Sq Mean Sq F value Pr(>F)
Residuals 36 438.58   12.18
> coef(kiwishade.aov)
(Intercept) :
(Intercept)
    96.5327

block:shade :
  blocknorth    blockwest shadeAug2Dec shadeDec2Feb shadeFeb2May
    0.993125    -3.430000     3.030833   -10.281667    -7.428333

Within :
numeric(0)
```

5.9 Exercises

1. Here are two sets of data that were obtained the same apparatus, including the same rubber band, as the data frame elasticband. For the data set **elastic1**, the values are:
stretch (mm): 46, 54, 48, 50, 44, 42, 52
distance (cm): 183, 217, 189, 208, 178, 150, 249.

For the data set **elastic2**, the values are:
stretch (mm): 25, 45, 35, 40, 55, 50 30, 50, 60
distance (cm): 71, 196, 127, 187, 249, 217, 114, 228, 291.

Using a different symbol and/or a different colour, plot the data from the two data frames **elastic1** and **elastic2** on the same graph. Do the two sets of results appear consistent.

---

[31] Data relate to the paper: Snelgar, W.P., Manson. P.J., Martin, P.J. 1992. Influence of time of shading on flowering and yield of kiwifruit vines. Journal of Horticultural Science 67: 481-487.
Further details, including a diagram showing the layout of plots and vines and details of shelter, are in Maindonald (1992). The two papers have different shorthands (e.g. Sept-Nov versus Aug-Dec) for describing the time periods for which the shading was applied.

For each of the data sets **elastic1** and **elastic2**, determine the regression of stretch on distance. In each case determine (i) fitted values and standard errors of fitted values and (ii) the R^2 statistic. Compare the two sets of results. What is the key difference between the two sets of data?

Using the data frame **beams** (in the data sets accompanying these notes), carry out a regression of **strength** on **SpecificGravity** and **Moisture**. Carefully examine the regression diagnostic plot, obtained by supplying the name of the **lm** object as the first parameter to **plot()**. What does this indicate?

Using the data frame **cars** (in the *datasets* package), plot **distance** (i.e. stopping distance) versus **speed**. Fit a line to this relationship, and plot the line. Then try fitting and plotting a quadratic curve. Does the quadratic curve give a useful improvement to the fit? If you have studied the dynamics of particles, can you find a theory that would tell you how stopping distance might change with speed?5. Using the data frame **hills** (in package *MASS*), regress **time** on **distance** and **climb**. What can you learn from the diagnostic plots that you get when you plot the **lm** object? Try also regressing **log(time)** on **log(distance)** and **log(climb)**. Which of these regression equations would you prefer?

Use the method of section 5.7 to determine, formally, whether one needs different regression lines for the two data frames **elastic1** and **elastic2**.

In section 5.7 check the form of the model matrix (i) for fitting two parallel lines and (ii) for fitting two arbitrary lines when one uses the *sum* contrasts. Repeat the exercise for the *helmert* contrasts.

6. Type

```
hosp<-rep(c("RNC","Hunter","Mater"),2)
hosp
fhosp<-factor(hosp)
levels(fhosp)
```

Now repeat the steps involved in forming the factor **fhosp**, this time keeping the factor levels in the order **RNC**, **Hunter**, **Mater**.

Use **contrasts(fhosp)** to form and print out the matrix of contrasts. Do this using helmert contrasts, treatment contrasts, and sum contrasts. Using an outcome variable

```
y <- c(2,5,8,10,3,9)
```

fit the model **lm(y~fhosp),** repeating the fit for each of the three different choices of contrasts. Comment on what you get.

For which choice(s) of contrasts do the parameter estimates change when you re-order the factor levels?

In the data set **cement** (*MASS* package), examine the dependence of *y* (amount of heat produced) on *x1*, *x2*, *x3* and *x4* (which are proportions of four constituents). Begin by examining the scatterplot matrix. As the explanatory variables are proportions, do they require transformation, perhaps by taking log(x/(100-x))? What alternative strategies one might use to find an effective prediction equation?

In the data set **pressure** (*datasets* package), examine the dependence of pressure on temperature. [Transformation of temperature makes sense only if one first converts to degrees Kelvin. Consider transformation of pressure. A logarithmic transformation is too extreme; the direction of the curvature changes. What family of transformations might one try?

Modify the code in section 5.5.3 to fit: (a) a line, with accompanying 95% confidence bounds, and (b) a cubic curve, with accompanying 95% pointwise confidence bounds. Which of the three possibilities (line, quadratic, curve) is most plausible? Can any of them be trusted?

*Repeat the analysis of the **kiwishade** data (section 5.8.2), but replacing **Error(block:shade)** with **block:shade**. Comment on the output that you get from **summary()**. To what extent is it potentially misleading? Also do the analysis where the **block:shade** term is omitted altogether. Comment on that analysis.

5.10 References

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Multivariate and Tree-Based Methods

6. Multivariate and Tree-based Methods

6.1 Multivariate EDA, and Principal Components Analysis

Principal components analysis is often a useful exploratory tool for multivariate data. The idea is to replace the initial set of variables by a small number of "principal components" that together may explain most of the variation in the data. The first principal component is the component (linear combination of the initial variables) that explains the greatest part of the variation. The second principal component is the component that, among linear combinations of the variables that are uncorrelated with the first principal component, explains the greatest part of the remaining variation, and so on.

The measure of variation used is the sum of the variances of variables, perhaps after scaling the variables so that they each have variance one. An analysis that works with the unscaled variables, and hence with the variance-covariance matrix, gives a greater weight to variables that have a large variance. The common alternative – scaling variables so that they each have variance equal to one – is equivalent to working with the correlation matrix.

With biological measurement data, it is usually desirable to begin by taking logarithms. The standard deviations then measure the logarithm of relative change. Because all variables measure much the same quantity (i.e. relative variability), and because the standard deviations are typically fairly comparable, scaling to give equal variances is unnecessary.

The data set **possum** that accompanies these notes has nine morphometric measurements on each of 102 mountain brushtail possums, trapped at seven sites from southern Victoria to central Queensland[32]. It is good practice to begin by examining relevant scatterplot matrices. This may draw attention to gross errors in the data. A plot in which the sites and/or the sexes are identified will draw attention to any very strong structure in the data. For example one site may be quite different from the others, for some or all of the variables.

Taking logarithms of these data does not make much difference to the appearance that they present when plotted. This is because the ratio of largest to smallest value is relatively small, never more than 1.6, for all variables.

Here are some of the scatterplot matrix possibilities:

```
pairs(possum[,6:14], col=palette()[as.integer(possum$sex)])
pairs(possum[,6:14], col=palette()[as.integer(possum$site)])
here<-!is.na(possum$footlgth)    # We need to exclude missing values
print(sum(!here))           # Check how many values are missing
```

We now look (Figure 23) at particular views of the data that we get from a principal components analysis:

```
possum.prc <- princomp(log(possum[here,6:14]))  # Principal components
# Print scores on second pc versus scores on first pc,
# by populations and sex, identified by site
xyplot(possum.prc$scores[,2] ~
       possum.prc$scores[,1]|possum$Pop[here]+possum$sex[here], groups=possum$site,
       auto.key=list(columns=3))
```

[32] Data relate to the paper: Lindenmayer, D. B., Viggers, K. L., Cunningham, R. B., and Donnelly, C. F. 1995. Morphological variation among columns of the mountain brushtail possum, *Trichosurus caninus* Ogilby (Phalangeridae: Marsupiala). Australian Journal of Zoology 43: 449-458.

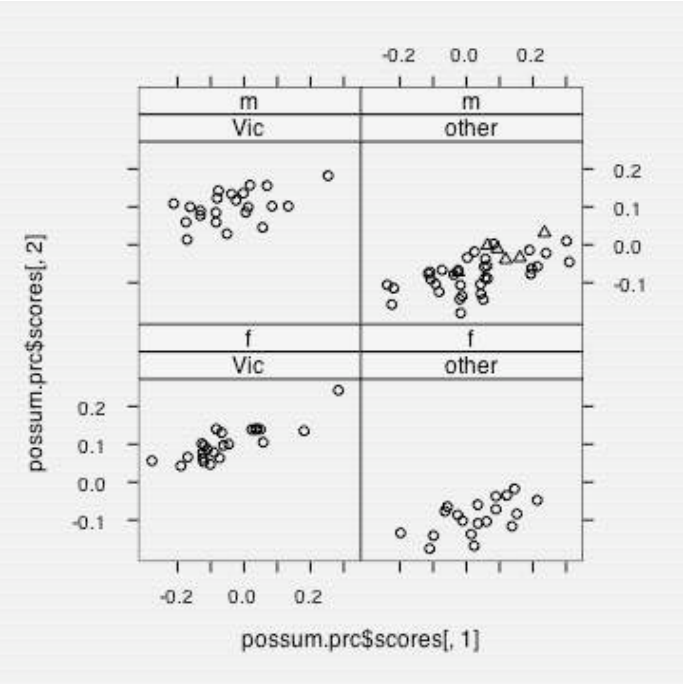

Figure 23: Second principal component versus first principal component, by population and by sex, for the possum data.

6.2 Cluster Analysis

In the language of Ripley (1996)[33], cluster analysis is a form of unsupervised classification. It is "unsupervised" because the clusters are not known in advance. There are two types of algorithms – algorithms based on *hierachical agglomeration*, and algorithms based on *iterative relocation*.

In *hierarchical agglomeration* each observation starts as a separate group. Groups that are "close" to one another are then successively merged. The output yields a hierarchical clustering tree that shows the relationships between observations and between the clusters into which they are successively merged. A judgement is then needed on the point at which further merging is unwarranted.

In *iterative relocation*, the algorithm starts with an initial classification, that it then tries to improve. How does one get the initial classification? Typically, by a prior use of a hierarchical agglomeration algorithm.

The *mva* package has the cluster analysis routines. The function dist() calculates distances. The function hclust() does hierarchical agglomerative clustering, with a choice of methods available. The function kmeans() (k-means clustering) implements iterative relocation.

6.3 Discriminant Analysis

We start with data that are classified into several groups, and want a rule that will allow us to predict the group to which a new data value will belong. In the language of Ripley (1996), our interest is in supervised classification. For example, we may wish to predict, based on prognostic measurements and outcome information for previous patients, which future patients will remain free of disease symptoms for twelve months or more.

Here are calculations for the **possum** data frame, using the **lda()** function from the Venables & Ripley *MASS* package. Our interest is in whether it is possible, on the basis of morphometric measurements, to distinguish animals from different sites. A cruder distinction is between populations, i.e. sites in Victoria (an Australian state) as opposed to sites in other states (New South Wales or Queensland). Because it has little on the distribution of variable values, I have not thought it necessary to take logarithms. I discuss this further below.

```
> library(MASS)                 # Only if not already attached.
> here<- !is.na(possum$footlgth)
```

[33] References are at the end of the chapter.

```
> possum.lda <- lda(site ~ hdlngth+skullw+totlngth+
+ taillgth+footlgth+earconch+eye+chest+belly,data=possum, subset=here)
> options(digits=4)
> possum.lda$svd   # Examine the singular values
[1] 15.7578  3.9372  3.1860  1.5078  1.1420  0.7772
>
> plot(possum.lda, dimen=3)
> # Scatterplot matrix for scores on 1st 3 canonical variates, as in Figure24
```

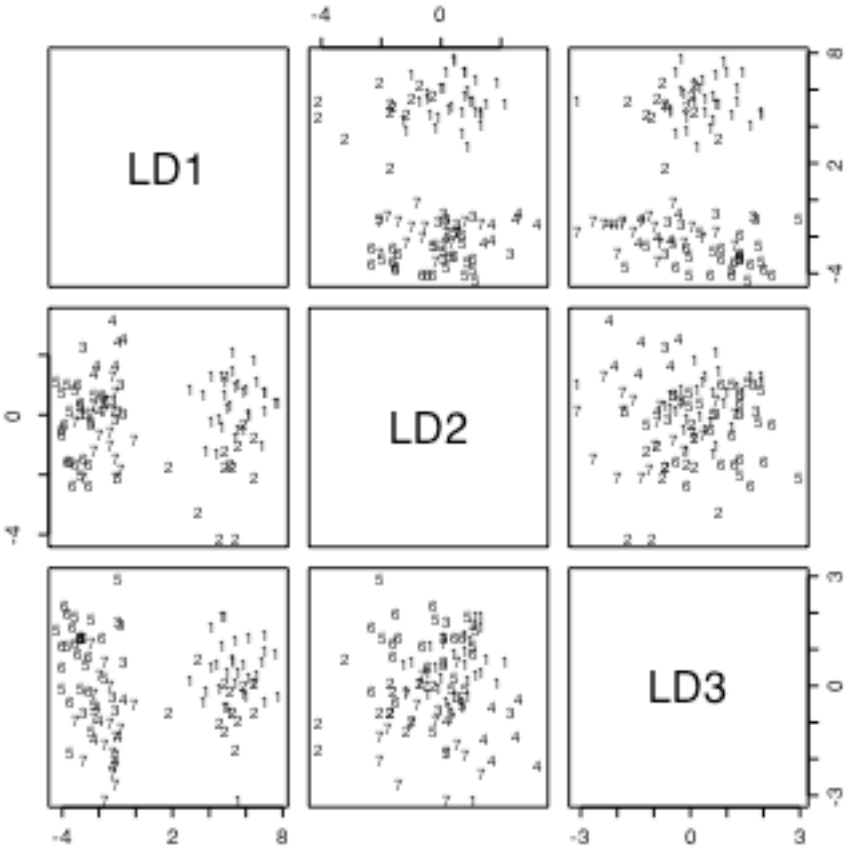

Figure 24: Scatterplot matrix of first three canonical variates.

The singular values are the ratio of between to within group sums of squares, for the canonical variates in turn. Clearly canonical variates after the third will have little if any discriminatory power. One can use **`predict.lda()`** to get (among other information) scores on the first few canonical variates.

Note that there may be interpretative advantages in taking logarithms of biological measurement data. The standard against which patterns of measurement are commonly compared is that of *allometric* growth, which implies a linear relationship between the logarithms of the measurements. Differences between different sites are then indicative of different patterns of allometric growth. The reader may wish to repeat the above analysis, but working with the logarithms of measurements.

Where there are two groups, logistic regression is often effective. A source of code for handling more general supervised classification problems is Hastie and Tibshirani's **`mda`** (mixture discriminant analysis) package. There is a brief overview of this package in the Venables and Ripley `Complements', referred to in section 13.2 .

6.4 Decision Tree models (Tree-based models)

We include tree-based classification here because it is a multivariate supervised classification, or discrimination, method. A tree-based regression approach is available for use for regression problems. Tree-based methods seem more suited to binary regression and classification than to regression with an ordinal or continuous dependent variable.

Tree-based models, also known as "Classification and Regression Trees" (CART), may be suitable for regression and classification problems when there are extensive data. One advantage of such methods is that they automatically handle non-linearity and interactions. Output includes a "decision tree" that is immediately useful for prediction.

```
library(rpart)
data(fgl)   # Forensic glass fragment data; from MASS package
glass.tree <- rpart(type ~ RI+Na+Mg+Al+Si+K+Ca+Ba+Fe, data=fgl)
plot(glass.tree);  text(glass.tree)
summary(glass.tree)
```

To use these models effectively, you also need to know about approaches to pruning trees, and about cross-validation. Methods for reduction of tree complexity that are based on significance tests at each individual node (i.e. branching point) typically choose trees that over-predict.

The Atkinson and Therneau *rpart* (recursive partitioning) package is closer to CART than is the S-PLUS *tree* library. It integrates cross-validation with the algorithm for forming trees.

6.5 Exercises

1. Using the data set **painters** (*MASS* package), apply principal components analysis to the scores for **Composition**, **Drawing**, **Colour**, and **Expression**. Examine the loadings on the first three principal components. Plot a scatterplot matrix of the first three principal components, using different colours or symbols to identify the different schools.

2. The data set **Cars93** is in the *MASS* package. Using the columns of continuous or ordinal data, determine scores on the first and second principal components. Investigate the comparison between (i) USA and non-USA cars, and (ii) the six different types (**Type**) of car. Now create a new data set in which binary factors become columns of 0/1 data, and include these in the principal components analysis.

3. Repeat the calculations of exercises 1 and 2, but this time using the function **lda()** from the *MASS* package to derive canonical discriminant scores, as in section 6.3.

4. The MASS package has the **Aids2** data set, containing de-identified data on the survival status of patients diagnosed with AIDS before July 1 1991. Use tree-based classification (**rpart()**) to identify major influences on survival.

5. Investigate discrimination between plagiotropic and orthotropic species in the data set **leafshape**[34].

6.6 References

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*7. R Data Structures

7.1 Vectors

Recall that vectors may have mode logical, numeric or character.

7.1.1 Subsets of Vectors

Recall (section 2.6.2) two common ways to extract subsets of vectors:

Specify the numbers of the elements that are to be extracted. One can use negative numbers to omit elements.

Specify a vector of logical values. The elements that are extracted are those for which the logical value is **T**. Thus suppose we want to extract values of **x** that are greater than 10.

The following demonstrates a third possibility, for vectors that have named elements:

```
> c(Andreas=178, John=185, Jeff=183)[c("John","Jeff")]
 John Jeff
  185  183
```

A vector of names has been used to extract the elements.

7.1.2 Patterned Data

Use 5:15 to generate the numbers 5, 6, …, 15. Entering 15:5 will generate the sequence in the reverse order.

To repeat the sequence (2, 3, 5) four times over, enter **rep(c(2,3,5), 4)** thus:

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

If instead one wants four 2s, then four 3s, then four 5s, enter **rep(c(2,3,5), c(4,4,4))**.

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

Note further that, in place of **c(4,4,4)** we could write **rep(4,3)**. So a further possibility is that in place of **rep(c(2,3,5), c(4,4,4))** we could enter **rep(c(2,3,5), rep(4,3)).**

In addition to the above, note that the function **rep()** has an argument **length.out**, meaning "keep on repeating the sequence until the length is **length.out**."

7.2 Missing Values

In R, the missing value symbol is **NA**. Any arithmetic operation or relation that involves **NA** generates an **NA**. This applies also to the relations **<**, **<=**, **>**, >=, **==**, **!=**. The first four compare magnitudes, **==** tests for equality, and **!=** tests for inequality. Users who do not carefully consider implications for expressions that include **Na**s may be puzzled by the results. Specifically, note that **x==NA** generates **NA**.

Be sure to use **is.na(x)** to test which values of **x** are **NA**. As **x==NA** gives a vector of **NA**s, you get no information at all about **x**. For example

```
> x <- c(1,6,2,NA)
> is.na(x)  # TRUE for when NA appears, and otherwise FALSE
[1] FALSE FALSE FALSE  TRUE
> x==NA     # All elements are set to NA
[1] NA NA NA NA
> NA==NA
[1] NA
```

WARNING: This is chiefly for those who may move between R and S-PLUS. In important respects, R's behaviour with missing values is more intuitive than that of S-PLUS. Thus in R

```
y[x>2] <- x[x>2]
```

gives the result that the naïve user might expect, i.e. replace elements of **y** with corresponding elements of **x** wherever **x>2**. Wherever **x>2** gives the result **NA**, no action is taken. In R, any **NA** in **x>2** yields a value of **NA** for **y[x>2]** on the left of the equation, and a value of **NA** for **x[x>2]** on the right of the equation.

In S-PLUS, the result on the right is the same, i.e. an **NA**. However, on the left, elements that have a subscript **NA** drop out. The vector on the left to which values will be assigned has, as a result, fewer elements than the vector on the right.

Thus the following has the effect in R that the naïve user might expect, but not in S-PLUS:

```
x <- c(1,6,2,NA,10)
y <- c(1,4,2,3,0)
y[x>2] <- x[x>2]
y
```

In S-PLUS it is essential to specify, in the example just considered:

```
y[!is.na(x)&x>2] <- x[!is.na(x)&x>2]
```

Here is a further example of R's behaviour:

```
>  x <- c(1,6,2,NA,10)
> x>2
[1] FALSE  TRUE FALSE    NA  TRUE
> x[x>3] <- c(21,22)       # Now, explain the result that follows
Warning message:
number of items to replace is not a multiple of replacement length
> x
[1]  1 21  2 NA 21
```

The safe way, in both S-PLUS and R, is to use **!is.na(x)** to limit the selection, on one or both sides as necessary, to those elements of **x** that are not **NA**s. We will have more to say on missing values in the section on data frames that now follows.

7.3 Data frames

The concept of a data frame is fundamental to the use of most of the R modelling and graphics functions. A data frame is a generalisation of a matrix, in which different columns may have different modes. All elements of any column must however have the same mode, i.e. all numeric or all factor, or all character.

Data frames where all columns hold numeric data have some, but not all, of the properties of matrices. There are important differences that arise because data frames are implemented as lists. To turn a data frame of numeric data into a matrix of numeric data, use **as.matrix()**.

Lists are discussed below, in section 7.6.

7.3.1 Extraction of Component Parts of Data frames

Consider the data frame **barley** that accompanies the lattice package:

```
> names(barley)
[1] "yield"   "variety" "year"    "site"
> levels(barley$site)
[1] "Grand Rapids"    "Duluth"          "University Farm" "Morris"
[5] "Crookston"       "Waseca"
```

We will extract the data for 1932, at the **Duluth** site.

```
> Duluth1932 <- barley[barley$year=="1932" & barley$site=="Duluth",
+ c("variety","yield")]
             variety    yield
66         Manchuria 22.56667
72           Glabron 25.86667
78          Svansota 22.23333
84            Velvet 22.46667
90             Trebi 30.60000
```

```
96           No. 457 22.70000
102          No. 462 22.50000
108         Peatland 31.36667
114          No. 475 27.36667
120 Wisconsin No. 38 29.33333
```

The first column holds the row labels, which in this case are the numbers of the rows that have been extracted. In place of **c("variety","yield")** we could have written, more simply, **c(2,4)**.

7.3.2 Data Sets that Accompany R Packages

Type in **data()** to get a list of data sets (mostly data frames) associated with all packages that are in the current search path. To get information on the data sets that are included in the *datasets* package, specify

```
data(package="datasets")
```

and similarly for any other package.

In versions of R previous to 2.0.0, it is usually necessary to specifically bring any of these data frames into the working directory. (Ensure though that the relevant package is attached.) Thus to bring in the data set **airquality** (*datasets* package), type

```
data(airquality)
```

The default Windows distribution includes many commonly required packages. Other packages must be explicitly installed. For remaining sections of these notes, the *MASS* package, which comes with the default distributution, will be used from time to time.

The *base* package, and several other packages, are automatically attached at the beginning of the session. To attach any other installed package, use the **library()** command.

7.4 Data Entry

The function **read.table()** offers a ready means to read a rectangular array into an R data frame. Suppose that the file **primates.dat** contains:

```
"Potar monkey"   10 115
Gorilla         207 406
Human           62 1320
"Rhesus monkey" 6.8 179
Chimp        52.2 440
```

Then

```
primates <- read.table("a:/primates.txt")
```

will create the data frame **primates**, from a file on the **a:** drive. The text strings in the first column will become the first column in the data frame.

Suppose that primates is a data frame with three columns – species name, body weight, and brain weight. You can give the columns names by typing in:

```
names(primates)<-c("Species","Bodywt","Brainwt")
```

Here then are the contents of the data frame.

```
> primates
        Species Bodywt Brainwt
1  Potar monkey   10.0     115
2       Gorilla  207.0     406
3         Human   62.0    1320
4 Rhesus monkey    6.8     179
5         Chimp   52.2     440
```

Specify **header=TRUE** if there is an initial how of header information. If the number of headers is one less than the number of columns of data, then the first column will be used, providing entries are unique, for row labels.

7.4.1 Idiosyncrasies

The function **read.table()** is straightforward for reading in rectangular arrays of data that are entirely numeric. When, as in the above example, one of the columns contains text strings, the column is by default stored as a factor with as many different levels as there are unique text strings[35].

Problems may arise when small mistakes in the data cause R to interpret a column of supposedly numeric data as character strings, which are automatically turned into factors. For example there may be an O (oh) somewhere where there should be a 0 (zero), or an el (**l**) where there should be a one (**1**). If you use any missing value symbols other than the default (**NA),** you need to make this explicit see section 7.3.2 below. Otherwise any appearance of such symbols as *****, period(.) and blank (in a case where the separator is something other than a space) will cause to whole column to be treated as character data.

Users who find this default behaviour of **read.table()** confusing may wish to use the parameter setting **as.is = TRUE.** [36] If the column is later required for use as a factor in a model or graphics formula, it may be necessary to make it into a factor at that time. Some functions do this conversion automatically.

7.4.2 Missing values when using `read.table()`

The function **read.table()** expects missing values to be coded as **NA**, unless you set **na.strings** to recognise other characters as missing value indicators. If you have a text file that has been output from SAS, you will probably want to set **na.strings=c(".").**

There may be multiple missing value indicators, e.g. **na.strings=c("NA",".","*","")**. The **""** will ensure that empty cells are entered as **NA**s.

7.4.3 Separators when using `read.table()`

With data from spreadsheets[37], it is sometimes necessary to use tab **("\t")** or comma as the separator. The default separator is white space. To set tab as the separator, specify **sep="\t"**.

7.5 Factors and Ordered Factors

We discussed factors in section 2.6.4. They provide an economical way to store vectors of character strings in which there are many multiple occurrences of the same strings. More crucially, they have a central role in the incorporation of qualitative effects into model and graphics formulae.

Factors have a dual identity. They are stored as integer vectors, with each of the values interpreted according to the information that is in the table of levels[38].

The data frame **islandcities** that accompanies these notes holds the populations of the 19 island nation cities with a 1995 urban centre population of 1.4 million or more. The row names are the city names, the first column (**country**) has the name of the country, and the second column (**population**) has the urban centre population, in millions. Here is a table that gives the number of times each country occurs

Australia	Cuba	Indonesia	Japan	Philippines	Taiwan	United Kingdom
3	1	4	6	2	1	2

[There are 19 cities in all.]

---

[35] Storage of columns of character strings as factors is efficient when a small number of distinct strings that are of modest length are each repeated a large number of times.

[36] Specifying **as.is = T** prevents columns of (intended or unintended) character strings from being converted into factors.

[37] One way to get mixed text and numeric data across from Excel is to save the worksheet in a **.csv** text file with comma as the separator. If for example file name is **myfile.csv** and is on drive a:, use **read.table("a:/myfile.csv", sep=",")** to read the data into R. This copes with any spaces which may appear in text strings. [But watch that none of the cell entries include commas.]

[38] Factors are vectors which have mode numeric and class "factor". They have an attribute levels that holds the level names.

Printing the contents of the column with the name **country** gives the names, not the integer values. As in most operations with factors, R does the translation invisibly. There are though annoying exceptions that can make the use of factors tricky. To be sure of getting the country names, specify

```
as.character(islandcities$country)
```

To get the integer values, specify

```
unclass(islandcities$country)
```

By default, R sorts the level names in alphabetical order. If we form a table that has the number of times that each country appears, this is the order that is used:

```
> table(islandcities$country)
 Australia Cuba Indonesia Japan Philippines Taiwan United Kingdom
         3    1         4     6           2      1              2
```

This order of the level names is purely a convenience. We might prefer countries to appear in order of latitude, from North to South. We can change the order of the level names to reflect this desired order:

```
> lev <- levels(islandcities$country)
> lev[c(7,4,6,2,5,3,1)]
[1] "United Kingdom" "Japan"          "Taiwan"         "Cuba"
[5] "Philippines"    "Indonesia"      "Australia"
> country <- factor(islandcities$country, levels=lev[c(7,4,6,2,5,3,1)])
> table(country)
 United Kingdom Japan Taiwan Cuba Philippines Indonesia Australia
              2     6      1    1           2         4         3
```

In ordered factors, i.e. factors with ordered levels, there are inequalities that relate factor levels.

Factors have the potential to cause a few surprises, so be careful! Here are two points to note:

When a vector of character strings becomes a column of a data frame, R by default turns it into a factor. Enclose the vector of character strings in the wrapper function **I()** if it is to remain character.

There are some contexts in which factors become numeric vectors. To be sure of getting the vector of text strings, specify e.g. **as.character(country)**.

To extract the numeric levels 1, 2, 3, …, specify **as.numeric(country)**.

7.6 Ordered Factors

Actually, it is their levels that are ordered. To create an ordered factor, or to turn a factor into an ordered factor, use the function **ordered()**. The levels of an ordered factor are assumed to specify positions on an ordinal scale. Try

```
> stress.level<-rep(c("low","medium","high"),2)
> ordf.stress<-ordered(stress.level, levels=c("low","medium","high"))
> ordf.stress
[1] low    medium high   low    medium high
Levels:  low < medium < high
> ordf.stress<"medium"
[1]  TRUE FALSE FALSE  TRUE FALSE FALSE
> ordf.stress>="medium"
[1] FALSE  TRUE  TRUE FALSE  TRUE  TRUE
```

Later we will meet the notion of inheritance. Ordered factors inherit the attributes of factors, and have a further ordering attribute. When you ask for the class of an object, you get details both of the class of the object, and of any classes from which it inherits. Thus:

```
> class(ordf.stress)
[1] "ordered" "factor"
```

7.7 Lists

Lists make it possible to collect an arbitrary set of R objects together under a single name. You might for example collect together vectors of several different modes and lengths, scalars, matrices or more general arrays, functions, etc. Lists can be, and often are, a rag-tag of different objects. We will use for illustration the list object that R creates as output from an **lm** calculation.

For example, consider the linear model (lm) object **elastic.lm** (c. f. sections 1.1.4 and 2.1.4) created thus:

```
elastic.lm <- lm(distance~stretch, data=elasticband)
```

It is readily verified that **elastic.lm** consists of a variety of different kinds of objects, stored as a list. You can get the names of these objects by typing in

```
> names(elastic.lm)
 [1] "coefficients"  "residuals"     "effects"       "rank"
 [5] "fitted.values" "assign"        "qr"            "df.residual"
 [9] "xlevels"       "call"          "terms"         "model"
```

The first list element is:

```
> elastic.lm$coefficients
(Intercept)     stretch
 -63.571429    4.553571
```

Alternative ways to extract this first list element are:

```
elastic.lm[["coefficients"]]
elastic.lm[[1]]
```

We can alternatively ask for the sublist whose only element is the vector **elastic.lm$coefficients**. For this, specify **elastic.lm["coefficients"]** or **elastic.lm[1]**. There is a subtle difference in the result that is printed out. The information is preceded by **$coefficients**, meaning "list element with name **coefficients**".

```
> elastic.lm[1]
$coefficients
(Intercept)     stretch
 -63.571429    4.553571
```

The second list element is a vector of length 7

```
> options(digits=3)
> elastic.lm$residuals
      1       2       3       4       5       6       7
  2.107  -0.321  18.000   1.893 -27.786  13.321  -7.214
```

The tenth list element documents the function call:

```
> elastic.lm$call
lm(formula = distance ~ stretch, data = elasticband)
> mode(elastic.lm$call)
[1] "call"
```

*7.8 Matrices and Arrays

All elements of a matrix have the same mode, i.e. all numeric, or all character. Thus a matrix is a more restricted structure than a data frame. One reason for numeric matrices is that they allow a variety of mathematical operations that are not available for data frames. Matrices are likely to be important for those users who wish to implement new regression and multivariate methods. The **matrix** construct generalises to **array**, which may have more than two dimensions.

Note that matrices are stored columnwise. Thus consider

```
> xx <- matrix(1:6,ncol=3)  # Equivalently, enter matrix(1:6,nrow=2)
> xx
     [,1] [,2] [,3]
[1,]    1    3    5
[2,]    2    4    6
```

If **xx** is any matrix, the assignment

```
x <- as.vector(xx)
```

places columns of **xx**, in order, into the vector **x**. In the example above, we get back the elements 1, 2, . . . , 6.

Matrices have the attribute "dimension". Thus

```
> dim(xx)
[1] 2 3
```

In fact a matrix *is* a vector (numeric or character) whose dimension attribute has length 2.

Now set

```
> x34 <- matrix(1:12,ncol=4)
> x34
     [,1] [,2] [,3] [,4]
[1,]    1    4    7   10
[2,]    2    5    8   11
[3,]    3    6    9   12
```

Here are examples of the extraction of columns or rows or submatrices

```
x34[2:3,c(1,4)]  # Extract rows 2 & 3 & columns 1 & 4
x34[2,]  # Extract the second row
x34[-2,]  # Extract all rows except the second
x34[-2,-3]  # Extract the matrix obtained by omitting row 2 & column 3
```

The **dimnames()** function assigns and/or extracts matrix row and column names. The **dimnames()** function gives a list, in which the first list element is the vector of row names, and the second list element is the vector of column names. This generalises in the obvious way for use with arrays, which we now discuss.

7.8.1 Arrays

The generalisation from a matrix (2 dimensions) to allow > 2 dimensions gives an array. A matrix is a 2-dimensional array.

Consider a numeric vector of length 24. So that we can easily keep track of the elements, we will make them 1, 2, .., 24. Thus

```
x <- 1:24
```

Then

```
dim(x) <- c(2,12)
```

turns this into a 2 x 12 matrix.

```
> x
     [,1] [,2] [,3] [,4] [,5] [,6] [,7] [,8] [,9] [,10] [,11] [,12]
[1,]    1    3    5    7    9   11   13   15   17    19    21    23
[2,]    2    4    6    8   10   12   14   16   18    20    22    24
```

Now try

```
> dim(x) <-c(3,4,2)
> x

, , 1
     [,1] [,2] [,3] [,4]
[1,]    1    4    7   10
[2,]    2    5    8   11
[3,]    3    6    9   12

, , 2
     [,1] [,2] [,3] [,4]
[1,]   13   16   19   22
[2,]   14   17   20   23
```

```
[3,]   15   18   21   24
```

7.8.2 Conversion of Numeric Data frames into Matrices

There are various manipulations that are available for matrices, but not for data frames. Use **`as.matrix()`** to handle any conversion that may be necessary.

7.9 Exercises

Generate the numbers 101, 102, …, 112, and store the result in the vector **`x`**.

Generate four repeats of the sequence of numbers (4, 6, 3).

Generate the sequence consisting of eight 4s, then seven 6s, and finally nine 3s. Store the numbers obtained , in order, in the columns of a 6 by 4 matrix.

Create a vector consisting of one 1, then two 2's, three 3's, etc., and ending with nine 9's.

For each of the following calculations, what you would expect? Check to see if you were right!

a)
```
answer <- c(2, 7, 1, 5, 12, 3, 4)
for (j in 2:length(answer)){ answer[j] <- max(answer[j],answer[j-1])}
```

b)
```
answer <- c(2, 7, 1, 5, 12, 3, 4)
for (j in 2:length(answer)){ answer[j] <- sum(answer[j],answer[j-1])}
```

In the built-in data frame **`airquality`** (*datasets* package)**:** (a) Determine, for each of the columns of the data frame **`airquality`** (*datasets* package), the median, mean, upper and lower quartiles, and range; (b) Extract the row or rows for which **`Ozone`** has its maximum value; (c) extract the vector of values of **`Wind`** for values of **`Ozone`** that are above the upper quartile.

Refer to the Eurasian snow data that is given in Exercise 1.6 . Find the mean of the snow cover (a) for the odd-numbered years and (b) for the even-numbered years.

Determine which columns of the data frame **`Cars93`** (*MASS* package) are factors. For each of these factor columns, print out the levels vector. Which of these are ordered factors?

Use **`summary()`** to get information about data in the data frames **`attitude (both in the datasets package),`** and **`cpus`** (*MASS* package). Write brief notes, for each of these data sets, on what this reveals.

From the data frame **`mtcars`** (*MASS* package) extract a data frame **`mtcars6`** that holds only the information for cars with 6 cylinders.

From the data frame **`Cars93`** (*MASS* package), extract a data frame which holds only information for small and sporty cars.

8. Functions

8.1 Functions for Confidence Intervals and Tests

Use the help to get complete information. Below, I note two of the simpler functions.

8.1.1 The t-test and associated confidence interval

Use **t.test()**. This allows both a one-sample and a two-sample test.

8.1.2 Chi-Square tests for two-way tables

Use **chisq.test()** for a test for no association between rows and columns in the output from **table()**. Alternatively, the argument may be a matrix. This test assumes that counts enter independently into the cells of a table. For example, the test is invalid if there is clustering in the data.

8.2 Matching and Ordering

```
> match(<vec1>, <vec2>)  ## For each element of <vec1>, returns the
                         ## position of the first occurrence in <vec2>
> order(<vector>)        ## Returns the vector of subscripts giving
                         ## the order in which elements must be taken
                         ## so that <vector> will be sorted.
> rank(<vector>)         ## Returns the ranks of the successive elements.
```

Numeric vectors will be sorted in numerical order. Character vectors will be sorted in alphanumeric order.

The operator %in% can be highly useful in picking out subsets of data. For example:

```
> x <- rep(1:5,rep(3,5))
> x
 [1] 1 1 1 2 2 2 3 3 3 4 4 4 5 5 5
> two4 <- x %in% c(2,4)
> two4
 [1] FALSE FALSE FALSE  TRUE  TRUE  TRUE FALSE FALSE FALSE  TRUE
[11]  TRUE  TRUE FALSE FALSE FALSE
> # Now pick out the 2s and the 4s
> x[two4]
[1] 2 2 2 4 4 4
```

8.3 String Functions

```
substring(<vector of text strings>, <first position>, <last position>)
nchar(<vector of text strings>)
              ## Returns vector of number of characters in each element.
```

*8.3.1 Operations with Vectors of Text Strings – A Further Example

We will work with the column **Make** in the dataset **Cars93** from the **MASS** package.

```
library(MASS)  # if needed
data(Cars93)   # if needed
```

To extract the first part of the name, up to the first space, specify

```
car.brandnames <- substring(Cars93$Make, 1, nblank-1)
> car.brandnames[1:5]
[1] "Acura" "Acura" "Audi"  "Audi"  "BMW"
```

To find the position at which the first space appears, we might do the following:

```
nblank <- sapply(Cars93$Make, function(x){n <- nchar(x);
      a <- substring(x, 1:n, 1:n); m <- match(" ", a,nomatch=1); m})
```

8.4 Application of a Function to the Columns of an Array or Data Frame

```
apply(<array>, <dimension>, <function>)
lapply(<list>, <function>)
               ## N. B. A dataframe is a list.  Output is a list.
sapply(<list>, <function>)
               ## As lapply(), but simplify (e.g. to a vector
               ## or matrix), if possible.
```

8.4.1 apply()

The function apply() can be used on data frames as well as matrices. Here is an example:

```
> apply(airquality,2,mean)   # All elements must be numeric!
  Ozone Solar.R    Wind    Temp   Month     Day
     NA      NA    9.96   77.88    6.99   15.80
> apply(airquality,2,mean,na.rm=T)
  Ozone Solar.R    Wind    Temp   Month     Day
  42.13  185.93    9.96   77.88    6.99   15.80
```

The use of **`apply(airquality,1,mean)`** will give means for each row. These are not, for these data, useful information!

8.4.2 sapply()

The function **`sapply()`** can be useful for getting information about the columns of a data frame. Here we use it to count that number of missing values in each column of the built-in data frame **`airquality`**.

```
> sapply(airquality, function(x)sum(is.na(x)))
  Ozone Solar.R    Wind    Temp   Month     Day
     37       7       0       0       0       0
```

Here are several further examples that use the data frame **`moths`** that accompanies these notes:

```
> sapply(moths,is.factor)          # Determine which columns are factors
 meters       A       P habitat
  FALSE   FALSE   FALSE    TRUE
> # How many levels does each factor have?
> sapply(moths, function(x)if(!is.factor(x))return(0) else length(levels(x)))
 meters       A       P habitat
      0       0       0       8
```

*8.5 aggregate() and tapply()

The arguments are in each case a variable, a list of factors, and a function that operates on a vector to return a single value. For each combination of factor levels, the function is applied to corresponding values of the variable. The function aggregate() returns a data frame. For example:

```
> str(cabbages)
`data.frame':   60 obs. of  4 variables:
 $ Cult  : Factor w/ 2 levels "c39","c52": 1 1 1 1 1 1 1 1 1 1 ...
 $ Date  : Factor w/ 3 levels "d16","d20","d21": 1 1 1 1 1 1 1 1 1 1 ...
 $ HeadWt: num  2.5 2.2 3.1 4.3 2.5 4.3 3.8 4.3 1.7 3.1 ...
 $ VitC  : int  51 55 45 42 53 50 50 52 56 49 ...
> attach(cabbages)
> aggregate(HeadWt, by=list(Cult=Cult, Date=Date), FUN=mean)
  Cult Date    x
1  c39  d16 3.18
2  c52  d16 2.26
3  c39  d20 2.80
4  c52  d20 3.11
```

```
5  c39  d21 2.74
6  c52  d21 1.47
```

The syntax for tapply() is similar, except that the name of the second argument is **INDEX** rather than **b**y.

The output is an array with as many dimensions as there are factors. Where there are no data values for a particular combination of factor levels, **NA** is returned.

*8.7 Merging Data Frames

The data frame **Cars93** (*MASS* package) holds extensive information on data from 93 cars on sale in the USA in 1993. One of the variables, stored as a factor, is **Type**. I have created a data frame **Cars93.summary**, in which the row names are the distinct values of Type, while a later column holds two character abbreviations of each of the car types, suitable for use in plotting.

```
> Cars93.summary
        Min.passengers Max.passengers No.of.cars abbrev
Compact              4              6         16      C
Large                6              6         11      L
Midsize              4              6         22      M
Small                4              5         21     Sm
Sporty               2              4         14     Sp
Van                  7              8          9      V
```

We proceed thus to add a column that has the abbreviations to the data frame. Here however our demands are simple, and we can proceed thus:

```
new.Cars93 <- merge(x=Cars93,y=Cars93.summary[,4,drop=F],
                    by.x="Type",by.y="row.names")
```

This creates a data frame that has the abbreviations in the additional column with name **"abbrev"**.

If there had been rows with missing values of **Type**, these would have been omitted from the new data frame. This can be avoided by making sure that **Type** has NA as one of its levels, in both data frames.

8.8 Dates

Since version 1.9.0, the *date* package has been superseded by functions for working with dates that are in R *base*. See **help(Dates), help(as.Date)** and **help(format.Date**) for detailed information.

Use **as.Date()** to convert text strings into dates. The default is that the year comes first, then the month, and then the day of the month, thus:

```
> # Electricity Billing Dates
> dd <- as.Date(c("2003/08/24","2003/11/23","2004/02/22","2004/05/> diff(dd)
Time differences of 91, 91, 91 days
```

Use **format()** to set or change the way that a date is formatted. The following are a selection of the symbols used:

%d: day, as number

%a: abbreviated weekday name (**%A**: unabbreviated)

%m: month (00-12)

%b: month abbreviated name (**%B**: unabbreviated)

%y: final two digits of year (**%Y**: all four digits)

The default format is **"%Y-%m-%d**".

The function **as.Date()** will take a vector of character strings that has an appropriate format, and convert it into a dates object. By default, dates are stored using January 1 1970 as origin. This becomes apparent when **as.integer()** is used to convert a date into an integer value. Here are examples:

```
> as.Date("1/1/1960", format="%d/%m/%Y")
[1] "1960-01-01"
```

```
> as.Date("1:12:1960",format="%d:%m:%Y")
[1] "1960-12-01"
> as.Date("1960-12-1")-as.Date("1960-1-1")
as.Date("1960-12-1")-as.Date("1960-1-1")
> as.Date("31/12/1960","%d/%m/%Y")
[1] "1960-12-31"
> as.integer(as.Date("1/1/1970","%d/%m/%Y")
[1] 0
> as.integer(as.Date("1/1/2000","%d/%m/%Y"))
[1] 10957
```

The function **format()** allows control of the formatting of dates. See **help(format.Date)**.

```
> dec1 <- as.Date("2004-12-1")
> format(dec1, format="%b %d %Y")
[1] "Dec 01 2004"
> format(dec1, format="%a %b %d %Y")
[1] "Wed Dec 01 2004"
```

8.9. Writing Functions and other Code

We have already met several functions. Here is a function to convert Fahrenheit to Celsius:

```
> fahrenheit2celsius <- function(fahrenheit=32:40)(fahrenheit-32)*5/9
> # Now invoke the function
> fahrenheit2celsius(c(40,50,60))
[1]  4.444444 10.000000 15.555556
```

The function returns the value **(fahrenheit-32)*5/9**. More generally, a function returns the value of the last statement of the function. Unless the result from the function is assigned to a name, the result is printed.

Here is a function that prints out the mean and standard deviation of a set of numbers:

```
> mean.and.sd <- function(x=1:10){
+ av <- mean(x)
+ sd <- sqrt(var(x))
+ c(mean=av, SD=sd)
+ }
>
> # Now invoke the function
> mean.and.sd()
    mean       SD
5.500000 3.027650

> mean.and.sd(hills$climb)
    mean       SD
1815.314 1619.151
```

8.9.1 Syntax and Semantics

A function is created using an assignment. On the right hand side, the parameters appear within round brackets. You can, if you wish, give a default. In the example above the default was x = 1:10, so that users can run the function without specifying a parameter, just to see what it does.

Following the closing ")" the function body appears. Except where the function body consists of just one statement, this is enclosed between curly braces ({ }). The return value usually appears on the final line of the function body. In the example above, this was the vector consisting of the two named elements mean and sd.

8.9.3 A Function that gives Data Frame Details

First we will define a function that accepts a vector **x** as its only argument. It will allow us to determine whether x is a factor, and if a factor, how many levels it has. The built-in function **is.factor()** will return T if **x** is a factor, and otherwise F. The following function **faclev()** uses **is.factor()** to test whether **x** is a factor. It prints out 0 if **x** is not a factor, and otherwise the number of levels of **x**.

```
> faclev <- function(x)if(!is.factor(x))return(0) else
                                  length(levels(x))
```

Earlier, we encountered the function **sapply() that** can be used to repeat a calculation on all columns of a data frame. [More generally, the first argument of **sapply()** may be a list.] To apply **faclev()** to all columns of the data frame **moths** we can specify

```
> sapply(moths, faclev)
```

We can alternatively give the definition of **faclev** directly as the second argument of **sapply**, thus

```
> sapply(moths, function(x)if(!is.factor(x))return(0)
else length(levels(x)))
```

Finally, we may want to do similar calculations on a number of different data frames. So we create a function **check.df()** that encapsulates the calculations. Here is the definition of **check.df()**.

```
check.df <- function(df=moths)
            sapply(df, function(x)if(!is.factor(x))return(0) else
                                                  length(levels(x)))
```

8.9.4 Compare Working Directory Data Sets with a Reference Set

At the beginning of a new session, we might store the names of the objects in the working directory in the vector **dsetnames**, thus:

```
dsetnames <- objects()
```

Now suppose that we have a function **additions()**, defined thus:

```
additions <- function(objnames = dsetnames)
{
        newnames <- objects(pos=1)
        existing <- as.logical(match(newnames, objnames, nomatch = 0))
        newnames[!existing]
}
```

At some later point in the session, we can enter

```
additions(dsetnames)
```

to get the names of objects that have been added since the start of the session.

8.9.5 Issues for the Writing and Use of Functions

There can be many functions. Choose their names carefully, so that they are meaningful.

Choose meaningful names for arguments, even if this means that they are longer than one would like. Remember that they can be abbreviated in actual use.

As far as possible, make code self-documenting. Use meaningful names for R objects. Ensure that the names used reflect the hierarchies of files, data structures and code.

R allows the use of names for elements of vectors and lists, and for rows and columns of arrays and dataframes. Consider the use of names rather than numbers when you pull out individual elements, columns etc. Thus **dead.tot[,"dead"]** is more meaningful and safer than **dead.tot[,2]**.

Settings that may need to change in later use of the function should appear as default settings for parameters. Use lists, where this seems appropriate, to group together parameters that belong together conceptually.

Where appropriate, provide a demonstration mode for functions. Such a mode will print out summary information on the data and/or on the results of manipulations prior to analysis, with appropriate labelling. The code needed to implement this feature has the side-effect of showing by example what the function does, and may be useful for debugging.

Break functions up into a small number of sub-functions or "primitives". Re-use existing functions wherever possible. Write any new "primitives" so that they can be re-used. This helps ensure that functions contain well-tested and well-understood components. Watch the r-help electronic mail list (section 13.3) for useful functions for routine tasks.

Wherever possible, give parameters sensible defaults. Often a good strategy is to use as defaults parameters that will serve for a demonstration run of the function.

NULL is a useful default where the parameter mostly is not required, but where the parameter if it appears may be any one of several types of data structure. The test **`if(!is.null())`** then determines whether one needs to investigate that parameter further.

Structure computations so that it is easy to retrace them. For this reason substantial chunks of code should be incorporated into functions sooner rather than later.

Structure code to avoid multiple entry of information.

8.9.6 Functions as aids to Data Management

Where data, labelling etc must be pulled together from a number of sources, and especially where you may want to retrace your steps some months later, take the same care over structuring data as over structuring code. Thus if there is a factorial structure to the data files, choose file names that reflect it. You can then generate the file names automatically, using **`paste()`** to glue the separate portions of the name together.

Lists are a useful mechanism for grouping together all data and labelling information that one may wish to bring together in a single set of computations. Use as the name of the list a unique and meaningful identification code. Consider whether you should include objects as list items, or whether identification by name is preferable. Bear in mind, also, the use of **`switch()`**, with the identification code used to determine what **`switch()`** should pick out, to pull out specific information and data that is required for a particular run.

Concentrate in one function the task of pulling together data and labelling information, perhaps with some subsequent manipulation, from a number of separate files. This structures the code, and makes the function a source of documentation for the data.

Use user-defined data frame attributes to document your data. For example, given the data frame **`elastic`** containing the amount of stretch and resulting distance of movement of a rubber band, one might specify

```
attributes(elasticband)$title <-
    "Extent of stretch of band, and Resulting Distance"
```

8.9.7 Graphs

Use graphs freely to shed light both on computations and on data. One of R's big pluses is its tight integration of computation and graphics.

8.9.8 A Simulation Example

We would like to know how well such a student might do by random guessing, on a multiple choice test consisting of 100 questions each with five alternatives. We can get an idea by using simulation. Each question corresponds to an independent Bernoulli trial with probability of success equal to 0.2. We can simulate the correctness of the student for each question by generating an independent uniform random number. If this number is less than .2, we say that the student guessed correctly; otherwise, we say that the student guessed incorrectly.

This will work, because the probability that a uniform random variable is less than .2 is exactly .2, while the probability that a uniform random variable exceeds .2 is exactly .8, which is the same as the probability that the student guesses incorrectly. Thus, the uniform random number generator is simulating the student. R can do this as follows:

```
guesses <- runif(100)
correct.answers <- 1*(guesses < .2)
correct.answers
```

The multiplication by 1 causes **`(guesses<.2)`**, which is calculated as **`TRUE`** or **`FALSE`**, to be coerced to 1 (**`TRUE`**) or 0 (**`FALSE`**). The vector **`correct.answers`** thus contains the results of the student's guesses. A 1 is recorded each time the student correctly guesses the answer, while a 0 is recorded each time the student is wrong.

One can thus write an R function that simulates a student guessing at a True-False test consisting of some arbitrary number of questions. We leave this as an exercise.

8.9.9 Poisson Random Numbers

One can think of the Poisson distribution as the distribution of the total for occurrences of rare events. For example, an accident at an intersection on any one day should be a rare event. The total number of accidents over the course of a year may well follow a distribution that is close to Poisson. [However the total number of people injured is unlikely to follow a Poisson distribution. Why?] The function using **`rpois()`** generates Poisson random numbers. Suppose for example traffic accidents occur at an intersection with a Poisson distribution that has a mean rate of 3.7 per year. To simulate the annual number of accidents for a 10-year period, we can specify **`rpois(10,3.7)`**. We pursue the Poisson distribution in an exercise below.

8.10 Exercises

1. Use the **`round`** function together with **`runif()`** to generate 100 random integers between 0 and 99. Now look up the help for **`sample()`**, and use it for the same purpose.

2. Write a function that will take as its arguments a list of response variables, a list of factors, a data frame, and a function such as mean or median. It will return a data frame in which each value for each combination of factor levels is summarised in a single statistic, for example the mean or the median.

3. Determine the number of days, according to R, between the following dates:

January 1 in the year 1700, and January 1 in the year 1800

January 1 in the year 1998, and January 1 in the year 2000

4. The supplied data frame **`milk`** has columns **`four`** and **`one`**. Seventeen people rated the sweetness of each of two samples of a milk product on a continuous scale from 1 to 7, one sample with four units of additive and the other with one unit of additive. Here is a function that plots, for each patient, the **`four`** result against the **`one`** result, but insisting on the same range for the x and y axes.

```
plot.one <- function(){
  xyrange <- range(milk)   # Calculates the range of all values in the data frame
  par(pin=c(6.75, 6.75))      # Set plotting area = 6.75 in. by 6.75 in.
  plot(four, one, data=milk, xlim=xyrange, ylim=xyrange, pch=16)
  abline(0,1)                  # Line where four = one
}
```

Rewrite this function so that, given the name of a data frame and of any two of its columns, it will plot the second named column against the first named column, showing also the line $y=x$.

5. Write a function that prints, with their row and column labels, only those elements of a correlation matrix for which abs(correlation) >= 0.9.

6. Write your own wrapper function for one-way analysis of variance that provides a side by side boxplot of the distribution of values by groups. If no response variable is specified, the function will generate random normal data (no difference between groups) and provide the analysis of variance and boxplot information for that.

7. Write a function that computes a moving average of order 2 of the values in a given vector. Apply the function to the data (in the data set **`huron`** that accompanies these notes) for the levels of Lake Huron. Repeat for a moving average of order 3.

9. Find a way of computing the moving averages in exercise 3 that does not involve the use of a for loop.

10. Create a function to compute the average, variance and standard deviation of 1000 randomly generated uniform random numbers, on [0,1]. (Compare your results with the theoretical results: the expected value of a uniform random variable on [0,1] is 0.5, and the variance of such a random variable is 0.0833.)

11. Write a function that generates 100 independent observations on a uniformly distributed random variable on the interval [3.7, 5.8]. Find the mean, variance and standard deviation of such a uniform random variable. Now modify the function so that you can specify an arbitrary interval.

12. Look up the help for the **`sample()`** function. Use it to generate 50 random integers between 0 and 99, sampled without replacement. (This means that we do not allow any number to be sampled a second time.) Now, generate 50 random integers between 0 and 9, with replacement.

13. Write an R function that simulates a student guessing at a True-False test consisting of 40 questions. Find the mean and variance of the student's answers. Compare with the theoretical values of .5 and .25.

14. Write an R function that simulates a student guessing at a multiple choice test consisting of 40 questions, where there is chance of 1 in 5 of getting the right answer to each question. Find the mean and variance of the student's answers. Compare with the theoretical values of .2 and .16.

15. Write an R function that simulates the number of working light bulbs out of 500, where each bulb has a probability .99 of working. Using simulation, estimate the expected value and variance of the random variable X, which is 1 if the light bulb works and 0 if the light bulb does not work. What are the theoretical values?

16. Write a function that does an arbitrary number **n** of repeated simulations of the number of accidents in a year, plotting the result in a suitable way. Assume that the number of accidents in a year follows a Poisson distribution. Run the function assuming an average rate of 2.8 accidents per year.

17. Write a function that simulates the repeated calculation of the coefficient of variation (= the ratio of the mean to the standard deviation), for independent random samples from a normal distribution.

18. Write a function that, for any sample, calculates the median of the absolute values of the deviations from the sample median.

*19. Generate random samples from normal, exponential, t (2 d. f.), and t (1 d. f.), thus:

a) `xn<-rnorm(100)` b) `xe<-rexp(100)`

c) `xt2<-rt(100, df=2)` d) `xt2<-rt(100, df=1`)

Apply the function from exercise 17 to each sample. Compare with the standard deviation in each case.

*20. The vector **x** consists of the frequencies

```
5, 3, 1, 4, 6
```

The first element is the number of occurrences of level 1, the second is the number of occurrences of level 2, and so on. Write a function that takes any such vector x as its input, and outputs the vector of factor levels, here

```
1 1 1 1 1 2 2 2 3 . . .
```

[You'll need the information that is provided by cumsum(x). Form a vector in which 1's appear whenever the factor level is incremented, and is otherwise zero. . . .]

*21. Write a function that calculates the minimum of a quadratic, and the value of the function at the minimum.

*22. A "between times" correlation matrix, has been calculated from data on heights of trees at times 1, 2, 3, 4, . . . Write a function that calculates the average of the correlations for any given lag.

*23. Given data on trees at times 1, 2, 3, 4, . . ., write a function that calculates the matrix of "average" relative growth rates over the several intervals.

[The relative growth rate may be defined as $\frac{1}{w}\frac{dw}{dt} = \frac{d\log w}{dt}$. Hence it is reasonable to calculate the average over the interval from t_1 to t_2 as $\frac{\log w_2 - \log w_1}{t_2 - t_1}$.]

*9. GLM, and General Non-linear Models

GLM models are Generalized Linear Models. They extend the multiple regression model. The GAM (Generalized Additive Model) model is a further extension.

9.1 A Taxonomy of Extensions to the Linear Model

R allows a variety of extensions to the multiple linear regression model. In this chapter we describe the alternative functional forms.

The basic model formulation[39] is:

Observed value = Model Prediction + Statistical Error

Often it is assumed that the statistical error values (values of □ in the discussion below) are independently and identically distributed as Normal. Generalized Linear Models, and the other extensions we describe, allow a variety of non-normal distributions. In the discussion of this section, our focus is on the form of the model prediction, and we leave until later sections the discussion of different possibilities for the "error" distribution.

Multiple regression model

$y = \square + \square_1 x_1 + \square_2 x_2 + \ldots + \square_p x_p + \square$

Use `lm()` to fit multiple regression models. The various other models we describe are, in essence, generalizations of this model.

Generalized Linear Model (e.g. logit model)

$y = g(a + b_1 x_1) + \square$

Here $g(.)$ is selected from one of a small number of options.

For logit models, $y = \pi + \varepsilon$, where

$$\log(\frac{\pi}{1-\pi}) = a + b_1 x_1$$

Here □ is an expected proportion, and

$$\log(\frac{\pi}{1-\pi}) \quad = \text{logit}(\pi) \text{ is log(odds).}$$

We can turn this model around, and write

$$y = g(a + b_1 x_1) + \varepsilon = \frac{\exp(a + b_1 x_1)}{1 + \exp(a + b_1 x_1)} + \varepsilon$$

Here $g(.)$ undoes the logit transformation.

We can add more explanatory variables: $a + b_1 x_1 + \ldots + b_p x_p$.

Use `glm()` to fit generalized linear models.

Additive Model

$$y = \phi_1(x_1) + \phi_2(x_2) + \ldots. + \phi_p(x_p) + \varepsilon$$

Additive models are a generalization of `lm` models. In 1 dimension $y = \phi_1(x_1) + \varepsilon$

Some of $z_1 = \phi_1(x_1), z_2 = \phi_2(x_2), \ldots, z_p = \phi_p(x_p)$ may be smoothing functions, while others may be the usual linear model terms. The constant term gets absorbed into one or more of the ϕs.

Generalized Additive Model

---

[39] There are various generalizations. Models which have this form may be nested within other models which have this basic form. Thus there may be `predictions' and `errors' at different levels within the total model.

$$y = g(\phi_1(x_1) + \phi_2(x_2) + ... + \phi_p(x_p)) + \varepsilon$$

Generalized Additive Models are a generalisation of Generalized Linear Models. For example, *g*(.) may be the function that undoes the logit transformation, as in a logistic regression model.

Some of $z_1 = \phi_1(x_1), z_2 = \phi_2(x_2), ..., z_p = \phi_p(x_p)$ may be smoothing functions, while others may be the usual linear model terms.

We can transform to get the model $y = g(z_1 + z_2 + ... + z_p) + \varepsilon$

Notice that even if *p* = 1, we may still want to retain both $\phi_1(.)$ and *g*(.), i.e. $y = g(\phi_1(x_1)) + \varepsilon$.
The reason is that *g*(.) is a specific function, such as the inverse of the logit function. The function *g*(.) does as much as it can of the task of transformation, with $\phi_1(.)$ doing anything more that seems necessary.

The fitting of spline (**bs()** or **ns()**) terms in a linear model or a generalized linear model can be a good alternative to the use of a full generalized additive model.

9.2 Logistic Regression

We will use a logistic regression model as a starting point for discussing Generalized Linear Models.

With proportions that range from less than 0.1 to 0.99, it is not reasonable to expect that the expected proportion will be a linear function of *x*. Some such transformation (`link' function) as the logit is required. A good way to think about logit models is that they work on a log(odds) scale. If *p* is a probability (e.g. that horse A will win the race), then the corresponding odds are *p*/(1-*p*), and

$$\text{log(odds)} = \log(\frac{p}{1-p}) = \log(p) - \log(1-p)$$

The linear model predicts, not *p*, but $\log(\frac{p}{1-p})$. Figure 25 shows the logit transformation.

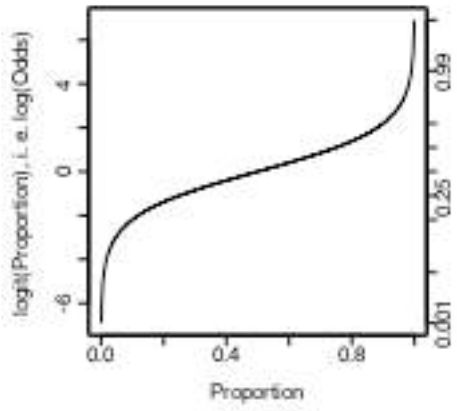

Figure 25: The logit or log(odds) transformation. Shown here is a plot of log(odds) versus proportion. Notice how the range is stretched out at both ends.

The logit or log(odds) function turns expected proportions into values that may range from -□ to +□. It is not satisfactory to use a linear model to predict proportions. The values from the linear model may well lie outside the range from 0 to 1. It is however in order to use a linear model to predict logit(proportion). The logit function is an example of a link function.

There are various other link functions that we can use with proportions. One of the commonest is the complementary log-log function.

9.2.1 Anesthetic Depth Example

Thirty patients were given an anesthetic agent that was maintained at a pre-determined [alveolar] concentration for 15 minutes before making an incision[40]. It was then noted whether the patient moved, i.e. jerked or twisted. The interest is in estimating how the probability of jerking or twisting varies with increasing concentration of the anesthetic agent.

The response is best taken as nomove, for reasons that will emerge later. There is a small number of concentrations; so we begin by tabulating proportion that have the nomove outcome against concentration.

	Alveolar Concentration					
Nomove	0.8	1	1.2	1.4	1.6	2.5
0	6	4	2	2	0	0
1	1	1	4	4	4	2
Total	7	5	6	6	4	2

Table 1: Patients moving (0) and not moving (1), for each of six different alveolar concentrations.

Figure 26 then displays a plot of these proportions.

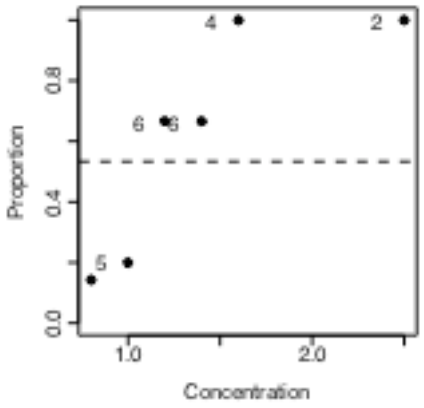

Figure 26: Plot, versus concentration, of proportion of patients not moving. The horizontal line estimates the expected proportion of nomoves if the concentration had no effect.

We fit two models, the logit model and the complementary log-log model. We can fit the models either directly to the 0/1 data, or to the proportions in Table 1. To understand the output, you need to know about "deviances". A deviance has a role very similar to a sum of squares in regression. Thus we have:

Regression	Logistic regression
degrees of freedom	degrees of freedom
sum of squares	deviance
mean sum of squares	mean deviance
(divide by d.f.)	(divide by d.f.)
We prefer models with a small mean residual sum of squares.	We prefer models with a small mean deviance.

[40] I am grateful to John Erickson (Anesthesia and Critical Care, University of Chicago) and to Alan Welsh (Centre for Mathematics & its Applications, Australian National University) for allowing me use of these data.

If individuals respond independently, with the same probability, then we have Bernoulli trials. Justification for assuming the same probability will arise from the way in which individuals are sampled. While individuals will certainly be different in their response the notion is that, each time a new individual is taken, they are drawn at random from some larger population. Here is the R code:

```
> anaes.logit <- glm(nomove ~ conc, family = binomial(link = logit),
+        data = anesthetic)
```

The output summary is:

```
> summary(anaes.logit)

Call: glm(formula = nomove ~ conc, family = binomial(link = logit),
         data = anesthetic)
Deviance Residuals:
   Min     1Q Median    3Q  Max
 -1.77 -0.744 0.0341 0.687 2.07

Coefficients:
            Value Std. Error t value
(Intercept) -6.47       2.42   -2.68
       conc  5.57       2.04    2.72

(Dispersion Parameter for Binomial family taken to be 1 )

    Null Deviance: 41.5 on 29 degrees of freedom
Residual Deviance: 27.8 on 28 degrees of freedom
Number of Fisher Scoring Iterations: 5

Correlation of Coefficients:
     (Intercept)
conc -0.981
```

Fig. 27 is a graphical summary of the results:

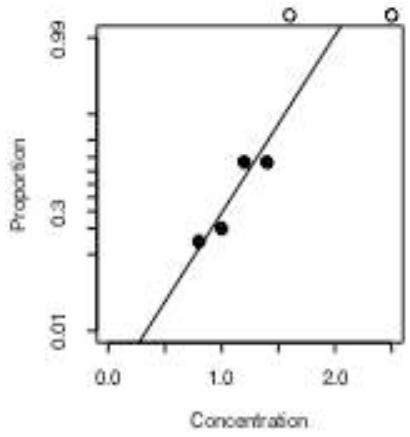

Figure 27: Plot, versus concentration, of log(odds) [= logit(proportion)] of patients not moving. The line is the estimate of the proportion of moves, based on the fitted logit model.

With such a small sample size it is impossible to do much that is useful to check the adequacy of the model.

Try also **`plot(anaes.logit)`**.

9.3 glm models (Generalized Linear Regression Modelling)

In the above we had

```
anaes.logit <- glm(nomove ~ conc, family = binomial(link = logit),
                   data=anesthetic)
```

The **family** parameter specifies the distribution for the dependent variable. There is an optional argument that allows us to specify the link function. Below we give further examples.

9.3.2 Data in the form of counts

Data that are in the form of counts can often be analysed quite effectively assuming the **poisson** family. The link that is commonly used here is **log**. The **log** link transforms from positive numbers to numbers in the range -□ to +□ that a linear model may predict.

9.3.3 The gaussian family

If no family is specified, then the family is taken to be **gaussian**. The default link is then the **identity,** as for an **lm** model. This way of formulating an **lm** type model does however have the advantage that one is not restricted to the identity link.

```
data(airquality)
air.glm<-glm(Ozone^(1/3) ~ Solar.R + Wind + Temp, data = airquality)
    # Assumes gaussian family, i.e. normal errors model
summary(air.glm)
```

9.4 Models that Include Smooth Spline Terms

These make it possible to fit spline and other smooth transformations of explanatory variables. One can request a `smooth' b-spline or n-spline transformation of a column of the X matrix. In place of **x** one specifies **bs(x)**or **ns(x)**. One can control the smoothness of the curve, but often the default works quite well. You need to install the *splines* package. R does not at present have a facility for plots that show the contribution of each term to the model.

9.4.1 Dewpoint Data

The data set **dewpoint**[41] has columns **mintemp**, **maxtemp** and **dewpoint**. The dewpoint values are averages, for each combination of mintemp and maxtemp, of monthly data from a number of different times and locations. We fit the model:

dewpoint = mean of **dewpoint** + smooth(**mintemp**) + smooth(**maxtemp**)

Taking out the mean is a computational convenience. Also it provides a more helpful form of output. Here are details of the calculations:

```
dewpoint.lm <- lm(dewpoint ~ bs(mintemp) + bs(maxtemp),
                  data = dewpoint)
options(digits=3)
summary(dewpoint.lm)
```

9.5 Survival Analysis

For example times at which subjects were either lost to the study or died ("failed") may be recorded for individuals in each of several treatment groups. Engineering or business failures can be modelled using this same methodology. The R *survival* package has state of the art abilities for survival analysis.

---

[41] I am grateful to Dr Edward Linacre, Visiting Fellow, Geography Department, Australian National University, for making these data available.

9.6 Non-linear Models

You can use **nls()** (non-linear least squares) to obtain a least squares fit to a non-linear function.

9.7 Model Summaries

Type in

```
methods(summary)
```

to get a list of the summary methods that are available. You may want to mix and match, e.g. **summary.lm()** on an aov or glm object. The output may not be what you might expect. So be careful!

9.8 Further Elaborations

Generalised Linear Models were developed in the 1970s. They unified a huge range of diverse methodology. They have now become a stock-in-trade of statistical analysts. Their practical implementation built on the powerful computational abilities that, by the 1970s, had been developed for handling linear model calculations.

Practical data analysis demands further elaborations. An important elaboration is to the incorporation of more than one term in the error structure. The R **nlme** package implements such extensions, both for linear models and for a wide class of nonlinear models.

Each such new development builds on the theoretical and computational tools that have arisen from earlier developments. Exciting new analysis tools will continue to appear for a long time yet. This is fortunate. Most professional users of R will regularly encounter data where the methodology that the data ideally demands is not yet available.

9.9 Exercises

1. Fit a Poisson regression model to the data in the data frame **moths** that Accompanies these notes. Allow different intercepts for different habitats. Use log(meters) as a covariate.

9.10 References

Dobson, A. J. 1983. An Introduction to Statistical Modelling. Chapman and Hall, London.

Hastie, T. J. and Tibshirani, R. J. 1990. Generalized Additive Models. Chapman and Hall, London.

Maindonald J H and Braun W J 2003. Data Analysis and Graphics Using R – An Example-Based Approach. Cambridge University Press.

McCullagh, P. and Nelder, J. A., 2nd edn., 1989. Generalized Linear Models. Chapman and Hall.

Venables, W. N. and Ripley, B. D., 2nd edn 1997. Modern Applied Statistics with S-Plus. Springer, New York.

*10. Multi-level Models, Repeated Measures and Time Series

10.1 Multi-Level Models, Including Repeated Measures Models

Models have both a fixed effects structure and an error structure. For example, in an inter-laboratory comparison there may be variation between laboratories, between observers within laboratories, and between multiple determinations made by the same observer on different samples. If we treat laboratories and observers as random, the only fixed effect is the mean.

The functions **`lme()`** and **`nlme()`**, from the Pinheiro and Bates *nlme* package, handle models in which a repeated measures error structure is superimposed on a linear (**`lme`**) or non-linear (**`nlme`**) model. Version 3 of lme is broadly comparable to *Proc Mixed* in the widely used SAS statistical package. The function **`lme`** has associated with it highly useful abilities for diagnostic checking and for various insightful plots.

There is a strong link between a wide class of repeated measures models and time series models. In the time series context there is usually just one realisation of the series, which may however be observed at a large number of time points. In the repeated measures context there may be a large number of realisations of a series that is typically quite short.

10.1.1 The Kiwifruit Shading Data, Again

Refer back to section 5.8.2 for details of these data. The fixed effects are **`block`** and treatment (**`shade`**). The random effects are **`block`** (though making block a random effect is optional, for purposes of comparing treatments), **`plot`** within **`block`**, and units within each block/plot combination. Here is the analysis:

```
> library(nlme)
Loading required package: nls
> kiwishade$plot<-factor(paste(kiwishade$block, kiwishade$shade,
    sep="."))
> kiwishade.lme<-lme(yield~shade,random=~1|block/plot, data=kiwishade)
> summary(kiwishade.lme)
Linear mixed-effects model fit by REML
 Data: kiwishade
       AIC      BIC    logLik
  265.9663 278.4556 -125.9831

Random effects:
 Formula: ~1 | block
        (Intercept)
StdDev:    2.019373

 Formula: ~1 | plot %in% block
        (Intercept) Residual
StdDev:    1.478639 3.490378

Fixed effects: yield ~ shade
                 Value Std.Error DF  t-value p-value
(Intercept)  100.20250  1.761621 36 56.88086  <.0001
shadeAug2Dec   3.03083  1.867629  6  1.62282  0.1558
shadeDec2Feb -10.28167  1.867629  6 -5.50520  0.0015
shadeFeb2May  -7.42833  1.867629  6 -3.97741  0.0073
 Correlation:
             (Intr) shdA2D shdD2F
shadeAug2Dec -0.53
shadeDec2Feb -0.53   0.50
shadeFeb2May -0.53   0.50   0.50

Standardized Within-Group Residuals:
```

```
       Min         Q1        Med         Q3        Max
-2.4153887 -0.5981415 -0.0689948  0.7804597  1.5890938
Number of Observations: 48
Number of Groups:
          block plot %in% block
              3              12
> anova(kiwishade.lme)
            numDF denDF  F-value p-value
(Intercept)     1    36 5190.552  <.0001
shade           3     6   22.211  0.0012
```

This was a balanced design, which is why section 5.8.2 could use **aov()**. We can get an output summary that is helpful for showing how the error mean squares match up with standard deviation information given above thus:

```
> intervals(kiwishade.lme)
Approximate 95% confidence intervals

 Fixed effects:
                lower       est.      upper
(Intercept)   96.62977 100.202500 103.775232
shadeAug2Dec  -1.53909   3.030833   7.600757
shadeDec2Feb -14.85159 -10.281667  -5.711743
shadeFeb2May -11.99826  -7.428333  -2.858410

 Random Effects:
  Level: block
                   lower     est.   upper
sd((Intercept)) 0.5473014 2.019373 7.45086
  Level: plot
                   lower     est.    upper
sd((Intercept)) 0.3702555 1.478639 5.905037

 Within-group standard error:
   lower     est.    upper
2.770678 3.490378 4.397024
```

We are interested in the three sd estimates. By squaring the standard deviations and converting them to variances we get the information in the following table:

	Variance component	Notes
block	$2.019^2 = 4.076$	Three blocks
plot	$1.479^2 = 2.186$	4 plots per block
residual (within group)	$3.490^2 = 12.180$	4 vines (subplots) per plot

The above gives the information for an analysis of variance table. We have:

	Variance component	Mean square for anova table	d.f.
block	4.076	12.180 + 4 □ 2.186 + 16 □ 4.076 = 86.14	2 (3-1)
plot	2.186	12.180 + 4 □ 2.186 = 20.92	6 (3-1) □(2-1)
residual (within gp)	12.180	12.18	3□4□(4-1)

Now fsee where these same pieces of information appeared in the analysis of variance table of section 5.8.2:

```
> kiwishade.aov<-aov(yield~block+shade+Error(block:shade),data=kiwishade)
> summary(kiwishade.aov)

Error: block:shade
          Df  Sum Sq Mean Sq F value   Pr(>F)
block      2  172.35   86.17  4.1176 0.074879
shade      3 1394.51  464.84 22.2112 0.001194
Residuals  6  125.57   20.93

Error: Within
          Df Sum Sq Mean Sq F value Pr(>F)
Residuals 36 438.58   12.18
```

10.1.2 The Tinting of Car Windows

In section 4.1 we encountered data from an experiment that aimed to model the effects of the tinting of car windows on visual performance[42]. The authors are mainly interested in effects on side window vision, and hence in visual recognition tasks that would be performed when looking through side windows.

Data are in the data frame **tinting**. In this data frame, **csoa** (critical stimulus onset asynchrony, i.e. the time in milliseconds required to recognise an alphanumeric target), **it** (inspection time, i.e. the time required for a simple discrimination task) and **age** are variables, while **tint** (3 levels) and **target** (2 levels) are ordered factors. The variable **sex** is coded 1 for males and 2 for females, while the variable **agegp** is coded 1 for young people (all in their early 20s) and 2 for older participants (all in the early 70s).

We have two levels of variation – within individuals (who were each tested on each combination of **tint** and **target**), and between individuals. So we need to specify **id** (identifying the individual) as a random effect. Plots such as we examined in section 4.1 make it clear that, to get variances that are approximately homogeneous, we need to work with log(**csoa**) and log(**it**). Here we examine the analysis for log(**it**). We start with a model that is likely to be more complex than we need (it has all possible interactions):

```
itstar.lme<-lme(log(it)~tint*target*agegp*sex,
  random=~1|id, data=tinting,method="ML")
```

A reasonable guess is that first order interactions may be all we need, i.e.

```
it2.lme<-lme(log(it)~(tint+target+agegp+sex)^2,
  random=~1|id, data=tinting,method="ML")
```

Finally, there is the very simple model, allowing only for main effects:

```
it1.lme<-lme(log(it)~(tint+target+agegp+sex),
  random=~1|id, data=tinting,method="ML")
```

Note that we have fitted all these models by maximum likelihood. This is so that we can do the equivalent of an analysis of variance comparison. Here is what we get:

```
> anova(itstar.lme,it2.lme,it1.lme)
           Model df       AIC      BIC    logLik   Test  L.Ratio p-value
itstar.lme     1 26  8.146187 91.45036 21.926906
it2.lme        2 17 -3.742883 50.72523 18.871441 1 vs 2  6.11093  0.7288
it1.lme        3  8  1.138171 26.77022  7.430915 2 vs 3 22.88105  0.0065
```

[42] Data relate to the paper: Burns, N. R., Nettlebeck, T., White, M. and Willson, J. 1999. Effects of car window tinting on visual performance: a comparison of elderly and young drivers. Ergonomics 42: 428-443.

The model that limits attention to first order interactions is adequate. We will need to examine the first order interactions individually. For this we re-fit the model used for **it2.lme**, but now with **method="REML"**.

```
it2.reml<-update(it2.lme,method="REML")
```

We now examine the estimated effects:

```
> options(digits=3)
> summary(it2.reml)$tTable
                     Value Std.Error  DF t-value  p-value
(Intercept)         6.05231    0.7589 145   7.975 4.17e-13
tint.L              0.22658    0.0890 145   2.547 1.19e-02
tint.Q              0.17126    0.0933 145   1.836 6.84e-02
targethicon        -0.24012    0.1010 145  -2.378 1.87e-02
agegp              -1.13449    0.5167  22  -2.196 3.90e-02
sex                -0.74542    0.5167  22  -1.443 1.63e-01
tint.L.targethicon -0.09193    0.0461 145  -1.996 4.78e-02
tint.Q.targethicon -0.00722    0.0482 145  -0.150 8.81e-01
tint.L.agegp       -0.13075    0.0492 145  -2.658 8.74e-03
tint.Q.agegp       -0.06972    0.0520 145  -1.341 1.82e-01
tint.L.sex          0.09794    0.0492 145   1.991 4.83e-02
tint.Q.sex         -0.00542    0.0520 145  -0.104 9.17e-01
targethicon.agegp   0.13887    0.0584 145   2.376 1.88e-02
targethicon.sex    -0.07785    0.0584 145  -1.332 1.85e-01
agegp.sex           0.33164    0.3261  22   1.017 3.20e-01
```

Because **tint** is an ordered factor, polynomial contrasts are used.

10.1.3 The Michelson Speed of Light Data

Here is an example, using the Michelson speed of light data from the Venables and Ripley *MASS* package. The model allows the determination to vary linearly with **Run** (from 1 to 20), with the slope varying randomly between the five experiments of 20 runs each. We assume an autoregressive dependence structure of order 1. We allow the variance to change from one experiment to another. Maximum likelihood tests suggest that one needs at least this complexity in the variance and dependence structure to represent the data accurately. A model that has neither fixed nor random **Run** effects seems all that is justified statistically. To test this, one needs to fit models with and without these effects, setting **method="ML"** in each case, and compare the likelihoods. (I leave this as an exercise!) For purposes of doing this test, a first order autoregressive model would probably be adequate. A model that ignores the sequential dependence entirely does give misleading results.

```
> library(MASS)  # if needed
> data(michelson)  # if needed
> michelson$Run <- as.numeric(michelson$Run) # Ensure Run is a variable
> mich.lme1 <- lme(fixed = Speed ~ Run, data = michelson,
       random =  ~ Run| Expt, correlation = corAR1(form =  ~ 1 | Expt),
      weights = varIdent(form =  ~ 1 | Expt))
> summary(mich.lme1)
Linear mixed-effects model fit by REML
 Data: michelson
   AIC  BIC logLik
  1113 1142   -546

Random effects:
 Formula: ~Run | Expt
 Structure: General positive-definite
            StdDev Corr
```

```
(Intercept)  46.49 (Intr)
Run           3.62 -1
Residual    121.29

Correlation Structure: AR(1)
 Formula: ~1 | Expt
 Parameter estimate(s):
  Phi
0.527
Variance function:
 Structure: Different standard deviations per stratum
 Formula: ~1 | Expt
 Parameter estimates:
    1     2     3     4     5
1.000 0.340 0.646 0.543 0.501
Fixed effects: Speed ~ Run
            Value Std.Error DF t-value p-value
(Intercept)   868     30.51 94   28.46  <.0001
Run            -2      2.42 94   -0.88   0.381
 Correlation:
    (Intr)
Run -0.934

Standardized Within-Group Residuals:
   Min     Q1    Med     Q3    Max
-2.912 -0.606  0.109  0.740  1.810

Number of Observations: 100
Number of Groups: 5
```

10.2 Time Series Models

The R *stats* package has a number of functions for manipulating and plotting time series, and for calculating the autocorrelation function.

There are (at least) two types of method – time domain methods and frequency domain methods. In the time domain models may be conventional "short memory" models where the autocorrelation function decays quite rapidly to zero, or the relatively recently developed "long memory" time series models where the autocorrelation function decays very slowly as observations move apart in time. A characteristic of "long memory" models is that there is variation at all temporal scales. Thus in a study of wind speeds it may be possible to characterise windy days, windy weeks, windy months, windy years, windy decades, and perhaps even windy centuries. R does not yet have functions for fitting the more recently developed long memory models.

The function **`stl()`** decomposes a times series into a trend and seasonal components, etc. The functions **`ar()`** (for "autoregressive" models) and associated functions, and **`arima0()`** ("autoregressive integrated moving average models") fit standard types of time domain short memory models. Note also the function **`gls()`** in the *nlme* package, which can fit relatively complex models that may have autoregressive, arima and various other types of dependence structure.

The function **`spectrum()`** and related functions is designed for frequency domain or "spectral" analysis.

10.3 Exercises

1. Use the function **`acf()`** to plot the autocorrelation function of lake levels in successive years in the data set **`huron`**. Do the plots both with **`type="correlation"`** and with **`type="partial"`**.

10.4 References

Chambers, J. M. and Hastie, T. J. 1992. Statistical Models in S. Wadsworth and Brooks Cole Advanced Books and Software, Pacific Grove CA.

Diggle, Liang & Zeger 1996. Analysis of Longitudinal Data. Clarendon Press, Oxford.

Everitt, B. S. and Dunn, G. 1992. Applied Multivariate Data Analysis. Arnold, London.

Hand, D. J. & Crowder, M. J. 1996. Practical longitudinal data analysis. Chapman and Hall, London.

Little, R. C., Milliken, G. A., Stroup, W. W. and Wolfinger, R. D. (1996). SAS Systems for Mixed Models. SAS Institute Inc., Cary, New Carolina.

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Pinheiro, J. C. and Bates, D. M. 2000. Mixed effects models in S and S-PLUS. Springer, New York.

Venables, W. N. and Ripley, B. D., 2nd edn 1997. Modern Applied Statistics with S-Plus. Springer, New York.

*11. Advanced Programming Topics

11.1. Methods

R is an object-oriented language. Objects may have a "class". For functions such as **print()**, **summary()**, etc., the class of the object determines what action will be taken. Thus in response to **print(x)**, R determines the class attribute of **x**, if one exists. If for example the class attribute is "factor", then the function which finally handles the printing is **print.factor()**. The function **print.default()** is used to print objects that have not been assigned a class.

More generally, the class attribute of an object may be a vector of strings. If there are "ancestor" classes – parent, grandparent, . . ., these are specified in order in subsequent elements of the class vector. For example, ordered factors have the class "ordered", which inherits from the class "factor". Thus:

```
> fac<-ordered(1:3)
> class(fac)
[1] "ordered" "factor"
```

Here **fac** has the class "ordered", which inherits from the parent class "factor".

The function **print.ordered()**, which is the function that is called when you invoke **print()** with an ordered factor, could be rewritten to use the fact that "ordered" inherits from "factor", thus:

```
> print.ordered
function (x, quote = FALSE)
{
    if (length(x) <= 0)
        cat("ordered(0)\n")
    else NextMethod("print")
    cat("Levels: ", paste(levels(x), collapse = " < "), "\n")
    invisible(x)
}
```

The system version of **print.ordered()** does not use **print.factor()**. The function **print.glm()** does not call **print.lm()**, even though glm objects inherit from lm objects. The mechanism is avaialble for use if required.

11.2 Extracting Arguments to Functions

How, inside a function, can one extract the value assigned to a parameter when the function was called? Below there is a function **extract.arg()**. When it is called as **extract.arg(a=xx)**, we want it to return **"xx"**. When it is called as **extract.arg(a=xy)**, we want it to return **"xy"**. Here is how it is done.

```
extract.arg <-
function (a)
{
    s <- substitute(a)
    as.character(s)
}


> extract.arg(a=xy)
[1] "xy"
```

If the argument is a function, we may want to get at the arguments to the function. Here is how one can do it

```
deparse.args <-
function (a)
{
    s <- substitute (a)
    if(mode(s) == "call"){
```

```
            # the first element of a 'call' is the function called
            # so we don't deparse that, just the arguments.
            print(paste("The function is:  ", s[1],"()", collapse=""))
            lapply (s[-1], function (x)
            paste (deparse(x), collapse = "\n"))
            }
    else stop ("argument is not a function call")
}
```

For example:

```
> deparse.args(list(x+y, foo(bar)))
[1] "The function is:   list ()"
[[1]]
[1] "x + y"

[[2]]
[1] "foo(bar)"
```

11.3 Parsing and Evaluation of Expressions

When R encounters an expression such as **`mean(x+y)`** or **`cbind(x,y)`**, there are two steps:

The text string is parsed and turned into an expression, i.e. the syntax is checked and it is turned into code that the R computing engine can more immediately evaluate.

The expression is evaluated.

Upon typing in

```
expression(mean(x+y))
```

the output is the unevaluated expression **`expression(mean(x+y))`**. Setting

```
my.exp <- expression(mean(x+y))
```

stores this unevaluated expression in **`my.exp`** . The actual contents of **`my.exp`** are a little different from what is printed out. R gives you as much information as it thinks helpful.

Note that **`expression(mean(x+y))`** is different from **`expression("mean(x+y)"),`** as is obvious when the expression is evaluated. A text string is a text string is a text string, unless one explicitly changes it into an expression or part of an expression.

Let's see how this works in practice

```
> x <- 101:110
> y <- 21:30
> my.exp <- expression(mean(x+y))
> my.txt <- expression("mean(x+y)")
> eval(my.exp)
[1] 131
> eval(my.txt)
[1] "mean(x+y)"
```

What if we already have **`"mean(x+y)"`** stored in a text string, and want to turn it into an expression? The answer is to use the function **`parse(),`** but indicate that the parameter is text rather than a file name. Thus

```
> parse(text="mean(x+y)")
expression(mean(x + y))
```

We store the expression in **`my.exp2`**, and then evaluate it

```
> my.exp2 <- parse(text="mean(x+y)")
> eval(my.exp2)
[1] 131
```

Here is a function that creates a new data frame from an arbitrary set of columns of an existing data frame. Once in the function, we attach the data frame so that we can leave off the name of the data frame, and use only the column names

```
make.new.df <- function(old.df = austpop, colnames = c("NSW", "ACT"))
{
     attach(old.df)
     on.exit(detach(old.df))
     argtxt <- paste(colnames, collapse = ",")
     exprtxt <- paste("data.frame(", argtxt, ")", sep = "")
     expr <- parse(text = exprtxt)
     df <- eval(expr)
     names(df) <- colnames
     df
}
```

To verify that the function does what it should, type in

```
> make.new.df()
   NSW ACT
1 1904   3
. . . .
```

The function **do.call()** makes it possible to supply the function name and the argument list in separate text strings. When **do.call** is used it is only necessary to use **parse()** in generating the argument list.

For example

```
make.new.df <-
function(old.df = austpop, colnames = c("NSW", "ACT"))
{
     attach(old.df)
     on.exit(detach(old.df))
     argtxt <- paste(colnames, collapse = ",")
     listexpr <- parse(text=paste("list(", argtxt, ")", sep = ""))
     df <- do.call("data.frame", eval(listexpr))
     names(df) <- colnames
     df
}
```

11.4 Plotting a mathematical expression

The following, given without explanation, illustrates some of the possibilities. It needs better error checking than it has at present:

```
plotcurve <-
function(equation = "y = sqrt(1/(1+x^2))", ...){
leftright <- strsplit(equation, split = "=")[[1]]
left <- leftright[1]    # The part to the left of the "="
right <- leftright[2]   # The part to the right of the "="
expr <- parse(text=right)
xname <- all.vars(expr)
if(length(xname) > 1)stop(paste("There are multiple variables, i.e.",paste(xname,
collapse=" & "),
  "on the right of the equation"))
if(length(list(...))==0)assign(xname, 1:10)
 else {
 nam <- names(list(...))
 if(nam!=xname)stop("Clash of variable names")
```

```
 assign("x", list(...)[[1]])
 assign(xname, x)
}
y <- eval(expr)
yexpr <- parse(text=left)[[1]]
xexpr <- parse(text=xname)[[1]]
plot(x, y, ylab = yexpr, xlab = xexpr, type="n")
lines(spline(x,y))
mainexpr <- parse(text=paste(left, "==", right))
title(main = mainexpr)
}
```

Try

```
plotcurve()
plotcurve("ang=asin(sqrt(p))", p=(1:49)/50)
```

11.4 Searching R functions for a specified token.

A token is a syntactic entity; for example function names are tokens. For example, we search all functions in the working directory. The purpose of using **`unlist()`** in the code below is to change **`myfunc`** from a list into a vector of character strings.

```
mygrep <-
function(str)
{
##  Assign the names of all objects in current R
##  working directory to the string vector tempobj
##
  tempobj <- ls(envir=sys.frame(-1))
  objstring <- character(0)
  for(i in tempobj) {
          myfunc <- get(i)
    if(is.function(myfunc))
         if(length(grep(str,
             deparse(myfunc))))
     objstring <- c(objstring, i)
}
return(objstring)
}


mygrep("for")   # Find all functions that include a for loop
```

12. Appendix 1

12.1 R Packages for Windows

To get information on R packages, go to:

http://cran.r-project.org

The Australian link (accessible only to users in Australia) is:

http://mirror.aarnet.edu.au/pub/CRAN/

For Windows 95 etc binaries, look in

http://mirror.aarnet.edu.au/pub/CRAN/windows/windows-9x/

Look in the directory **contrib** for packages.

New packages are being added all the time. So it pays to check the CRAN site from time to time. Also, watch for announcements on the electronic mailing lists r-help and r-announce.

12.2 Contributed Documents and Published Literature

Much literature that has been written for S-PLUS is highly relevant for R.

Alzola, C. and Harrell, F. 1997. An Introduction to S and the Hmisc and Design Packages.
[Available from CRAN sites. The examples are largely medical.]

Burns, P. J. A Guide for the Unwilling S User. [Available from CRAN sites]
[The style is leisurely. However this assumes some prior knowledge of computing language terms. It may suit users with some initial knowledge of R.]

Chambers, J. M. 1998. Programming with Data. A Guide to the S Language. Springer-Verlag, New York.
[This is a book for specialists.]

Chambers, J. M. and Hastie, T. J. 1992. Statistical Models in S. Wadsworth and Brooks Cole Advanced Books and Software, Pacific Grove CA
[This is the basic reference on R and S-PLUS model formulae and models.]

Dalgaard, P. 2002. Introductory Statistics with R. Springer, New York.
[This is an R-based introductory text, with a biostatistical emphasis.]

Fox, J. 2002. An R and S-PLUS Companion to Applied Regression. Sage Books.

Maindonald J H and Braun W J 2003. Data Analysis and Graphics Using R – An Example-Based Approach. Cambridge University Press.
[This is an intermediate level text.]

Krause, A. and Olsen, M. 1997. The Basics of S and S-PLUS. Springer 1997.
[This is an introductory book, at about the same level as Spector.]

Spector, P. 1994. An Introduction to S and S-PLUS. Duxbury Press.
[This is a readable and compact beginner's guide to the S language.]

Venables, W.N., Smith, D.M. and the R Development Core Team. An Introduction to R. Notes on R: A Programming Environment for Data Analysis and Graphics.
[A current version is available from CRAN sites. This is derived from an original set of notes written by Bill Venables and Dave Smith for the S and S-PLUS environments.

Venables, W. N. and Ripley, B. D., 4th edn 2002. Modern Applied Statistics with S. Springer, NY.
[This has become a text book for the use of S-PLUS and R for applied statistical analysis. It assumes a fair level of statistical sophistication. Explanation is careful, but often terse. Together with the 'Complements' it gives brief introductions to extensive packages of functions that have been written or adapted by Ripley, Venables, and a number of other statisticians. Supplementary material (`Complements') is available from

http://www.stats.ox.ac.uk/pub/MASS4/.|

Venables, W.N. and Ripley, B.D. 2000. S Programming. Springer 2000. This is a terse and careful introduction to the dialects of the S language, including R.

R Development Core Team. An Introduction to R. [Available from CRAN sites]

A variety of further documents are available from CRAN sites.

12.3 Data Sets Referred to in these Notes

Data sets included in the image file usingR.RData

`Cars93.summary`	`ais`	`anesthetic`	`austpop`	`dewpoint`
`dolphins`	`elasticband`	`florida`	`hills`	`huron`
`islandcities`	`kiwishade`	`leafshape`	`milk`	`moths`
`oddbooks`	`orings`	`possum`	`primates`	`rainforest`
`seedrates`	`tinting`			

Data Sets from Package *datasets*

`Airquality`	`attitude`	`cars`	`Islands`	`LakeHuron`

Data Sets from Package *lattice*

`barley`

Data Sets from Package *MASS*

`Aids2`	`Animals`	`Cars93`	`PlantGrowth`	`Rubber`
`cement`	`cpus`	`fgl`	`michelson`	`mtcars`
`painters`	`pressure`	`ships`		

12.4 Answers to Selected Exercises

Section 1.6

1. `plot(distance~stretch,data=elasticband)`

2. (ii), (iii), (iv)

```
plot(snow.cover ~ year, data = snow)
hist(snow$snow.cover)
hist(log(snow$snow.cover))
```

Section 2.7

1. The value of answer is (a) 12, (b) 22, (c) 600.

2. `prod(c(10,3:5))`

3(i) `bigsum <- 0;  for (i in 1:100) {bigsum <- bigsum+i }; bigsum`

3(ii) `sum(1:100)`

4(i) `bigprod <- 1;  for (i in 1:50) {bigprod <- bigprod*i };  bigprod`

4(ii) `prod(1:50)`

5. `radius <- 3:20;  volume <- 4*pi*radius^3/3`
   `sphere.data <- data.frame(radius=radius, volume=volume)`

6. `sapply(tinting, is.factor)`
   `sapply(tinting[, 4:6], levels)`
   `sapply(tinting[, 4:6], is.ordered)`

Section 3.9

1.
```
plot(Animals$body, Animals$brain, pch=1,
     xlab="Body weight (kg)",ylab="Brain weight (g)")
```

2.
```
plot(log(Animals$body),log(Animals$brain),pch=1,
     xlab="Body weight (kg)", ylab="Brain weight (g)", axes=F)
brainaxis <- 10^seq(-1,4)
bodyaxis <-10^seq(-2,4)
axis(1, at=log(bodyaxis), lab=bodyaxis)
axis(2, at=log(brainaxis), lab=brainaxis)
box()
identify(log(Animals$body), log(Animals$brain), labels=row.names(Animals))
```

3. **par(mfrow = c(1,2)), etc.**

Section 7.9

1. **x <- seq(101,112) or x <- 101:112**

2. **rep(c(4,6,3),4)**

3. **c(rep(4,8),rep(6,7),rep(3,9)) or rep(c(4,6,3),c(8,7,9))**
   mat64 <- matrix(c(rep(4,8),rep(6,7),rep(3,9)), nrow=6, ncol=4)

4. **rep(seq(1,9),seq(1,9)) or rep(1:9, 1:9)**

6. (a) Use **summary(airquality) to get this information.**

   (b) **airquality[airquality$Ozone == max(airquality$Ozone),]**

   (c) **airquality$Wind[airquality$Ozone > quantile(airquality$Ozone, .75)]**

7. **mean(snow$snow.cover[seq(2,10,2)])**

   mean(snow$snow.cover[seq(1,9,2)])

9. **summary(attitude); summary(cpus)**

Comment on ranges of values, whether distributions seem skew, etc.

10. **mtcars6<-mtcars[mtcars$cyl==6,]**

11. **Cars93[Cars93$Type=="Small"|Cars93$Type=="Sporty",]**