Notes on R: A Programming Environment for Data Analysis and Graphics

Bill Venables & Dave Smith

Department of Statistics The University of Adelaide

Robert Gentleman & Ross Ihaka

Department of Statistics University of Auckland

Martin Mächler

Statistics Seminar ETH Zurich

© W. Venables, 1990, 1992.
© R. Gentleman & R. Ihaka, 1997.
© M. Mächler, 1997–1998.

Preface

These notes on R are derived from an original set of notes describing the S and S-PLUS environments written by Bill Venables and Dave Smith. We have made a number of small changes to reflect differences between the R and S programs.

R is an ongoing project and its capabilities do not presently match those of S. In these notes we have adopted the convention that any feature that we intend to implement is noted as such at the beginning of the section where the feature is described. Users can contribute to the project by implementing any of these that remain.

We would like to extend warm thanks to Bill Venables for granting permission to distributed this modified version of the notes in this way, and for being a supporter of R from way back.

Comments and corrections are always welcome. Please address email correspondence to

R@stat.auckland.ac.nz.

Suggestions to the reader

Most R novices will start with the introductory session in Appendix A. This should give some familiarity with the style of R sessions and more importantly some instant feedback on what actually happens.

Many users will come to R mainly for its graphical facilities. In this case section 11 on the graphics facilities can be read at almost any time and need not wait until all the preceding sections have been digested.

Robert Gentleman and Ross Ihaka, University of Auckland, April, 1997.

Contents

Preface

| 1 | Intr 1.1 | oduction and Preliminaries The R environment | 2 2 |
|----------|--|--|---|
| | 1.1 | Related Software and Documentation | 2 |
| | 1.3 | R and the Window System | 2 |
| | 1.4 | Using R interactively | 3 |
| | 1.5 | An Introductory Session | 3 |
| | 1.6 | Getting help with functions and features | 4 |
| | 1.7 | R Commands. Case Sensitivity. | 4 |
| | 1.8 | Recall and Correction of Previous Commands | 4 |
| | 1.9 | Executing Commands from, or Diverting Output to, a File | 4 |
| | 1.10 | Data Permanency. Removing Objects. | 5 |
| 2 | | ple Manipulations; Numbers and Vectors | 6 |
| | 2.1 | Vectors and Assignment | 6 |
| | 2.2 | Vector Arithmetic | 6 |
| | $\begin{array}{c} 2.3 \\ 2.4 \end{array}$ | Generating Regular Sequences | 7 8 |
| | $\frac{2.4}{2.5}$ | Logical Vectors | 8 |
| | $\frac{2.5}{2.6}$ | Missing Values | 9 |
| | $\frac{2.0}{2.7}$ | Index Vectors. Selecting and Modifying Subsets of a Data Set | 9 |
| | | | 9 |
| 3 | • | ects, their Modes and Attributes | 11 |
| | 3.1 | Intrinsic Attributes: mode and length | 11 |
| | 3.2 | Changing the Length of an Object | 11 |
| | 3.3 | attributes() and attr() | 12 |
| | 3.4 | The class of an object | 12 |
| | | | |
| 4 | | ered and Unordered Factors | 13 |
| 4 | 4.1 | A Specific Example | 13 |
| 4 | | | |
| 4 5 | 4.1 4.2 Arr a | A Specific Example | 13 13 15 |
| | 4.1 4.2 Arr 5.1 | A Specific Example | 13 13 15 15 |
| | 4.1 4.2 Arr 5.1 5.2 | A Specific Example | 13 13 15 15 |
| | 4.1 4.2 Arr 5.1 5.2 5.3 | A Specific Example | 13 13 15 15 15 |
| | 4.1 4.2 Arr 5.1 5.2 | A Specific Example | 13 13 15 15 15 15 17 |
| | 4.1 4.2 Arr 5.1 5.2 5.3 5.4 | A Specific Example | 13 13 15 15 15 15 17 |
| | 4.1 4.2 Arr 5.1 5.2 5.3 | A Specific Example | 13 13 15 15 15 15 17 17 |
| | 4.1 4.2 Arr : 5.1 5.2 5.3 5.4 5.5 | A Specific Example | 13 13 15 15 15 17 17 17 |
| | 4.1 4.2 Arr 5.1 5.2 5.3 5.4 5.5 5.6 | A Specific Example | 13 13 15 15 15 17 17 17 18 18 |
| | 4.1 4.2 Arr : 5.1 5.2 5.3 5.4 5.5 5.6 5.7 | A Specific Example | 13 13 15 15 15 17 17 17 18 18 19 |
| | 4.1 4.2 Arrs 5.1 5.2 5.3 5.4 5.5 5.6 5.7 5.8 | A Specific Example | 13 13 15 15 15 17 17 17 17 18 18 18 19 19 |
| | 4.1 4.2 Arrs 5.1 5.2 5.3 5.4 5.5 5.6 5.7 5.8 5.9 | A Specific Example | 13 13 15 15 15 17 17 17 18 18 19 |
| | 4.1 4.2 Arrs 5.1 5.2 5.3 5.4 5.5 5.6 5.7 5.8 5.9 5.10 | A Specific Example | 13 13 15 15 15 15 17 17 17 17 18 18 18 19 19 20 |
| 5 | 4.1 4.2 Arrs 5.1 5.2 5.3 5.4 5.5 5.6 5.7 5.8 5.9 5.10 | A Specific Example | 133 13 15 15 15 15 17 17 17 17 17 18 18 18 19 19 20 20 |
| 5 | 4.1 4.2 Arr : 5.1 5.2 5.3 5.4 5.5 5.6 5.7 5.8 5.9 5.10 List | A Specific Example | 133 13 15 15 15 15 15 15 17 17 17 17 18 18 19 20 20 20 22 |
| 5 | 4.1 4.2 Arr 5.1 5.2 5.3 5.4 5.5 5.6 5.7 5.8 5.9 5.10 List 6.1 | A Specific Example | 133 13 15 15 15 15 15 15 17 177 177 177 18 18 18 19 200 200 200 202 222 |
| 5 | 4.1 4.2 Arr 5.1 5.2 5.3 5.4 5.5 5.6 5.7 5.8 5.9 5.10 List 6.1 | A Specific Example | 133 133 155 155 155 157 177 177 177 177 177 177 |
| 5 | 4.1 4.2 Arr 5.1 5.2 5.3 5.4 5.5 5.6 5.7 5.8 5.9 5.10 List 6.1 6.2 | A Specific Example | 133 13 15 15 15 15 15 15 15 17 17 17 17 17 17 17 17 17 17 17 17 17 |
| 5 | 4.1 4.2 Arr 5.1 5.2 5.3 5.4 5.5 5.6 5.7 5.8 5.9 5.10 List 6.1 6.2 | A Specific Example | 133 133 155 155 155 157 177 177 177 177 177 177 |

| | 6.4.1 Making data frames 5 6.4.2 attach() and detach() 5 6.4.3 Working with data frames 5 | 24 25 25 26 26 |
|----|--|---|
| 7 | 7.1 The read.table() function 2 7.2 The scan() function 2 | 27 27 28 28 |
| 8 | 8.1 Grouped expressions 6 8.2 Control statements 6 8.2.1 Conditional execution: if statements 6 | 29 29 29 29 29 29 |
| 9 | 0.1 Simple examples | 31 32 32 33 33 33 33 33 33 35 35 37 38 |
| 10 | 0.1 Defining statistical models; formulæ 1 0.2 Regression models; fitted model objects 1 0.3 Generic functions for extracting information 1 0.4 Analysis of variance; comparing models 1 10.4.1 ANOVA tables 1 0.5 Updating fitted models. The ditto name "." 1 0.6 Generalized linear models; families 1 10.6.1 Families 1 10.6.2 The glm() function 1 0.7 Nonlinear least squares and maximum likelihood models 1 10.7.1 Least squares 1 10.7.2 Maximum likelihood 4 | 39 40 41 41 42 43 43 44 47 47 48 48 |
| 11 | 1.1 High-level plotting commands 5 11.1.1 The plot() function 5 11.1.2 Displaying multivariate data 5 11.1.3 Display graphics 5 11.1.4 Arguments to high-level plotting functions 5 11.2 Low-level plotting commands 5 1.3 Interactive graphics functions 5 1.4 Using graphics parameters 5 11.4.1 Permanent changes: The par() function 5 | 50 50 51 52 52 54 55 55 55 55 |

| | 11.5 Graphics parameters list | |
|---|---|---|
| | 11.5.1 Graphical elements | |
| | 11.5.2 Axes and tick marks $\ldots \ldots 5$ | |
| | 11.5.3 Figure margins | |
| | 11.5.4 Multiple figure environment | 8 |
| | 11.6 Device drivers | 0 |
| | 11.6.1 PostScript diagrams for typeset documents. | 1 |
| | 11.6.2 Multiple graphics devices | 1 |
| | | _ |
| Α | R: An introductory session 62 | 2 |
| в | The Inbuilt Command Line Editor in R 6 | 5 |
| | B.1 Preliminaries | 5 |
| | B.2 Editing Actions | 5 |
| | B.3 Command Line Editor Summary | 6 |
| a | | - |
| U | Exercises 6' | |
| | C.1 The cloud point data | |
| | | |
| | 00 0 1 | |
| | | |
| | v | |
| | 0 | |
| | | |
| | 0 11 | |
| | 0 | |
| | | |
| | | |
| | C.12 The Kalythos blindness data | |
| | C.14 The chlorine availability data | |
| | C.15 The saturated steam pressure data | |
| | C.16 Count Rumford's friction data | |
| | C.17 The jellyfish data | |
| | C.18 The Archæological pottery data | |
| | C.19 The Beaujolais quality data | |
| | C.20 The painters data of de Piles | |
| | -0.20 III painto atta of ut III $=$ 1 $=$ 1 $=$ 0 | J |

1 Introduction and Preliminaries

1.1 The R environment

 ${\sf R}$ is an integrated suite of software facilities for data manipulation, calculation and graphical display. Among other things it has

- an effective data handling and storage facility,
- a suite of operators for calculations on arrays, in particular matrices,
- a large, coherent, integrated collection of intermediate tools for data analysis,
- graphical facilities for data analysis and display either directly at the computer or on hardcopy, and
- a well developed, simple and effective programming language which includes conditionals, loops, user defined recursive functions and input and output facilities. (Indeed most of the system supplied functions are themselves written in the S language.)

The term "environment" is intended to characterize it as a fully planned and coherent system, rather than an incremental accretion of very specific and inflexible tools, as is frequently the case with other data analysis software.

R is very much a vehicle for newly developing methods of interactive data analysis. As such it is very dynamic, and new releases have not always been fully upwardly compatible with previous releases. Some users welcome the changes because of the bonus of new technology and new methods that come with new releases; others seem to be more worried by the fact that old code no longer works. Although R is intended as a programming language, one should regard programs written in R as essentially ephemeral.

1.2 Related Software and Documentation

R can be regarded as a re-implementation of the S language developed at AT&T by Rick Becker, John Chambers and Allan Wilks. A number of the books and manuals about S bear some relevance to R.

The basic reference is The New S Language: A Programming Environment for Data Analysis and Graphics by Richard A. Becker, John M. Chambers and Allan R. Wilks. The new features of the August 1991 release of S are covered in *Statistical Models in S* edited by John M. Chambers and Trevor J. Hastie. In addition, the manuals for S-PLUS, the commercially supported version of S may be useful.

1.3 R and the Window System

The most convenient way to use R is at a graphics workstation running a windowing system. These notes are aimed at users who have this facility. In particular we will occasionally refer to the use of R on an X-window system although the vast bulk of what is said applies generally to any implementation of the R environment.

Most users will find it necessary to interact directly with the operating system on their computer from time to time. In these notes, we mainly discuss interaction with the operating system on UNIX machines. If you are running R under either Macintosh or Windows you will need to make the appropriate adjustment. For both the Macintosh and Windows implementations we have attempted to adhere to the relevant user interface guidelines.

Setting up a workstation to take full advantage of the customizable features of R is a straightforward if somewhat tedious procedure, and will not be considered further here. Users in difficulty should seek local expert help.

1.4 Using R interactively

When you use the R program it issues a prompt when it expects input commands. The default prompt is ">", which on UNIX could be the same as the shell prompt, and so it may appear that nothing is happening. However, as we shall see, it is easy to change to a different R prompt if you wish. In these notes, we will assume that the UNIX shell prompt is "\$".

In using R under UNIX the suggested procedure for the first occasion is as follows:

1. Create a separate sub-directory, say work, to hold data files on which you will use R for this problem. This will be the working directory whenever you use R for this particular problem.

```
$ mkdir work
```

- \$ cd work
- 2. Start the R program with the command

\$ R

- 3. At this point R commands may be issued (see later).
- 4. To quit the R program the command is

> q() \$

Ψ

At this point you will be asked whether you want to save the data from your R session. You can respond yes, no or cancel (a single letter abbreviation will do) to save the data before quiting, quit without saving, or return to the R session. Data which is saved will be available in future R sessions.

Further ${\sf R}$ sessions are simple.

1. Make work the working directory and start the program as before:

\$ cd work

- \$ R
- 2. Use the R program, terminating with the q() command at the end of the session.

When using R under either the Macintosh or Windows the procedure to follow is basically the same. Create a folder or working directory. Then launch R by double clicking on the appropriate icon. Select **New** from the **File** menu to indicate that you want to start a new analysis (this will remove any previously defined objects from the workspace) and then select **Save** from the **File** menu to save the pristine image into the folder you have created. You may now commence your analysis and when you exit from R you will be prompted to save the image in your working directory.

To work on the same analysis at a later time simply double-click on the icon for the saved image. Alternatively you can start R elsewhere and then use **Open** from the **File** menu to select and subsequently open the saved image.

1.5 An Introductory Session

Readers wishing to get a feel for R at a computer before proceeding are strongly advised to work through the model introductory session given in Appendix A, starting on page 62.

1.6 Getting help with functions and features

R has an inbuilt help facility similar to the man facility of UNIX. To get more information on any specific named function, for example solve the command is

> help(solve)

An alternative is

> ?solve

For a feature specified by special characters, the argument must be enclosed in double or single quotes, making it a 'character string':

> help("[[")

+

Either form of quote mark may be used to escape the other, as in the string "It's important". Our convention in these notes is to use double quote marks for preference.

1.7 R Commands. Case Sensitivity.

Technically R is an expression language with a very simple syntax. It is case sensitive as are most UNIX based packages, so A and a are different symbols and would refer to different variables.

Elementary commands consist of either expressions or assignments. If an expression is given as a command, it is evaluated, printed, and the value is lost. An assignment also evaluates an expression and passes the value to a variable but the result is not automatically printed.

Commands are separated either by a semi-colon (";"), or by a newline. If a command is not complete at the end of a line, R will give a different prompt, for example

on second and subsequent lines and continue to read input until the command is syntactically complete. This prompt may be changed by the user. In these notes, we will generally omit the continuation prompt and indicate continuation by simple indenting.

1.8 Recall and Correction of Previous Commands

Under many versions of UNIX, R provides a mechanism for recalling and re-executing previous commands. The vertical arrow keys on the keyboard can be used to scroll forward and backward through a *command history*. Once a command is located in this way, the cursor can be moved within the command using the horizontal arrow keys, and characters can be removed with the **Delete** key or added with the other keys.

The recall and editing capabilities are highly customizable. You can find out how to do this by reading the UNIX manual entry for the readline library.

Alternatively, the emacs text editor provides rather more general support mechanisms for working interactively with R.

1.9 Executing Commands from, or Diverting Output to, a File

If commands are stored on an external file, say commands. R in the working directory work, they may be executed at any time in an R session with the command

```
> source("commands.R")
```

For Macintosh and Windows Source is also available on the File menu. The function sink,

4

```
> sink("record.lis")
```

will divert all subsequent output from the terminal to an external file, record.lis. The command

> sink()

restores it to the terminal once again.

1.10 Data Permanency. Removing Objects.

The entities that R creates and manipulates are known as *objects*. These may be variables, arrays of numbers, character strings, functions, or more general structures built from such components.

During an R session, objects are created and stored by name (we discuss this process in the next session). The R command

> objects()

can be used to display the names of the objects which are currently stored within R.

To remove objects the function **rm** is available:

> rm(x, y, z, ink, junk, temp, foo, bar)

All objects created during an R sessions can be stored permanently in a file for use in future R sessions. At the end of each R session you are given the opportunity to save all the currently available objects. If you indicate that you want to do this, the objects are written to a file called $.RData^{1}$. in the current directory.

When R is started at later time it reloads the objects from this file (at the same time the associated command history is also reloaded under UNIX).

It is recommended that you should use separate working directories for analyses conducted with R. It is quite common for objects with names x and y to be created during an analysis. Names like this are often meaningful in the context of a single analysis, but it can be quite hard to decide what they might be when the several analyses have been conducted in the same directory.

¹ The leading "dot" in this file name makes it *invisible* in UNIX.

2 Simple Manipulations; Numbers and Vectors

2.1 Vectors and Assignment

R operates on named data structures. The simplest such structure is the vector, which is a single entity consisting of an ordered collection of numbers. To set up a vector named x, say, consisting of five numbers, namely 10.4, 5.6, 3.1, 6.4 and 21.7, use the R command

> x \leftarrow c(10.4, 5.6, 3.1, 6.4, 21.7)

This is an assignment statement using the function c() which in this context can take an arbitrary number of vector arguments and whose value is a vector got by concatenating its arguments end to end.²

A number occurring by itself in an expression is taken as a vector of length one.

Notice that the assignment operator (\leftarrow) is **not** the usual = operator, which is reserved for another purpose. It consists of the two characters < ('less than') and - ('minus') occurring strictly side-by-side and it 'points' to the object receiving the value of the expression. In this text, the assignment operator is printed as " \leftarrow ", rather than "<-". ³

Assignment can also be made using the function assign(). An equivalent way of making the same assignment as above is with:

> assign("x", c(10.4, 5.6, 3.1, 6.4, 21.7))

The usual operator, \leftarrow ("<-"), can be thought of as a syntactic short-cut to this.

Assignments can also be made in the other direction, using the obvious change in the assignment operator. So the same assignment could be made using

> c(10.4, 5.6, 3.1, 6.4, 21.7) -> x

If an expression is used as a complete command, the value is printed *and lost*. So now if we were to use the command

> 1/x

the reciprocals of the five values would be printed at the terminal (and the value of x, of course, unchanged).

The further assignment

> y \leftarrow c(x, 0, x)

would create a vector \mathbf{y} with 11 entries consisting of two copies of \mathbf{x} with a zero in the middle place.

2.2 Vector Arithmetic

Vectors can be used in arithmetic expressions, in which case the operations are performed element by element. Vectors occurring in the same expression need not all be of the same length. If they are not, the value of the expression is a vector with the same length as the longest vector which occurs in the expression. Shorter vectors in the expression are *recycled* as often as need be (perhaps fractionally) until they match the length of the longest vector. In particular a constant is simply repeated. So with the above assignments the command

 $v \leftarrow 2*x + y + 1$

 $^{^{2}}$ With other than vector types of argument, such as list mode arguments, the action of c() is rather different. See §6.2.1.

³The underscore character, "_" is an allowable synonym for the left pointing assignment operator "<-", however we discourage this option, as it can easily lead to much less readible code.

2.3 Generating Regular Sequences

generates a new vector v of length 11 constructed by adding together, element by element, 2*x repeated 2.2 times,

y repeated just once, and 1 repeated 11 times.

The elementary arithmetic operators are the usual +, -, *, / and $\hat{}$ for raising to a power. In addition all of the common arithmetic functions are available. log, exp, sin, cos, tan, sqrt, and so on, all have their usual meaning. max and min select the largest and smallest elements of an vector respectively. range is a function whose value is a vector of length two, namely c(min(x), max(x)). length(x) is the number of elements in x, sum(x) gives the total of the elements in x and prod(x) their product.

Two statistical functions are mean(x) which calculates the sample mean, which is the same as sum(x)/length(x), and var(x) which gives

 $sum((x-mean(x))^2)/(length(x)-1)$

or sample variance. If the argument to var() is an $n \times p$ matrix the value is a $p \times p$ sample covariance matrix got by regarding the rows as independent p-variate sample vectors.

sort(x) returns a vector of the same size as x with the elements arranged in increasing order; however there are other more flexible sorting facilities available (see order() or sort.list() which produce a permutation to do the sorting).

rnorm(x) is a function which generates a vector (or more generally an array) of pseudo-random standard normal deviates, of the same size as x.

2.3 Generating Regular Sequences

R has a number of facilities for generating commonly used sequences of numbers. For example 1:30 is the vector $c(1,2, \ldots, 29, 30)$. The colon operator has highest priority within an expression, so, for example 2*1:15 is the vector $c(2,4,6, \ldots, 28, 30)$. Put $n \leftarrow 10$ and compare the sequences 1:n-1 and 1:(n-1).

The construction 30:1 may be used to generate a sequence backwards.

The function seq() is a more general facility for generating sequences. It has five arguments, only some of which may be specified in any one call. The first two arguments, if given, specify the beginning and end of the sequence, and if these are the only two arguments given the result is the same as the colon operator. That is seq(2,10) is the same vector as 2:10.

Parameters to seq(), and to many other R functions, can also be given in named form, in which case the order in which they appear is irrelevant. The first two parameters may be named from=value and to=value; thus seq(1,30), seq(from=1, to=30) and seq(to=30, from=1) are all the same as 1:30. The next two parameters to seq() may be named by=value and length=value, which specify a step size and a length for the sequence respectively. If neither of these is given, the default by=1 is assumed.

For example

> seq(-5, 5, by=.2) -> s3

generates in s3 the vector c(-5.0, -4.8, -4.6, ..., 4.6, 4.8, 5.0). Similarly

> s4 \leftarrow seq(length=51, from=-5, by=.2)

generates the same vector in s4.

The fifth parameter may be named along=vector, which if used must be the only parameter, and creates a sequence 1, 2, ..., length(vector), or the empty sequence if the vector is empty (as it can be).

A related function is **rep()** which can be used for replicating an object in various complicated ways. The simplest form is

> s5 \leftarrow rep(x, times=5)

which will put five copies of x end-to-end in s5.

2.4 Logical Vectors

As well as numerical vectors, R allows manipulation of logical quantities. The elements of a logical vectors have just two possible values, represented formally as FALSE and TRUE. These are usually abbreviated as F and T, respectively.

Logical vectors are generated by conditions. For example

> temp \leftarrow x>13

sets temp as a vector of the same length as x with values F corresponding to elements of x where the condition is *not* met and T where it is.

The logical operators are <, <=, >, >=, == for exact equality and != for inequality. In addition if c1 and c2 are logical expressions, then c1 & c2 is their intersection ("and"), c1 | c2 is their union ("or") and ! c1 is the negation of c1.

Logical vectors may be used in ordinary arithmetic, in which case they are *coerced* into numeric vectors, F becoming 0 and T becoming 1. However there are situations where logical vectors and their coerced numeric counterparts are not equivalent, for example see the next subsection.

2.5 Missing Values

In some cases the components of a vector may not be completely known. When an element or value is "not available" or a "missing value" in the statistical sense, a place within a vector may be reserved for it by assigning it the special value NA. In general any operation on an NA becomes an NA. The motivation for this rule is simply that if the specification of an operation is incomplete, the result cannot be known and hence is not available.

The function is.na(x) gives a logical vector of the same size as x with value T if and only if the corresponding element in x is NA.

```
> ind \leftarrow is.na(z)
```

Notice that the logical expression x = NA is quite different from is.na(x) since NA is not really a value but a marker for a quantity that is not available. Thus x = NA is a vector of the same length as $x \ all$ of whose values are NA as the logical expression itself is incomplete and hence undecidable.

Note that there is a second kind of "missing" values which are produced by numerical computation, the so-called *Not a Number*, NaN, values. Whereas these don't exist in S, they are printed the same as NA in S-PLUS. Examples are

> 0/0

or

> Inf - Inf

which both give NaN since the result cannot be defined sensibly.

In summary, is.na(xx) is TRUE *both* for NA and NaN values. To differentiate these, is.nan(xx) only is TRUE for NaNs.

2.6 Character Vectors

Character quantities and character vectors are used frequently in R, for example as plot labels. Where needed they are denoted by a sequence of characters delimited by the double quote character, E. g., "x-values", "New iteration results".

Character vectors may be concatenated into a vector by the c() function; examples of their use will emerge frequently.

The paste() function takes an arbitrary number of arguments and concatenates them into a single character string. Any numbers given among the arguments are coerced into character strings in the evident way, that is, in the same way they would be if they were printed. The arguments are by default separated in the result by a single blank character, but this can be changed by the named parameter, sep=string, which changes it to string, possibly empty.

For example

```
> labs \leftarrow paste(c("X","Y"), 1:10, sep="")
```

makes labs into the character vector

("X1", "Y2", "X3", "Y4", "X5", "Y6", "X7", "Y8", "X9", "Y10")

Note particularly that recycling of short lists takes place here too; thus c("X", "Y") is repeated 5 times to match the sequence 1:10.

2.7 Index Vectors. Selecting and Modifying Subsets of a Data Set

Subsets of the elements of a vector may be selected by appending to the name of the vector an *index vector* in square brackets. More generally any expression that evaluates to a vector may have subsets of its elements similarly selected by appending an index vector in square brackets immediately after the expression.

Such index vectors can be any of four distinct types.

1. A logical vector. In this case the index vector must be of the same length as the vector from which elements are to be selected. Values corresponding to T in the index vector are selected and those corresponding to F omitted. For example

> y \leftarrow x[!is.na(x)]

creates (or re-creates) an object y which will contain the non-missing values of x, in the same order. Note that if x has missing values, y will be shorter than x. Also

> (x+1)[(!is.na(x)) & x>0] -> z

creates an object z and places in it the values of the vector x+1 for which the corresponding value in x was both non-missing and positive.

2. A vector of positive integral quantities. In this case the values in the index vector must lie in the the set {1, 2, ..., length(x)}. The corresponding elements of the vector are selected and concatenated, in that order, in the result. The index vector can be of any length and the result is of the same length as the index vector. For example x[6] is the sixth component of x and

> x[1:10]

selects the first 10 elements of x, (assuming length(x) \geq 10). Also

> c("x","y")[rep(c(1,2,2,1), times=4)]

(an admittedly unlikely thing to do) produces a character vector of length 16 consisting of "x", "y", "y", "x" repeated four times.

3. A vector of negative integral quantities. Such an index vector specifies the values to be excluded rather than included. Thus

> y \leftarrow x[-(1:5)]

gives y all but the first five elements of x.

4. A vector of character strings. This possibility only applies where an object has a names attribute to identify its components. In this case a subvector of the names vector may be used in the same way as the positive integral labels in 2. above.

> fruit \leftarrow c(5, 10, 1, 20)

```
> names(fruit) \leftarrow c("orange", "banana", "apple", "peach")
```

```
> lunch <- fruit[c("apple","orange")]
```

The advantage is that alphanumeric *names* are often easier to remember than *numeric indices*. This option is particularly useful in connection with data frames, as we shall see later.

An indexed expression can also appear on the receiving end of an assignment, in which case the assignment operation is performed only on those elements of the vector. The expression must be of the form vector[index_vector] as having an arbitrary expression in place of the vector name does not make much sense here.

The vector assigned must match the length of the index vector, and in the case of a logical index vector it must again be the same length as the vector it is indexing.

For example

> x[is.na(x)] $\leftarrow 0$

replaces any missing values in x by zeros and

 $y[y<0] \leftarrow -y[y<0]$

has the same effect as

> y \leftarrow abs(y)⁴

 $^{^{4}}$ Note that abs() does not work as expected with complex arguments. The appropriate function for the complex modulus is Mod().

3 Objects, their Modes and Attributes

3.1 Intrinsic Attributes: mode and length

The entities R operates on are technically known as *objects*. Examples are vectors of numeric (real) or complex values, vectors of logical values and vectors of character strings. These are known as 'atomic' structures since their components are all of the same type, or *mode*, namely $numeric^5$, complex, logical and character respectively.

Vectors must have their values all of the same mode. Thus any given vector must be unambiguously either *logical*, *numeric*, *complex* or *character*. The only mild exception to this rule is the special "value" listed as NA for quantities not available. Note that a vector can be empty and still have a mode. For example the empty character string vector is listed as character(0) and the empty numeric vector as numeric(0).

R also operates on objects called *lists*, which are of mode *list*. These are ordered sequences of objects which individually can be of any mode. *lists* are known as 'recursive' rather than atomic structures since their components can themselves be lists in their own right.

The other recursive structures are those of mode function and expression. Functions are the functions that form part of the R system along with similar user written functions, which we discuss in some detail later in these notes. Expressions as objects form an advanced part of R which will not be discussed in these notes, except indirectly when we discuss formulæ used with modelling in R.

By the mode of an object we mean the basic type of its fundamental constituents. This is a special case of an *attribute* of an object. The *attributes* of an object provide specific information about the object itself. Another attribute of every object is its *length*. The functions mode(object) and length(object) can be used to find out the mode and length of any defined structure.

For example, if z is a complex vector of length 100, then in an expression mode(z) is the character string "complex" and length(z) is 100.

R caters for changes of mode almost anywhere it could be considered sensible to do so, (and a few where it might not be). For example with

 $> z \leftarrow 0:9$

we could put

```
> digits \leftarrow as.character(z)
```

after which digits is the character vector ("0", "1", "2", ..., "9"). A further *coercion*, or change of mode, reconstructs the numerical vector again:

> d \leftarrow as.integer(digits)

Now d and z are the same.⁶ There is a large collection of functions of the form as.something() for either coercion from one mode to another, or for investing an object with some other attribute it may not already possess. The reader should consult the different help files to become familiar with them.

3.2 Changing the Length of an Object

An "empty" object may still have a mode. For example

> e \leftarrow numeric()

 $^{^{5}}$ numeric mode is actually an amalgam of two distinct modes, namely integer and double precision, as explained in the manual.

 $^{^{6}}$ In general, coercion from numeric to character and back again will not be exactly reversible, because of roundoff errors in the character representation.

makes e an empty vector structure of mode numeric. Similarly character() is a empty character vector, and so on. Once an object of any size has been created, new components may be added to it simply by giving it an index value outside its previous range. Thus

> e[3] \leftarrow 17

now makes e a vector of length 3, (the first two components of which are at this point both NA). This applies to any structure at all, provided the mode of the additional component(s) agrees with the mode of the object in the first place.

This automatic adjustment of lengths of an object is used often, for example in the scan() function for input. (See §7.2.)

Conversely to truncate the size of an object requires only an assignment to do so. Hence if alpha is an object of length 10, then

> alpha \leftarrow alpha[2 * 1:5]

makes it an object of length 5 consisting of just the former components with even index. The old indices are not retained, of course.

3.3 attributes() and attr()

The function attributes (object) gives a list of all the non-intrinsic attributes currently defined for that object. The function attr(object,name) can be used to select a specific attribute. These functions are rarely used, except in rather special circumstances when some new attribute is being created for some particular purpose, for example to associate a creation date or an operator with an R object. The concept, however, is very important.

Some care should be exercised when assigning or deleting attributes since they are an integral part of the object system used in R.

When it is used on the left hand side of an assignment it can be used either to associate a new attribute with *object* or to change an existing one. For example

> attr(z,"dim") \leftarrow c(10,10)

allows R to treat ${\bf z}$ as if it were a 10×10 matrix.

3.4 The class of an object

A special attribute known as the *class* of the object is used to allow for an object oriented style of programming in R.

For example if an object has class data.frame, it will be printed in a certain way, the plot() function will display it graphically in a certain way, and other generic functions such as summary() will react to it as an argument in a way sensitive to its class.

To remove temporarily the effects of class, use the function unclass(). For example if winter has the class data.frame then

> winter

will print it in data frame form, which is rather like a matrix, whereas

```
> unclass(winter)
```

will print it as an ordinary list. Only in rather special situations do you need to use this facility, but one is when you are learning to come to terms with the idea of class and generic functions.

Generic functions and classes will be discussed further in §9.8, but only briefly.

4 Ordered and Unordered Factors

A *factor* is a vector object used to specify a discrete classification of the components of other vectors of the same length. R provides both *ordered* and *unordered* factors.

4.1 A Specific Example

Suppose, for example, we have a sample of 30 tax accountants from all the states and territories⁷ and their individual state of origin is specified by a character vector of state mnemonics as

Notice that in the case of a character vector, "sorted" means sorted in alphabetical order.

A factor is similarly created using the factor() function:

```
> statef \leftarrow factor(state)
```

The print() function handles factors slightly differently from other objects:

```
> statef
[1] tas sa qld nsw nsw nt wa wa qld vic nsw vic qld qld sa
[16] tas sa nt wa vic qld nsw nsw wa sa act nsw vic vic act
```

To find out the levels of a factor the function levels() can be used.

```
> levels(statef)
[1] "act" "nsw" "nt" "gld" "sa" "tas" "vic" "wa"
```

4.2 The function tapply() and ragged arrays

To continue the previous example, suppose we have the incomes of the same tax accountants in another vector (in suitably large units of money)

> incomes ← c(60, 49, 40, 61, 64, 60, 59, 54, 62, 69, 70, 42, 56, 61, 61, 61, 58, 51, 48, 65, 49, 49, 41, 48, 52, 46, 59, 46, 58, 43)

To calculate the sample mean income for each state we can now use the special function tapply():

```
> incmeans <- tapply(incomes, statef, mean)
```

giving a means vector with the components labelled by the levels

```
> incmeans
act nsw nt qld sa tas vic wa
44.5 57.333 55.5 53.6 55 60.5 56 52.25
```

The function tapply() is used to apply a function, here mean(), to each group of components of the first argument, here incomes, defined by the levels of the second component, here statef, as if they were separate vector structures. The result is a structure of the same length as the levels attribute of the factor containing the results. The reader should consult the help document for more details.

⁷ Foreign readers should note that there are eight states and territories in Australia, namely the Australian Capital Territory, New South Wales, the Northern Territory, Queensland, South Australia, Tasmania, Victoria and Western Australia.

Suppose further we needed to calculate the standard errors of the state income means. To do this we need to write an R function to calculate the standard error for any given vector. We discuss functions more fully later in these notes, but since there is an in built function var() to calculate the sample variance, such a function is a very simple one liner, specified by the assignment:

> stderr \leftarrow function(x) sqrt(var(x)/length(x))

(Writing functions will be considered later in $\S9$.) After this assignment, the standard errors are calculated by

and the values calculated are then

> incster act nsw nt qld sa tas vic wa 1.5 4.3102 4.5 4.1061 2.7386 0.5 5.244 2.6575

As an exercise you may care to find the usual 95% confidence limits for the state mean incomes. To do this you could use tapply() once more with the length() function to find the sample sizes, and the qt() function to find the percentage points of the appropriate t-distributions.

The function tapply() can be used to handle more complicated indexing of a vector by multiple categories. For example, we might wish to split the tax accountants by both state and sex. However in this simple instance what happens can be thought of as follows. The values in the vector are collected into groups corresponding to the distinct entries in the category. The function is then applied to each of these groups individually. The value is a vector of function results, labelled by the levels attribute of the category.

The combination of a vector and a labelling factor or category is an example of what is called a *ragged array*, since the subclass sizes are possibly irregular. When the subclass sizes are all the same the indexing may be done implicitly and much more efficiently, as we see in the next section.

5 Arrays and Matrices

5.1 Arrays

An array can be considered as a multiply subscripted collection of data entries, for example numeric. R allows simple facilities for creating and handling arrays, and in particular the special case of matrices.

A dimension vector is a vector of positive integers. If its length is k then the array is k-dimensional. The values in the dimension vector give the upper limits for each of the k subscripts. The lower limits are always 1.

A vector can be used by R as an array only if it has a dimension vector as its *dim* attribute. Suppose, for example, z is a vector of 1500 elements. The assignment

> dim(z) \leftarrow c(3,5,100)

gives it the dim attribute that allows it to be treated as a $3 \times 5 \times 100$ array.

Other functions such as matrix() and array() are available for simpler and more natural looking assignments, as we shall see in §5.4.

The values in the data vector give the values in the array in the same order as they would occur in Fortran, that is 'column major order', with the first subscript moving fastest and the last subscript slowest.

For example if the dimension vector for an array, say a is c(3,4,2) then there are $3 \times 4 \times 2 = 24$ entries in a and the data vector holds them in the order a[1,1,1], a[2,1,1], ..., a[2,4,2], a[3,4,2].

5.2 Array indexing. Subsections of an array

Individual elements of an array may be referenced, as above, by giving the name of the array followed by the subscripts in square brackets, separated by commas.

More generally, subsections of an array may be specified by giving a sequence of index vectors in place of subscripts; however if any index position is given an empty index vector, then the full range of that subscript is taken.

Continuing the previous example, a[2,,] is a 4×2 array with dimension vector c(4,2) and data vector containing the values

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

in that order. a[,,] stands for the entire array, which is the same as omitting the subscripts entirely and using a alone.

For any array, say Z, the dimension vector may be referenced explicitly as dim(Z) (on either side of an assignment).

Also, if an array name is given with just *one subscript or index vector*, then the corresponding values of the data vector only are used; in this case the dimension vector is ignored. This is not the case, however, if the single index is not a vector but itself an array, as we next discuss.

5.3 Index arrays

As well as an index vector in any subscript position, an array may be used with a single *index* array in order either to assign a vector of quantities to an irregular collection of elements in the array, or to extract an irregular collection as a vector.

A matrix example makes the process clear. In the case of a doubly indexed array, an index matrix may be given consisting of two columns and as many rows as desired. The entries in the index matrix are the row and column indices for the doubly indexed array. Suppose for example we have a 4×5 array X and we wish to do the following:

- Extract elements $\mathtt{X[1,3]}, \mathtt{X[2,2]}$ and $\mathtt{X[3,1]}$ as a vector structure, and
- Replace these entries in the array X by 0s.

In this case we need a 3×2 subscript array, as in the example given in Figure 1.

```
>
  x \leftarrow array(1:20,dim=c(4,5))
                                       # Generate a 4 \times 5 array.
>
  х
     [,1] [,2] [,3] [,4] [,5]
[1,]
               5
                     9
                          13
                               17
         1
[2,]
         2
               6
                    10
                          14
                               18
[3,]
         3
               7
                               19
                          15
                    11
[4,]
         4
               8
                    12
                          16
                               20
> i \leftarrow array(c(1:3,3:1),dim=c(3,2))
                                       # i is a 3 \times 2 index array.
>
  i
      [,1] [,2]
[1,]
         1
               3
[2,]
         2
               2
[3,]
         3
               1
> x[i]
                                       # Extract those elements
[1] 9 6 3
> x[i] \leftarrow 0
                                       # Replace those elements by zeros.
>
  х
      [,1] [,2] [,3] [,4] [,5]
[1,]
                     0
                          13
                               17
         1
               5
         2
[2,]
               0
                    10
                          14
                               18
[3,]
         0
               7
                    11
                          15
                               19
[4,]
         4
               8
                    12
                          16
                               20
>
```

Figure 1: Using an index array

As a less trivial example, suppose we wish to generate an (unreduced) design matrix for a block design defined by factors blocks (b levels) and varieties, (v levels). Further suppose there are n plots in the experiment. We could proceed as follows:

```
> Xb ← matrix(0, n, b)
> Xv ← matrix(0, n, v)
> ib ← cbind(1:n, blocks)
> iv ← cbind(1:n, varieties)
> Xb[ib] ← 1
> Xv[iv] ← 1
> X ← cbind(Xb, Xv)
```

Further, to construct the incidence matrix, N say, we could use

> N \leftarrow crossprod(Xb, Xv)

However a simpler direct way of producing this matrix is to use table():

> N \leftarrow table(blocks, varieties)

5.4 The array() function

As well as giving a vector structure a dim attribute, arrays can be constructed from vectors by the array function, which has the form

> Z <- array(data_vector,dim_vector)

For example, if the vector h contains 24, or fewer, numbers then the command

> Z \leftarrow array(h, dim=c(3,4,2))

would use **h** to set up $3 \times 4 \times 2$ array in Z. If the size of **h** is exactly 24 the result is the same as

> dim(Z) \leftarrow c(3,4,2)

However if h is shorter than 24, its values recycled from the beginning again to make it up to size 24. See §5.4.1 below. As an extreme but common example

> Z \leftarrow array(0, c(3,4,2)

makes Z an array of all zeros.

At this point dim(Z) stands for the dimension vector c(3,4,2), and Z[1:24] stands for the data vector as it was in h, and Z[] with an empty subscript or Z with no subscript stands for the entire array as an array.

Arrays may be used in arithmetic expressions and the result is an array formed by element by element operations on the data vector. The dim attributes of operands generally need to be the same, and this becomes the dimension vector of the result. So if A, B and C are all similar arrays, then

> D \leftarrow 2*A*B + C + 1

makes D a similar array with data vector the result of the evident element by element operations. However the precise rule concerning mixed array and vector calculations has to be considered a little more carefully.

5.4.1 Mixed vector and array arithmetic. The recycling rule

The precise rule affecting element by element mixed calculations with vectors and arrays is somewhat quirky and hard to find in the references. From experience I have found the following to be a reliable guide.

- The expression is scanned from left to right.
- Any short vector operands are extended by recycling their values until they match the size of any previous (or subsequent) operands.
- As long as short vectors and arrays, only, are encountered, the arrays must all have the same dim attribute or an error results.
- Any vector operand longer than some previous array immediately converts the calculation to one in which all operands are coerced to vectors. A diagnostic message is issued if the size of the long vector is not a multiple of the (common) size of all previous arrays.
- If array structures are present and no error or coercion to vector has been precipitated, the result is an array structure with the common dim attribute of its array operands.

5.5 The outer product of two arrays

An important operation on arrays is the *outer product*. If **a** and **b** are two numeric arrays, their outer product is an array whose dimension vector is got by concatenating their two dimension vectors, (order is important), and whose data vector is got by forming all possible products of

elements of the data vector of **a** with those of **b**. The outer product is formed by the special operator %o:

> ab \leftarrow a %o% b

An alternative is

> ab \leftarrow outer(a, b, '*')

The multiplication function can be replaced by an arbitrary function of two variables. For example if we wished to evaluate the function

$$f(x,y) = \frac{\cos(y)}{1+x^2}$$

over a regular grid of values with x- and y-coordinates defined by the R vectors x and y respectively, we could proceed as follows:

```
> f \leftarrow function(x,y) cos(y)/(1 + x<sup>2</sup>)
> z \leftarrow outer(x, y, f)
```

In particular the outer product of two ordinary vectors is a doubly subscripted array (that is a matrix, of rank at most 1). Notice that the outer product operator is of course non-commutative. Defining your own R functions will be considered further in Chapter 9.

5.5.1 An example: Determinants of 2×2 digit matrices

As an artificial but cute example, consider the determinants of 2×2 matrices $\begin{bmatrix} a & b \\ c & d \end{bmatrix}$ where each entry is a non-negative integer in the range $0, 1, \ldots, 9$, that is a digit.

The problem is to find the determinants, ad-bc, of all possible matrices of this form and represent the frequency with which each value occurs as a *high density* plot. This amounts to finding the probability distribution of the determinant if each digit is chosen independently and uniformly at random.

A neat way of doing this uses the outer() function twice:

```
> d \leftarrow outer(0:9, 0:9)
```

```
> fr \leftarrow table(outer(d, d, "-"))
```

```
> plot(as.numeric(names(fr)), fr, type="h",
```

```
xlab="Determinant", ylab="Frequency")
```

Notice the coercion of the names attribute of the frequency table to numeric in order to recover the range of the determinant values. The "obvious" way of doing this problem with for-loops, to be discussed in §8.2, is so inefficient as to be impractical.

It is also perhaps surprising that about 1 in 20 such matrices is singular.

5.6 Generalized transpose of an array

The function aperm(a, perm) may be used to permute an array, a. The argument perm must be a permutation of the integers $\{1, 2, \ldots, k\}$, where k is the number of subscripts in a. The result of the function is an array of the same size as a but with old dimension given by perm[j] becoming the new jth dimension. The easiest way to think of this operation is as a generalization of transposition for matrices. Indeed if A is a matrix, (that is, a doubly subscripted array) then B given by

> B \leftarrow aperm(A, c(2,1))

is just the transpose of A. For this special case a simpler function t() is available, so we could have used $B \leftarrow t(A)$.

5.7 Matrix facilities. Multiplication, inversion and solving linear equations.

5.7 Matrix facilities. Multiplication, inversion and solving linear equations.

As noted above, a matrix is just an array with two subscripts. However it is such an important special case it needs a separate discussion. R contains many operators and functions that are available only for matrices. For example t(X) is the matrix transpose function, as noted above. The functions nrow(A) and ncol(A) give the number of rows and columns in the matrix A respectively.

The operator %*% is used for matrix multiplication. An $n \times 1$ or $1 \times n$ matrix may of course be used as an *n*-vector if in the context such is appropriate. Conversely vectors which occur in matrix multiplication expressions are automatically promoted either to row or column vectors, whichever is multiplicatively coherent, if possible, (although this is not always unambiguously possible, as we see later).

If, for example, A and B are square matrices of the same size, then

> A * B

is the matrix of element by element products and

> A %*% B

is the matrix product. If \mathbf{x} is a vector, then

> x %*% A %*% x

is a quadratic form.⁸

The function crossprod() forms "crossproducts", meaning that

> crossprod(X, y) is the same as t(X) %% y

but the operation is more efficient. If the second argument to crossprod() is omitted it is taken to be the same as the first.

Other important matrix functions include solve(A, b) for solving equations, solve(A) for the matrix inverse, svd() for the singular value decomposition, qr() for QR decomposition and eigen() for eigenvalues and eigenvectors of symmetric matrices.

The meaning of diag() depends on its argument. diag(vector) gives a diagonal matrix with elements of the vector as the diagonal entries. On the other hand diag(matrix) gives the vector of main diagonal entries of matrix. This is the same convention as that used for diag() in MATLAB. Also, somewhat confusingly, if k is a single numeric value then diag(k) is the $k \times k$ identity matrix!

A surprising omission from the suite of matrix facilities is a function for the determinant of a square matrix, however the absolute value of the determinant is easy to calculate for example as the product of the singular values. (See later.)

5.8 Forming partitioned matrices. cbind() and rbind().

As we have already seen informally, matrices can be built up from other vectors and matrices by the functions cbind() and rbind(). Roughly cbind() forms matrices by binding together matrices horizontally, or column-wise, and rbind() vertically, or row-wise.

In the assignment

⁸Note that $x \ \% \ \% \ x$ is ambiguous, as it could mean either x'x or xx', where x is the column form. In such cases the smaller matrix seems implicitly to be the interpretation adopted, so the scalar x'x is in this case the result. The matrix xx' may be calculated either by $cbind(x) \ \% \ \% \ x$ or $x \ \% \ \% \ bind(x)$ since the result of rbind() or cbind() is always a matrix.

```
> X \leftarrow cbind(arg<sub>1</sub>, arg<sub>2</sub>, arg<sub>3</sub>, ...)
```

the arguments to cbind() must be either vectors of any length, or matrices with the same column size, that is the same number of rows. The result is a matrix with the concatenated arguments arg_1, arg_2, \ldots forming the columns.

If some of the arguments to cbind() are vectors they may be shorter than the column size of any matrices present, in which case they are cyclically extended to match the matrix column size (or the length of the longest vector if no matrices are given).

The function rbind() does the corresponding operation for rows. In this case any vector argument, possibly cyclically extended, are of course taken as row vectors.

Suppose X1 and X2 have the same number of rows. To combine these by columns into a matrix X, together with an initial column of 1s we can use

> $X \leftarrow cbind(1, X1, X2)$

The result of rbind() or cbind() always has matrix status. Hence cbind(x) and rbind(x) are possibly the simplest ways explicitly to allow the vector x to be treated as a column or row matrix respectively.

5.9 The concatenation function, c(), with arrays.

It should be noted that whereas cbind() and rbind() are concatenation functions that respect dim attributes, the basic c() function does not, but rather clears numeric objects of all dim and dimnames attributes. This is occasionally useful in its own right.

The official way to coerce an array back to a simple vector object is to use as.vector()

```
> vec \leftarrow as.vector(X)
```

However a similar result can be achieved by using c() with just one argument, simply for this side-effect:

> vec \leftarrow c(X)

There are slight differences between the two, but ultimately the choice between them is largely a matter of style (with the former being preferable).

5.10 Frequency tables from factors. The table() function

Recall that a factor defines a partition into groups. Similarly a pair of factors defines a two way cross classification, and so on. The function table() allows frequency tables to be calculated from equal length factors. If there are k category arguments, the result is a k-way array of frequencies.

Suppose, for example, that statef is a factor giving the state code for each entry in a data vector. The assignment

> statefr \leftarrow table(statef)

gives in statefr a table of frequencies of each state in the sample. The frequencies are ordered and labelled by the levels attribute of the category. This simple case is equivalent to, but more convenient than,

> statefr <- tapply(statef, statef, length)

Further suppose that incomef is a category giving a suitably defined "income class" for each entry in the data vector, for example with the cut() function:

```
> factor(cut(incomes,breaks=35+10*(0:7))) -> incomef
```

Then to calculate a two-way table of frequencies:

```
> table(incomef,statef)
```

| | act | nsw | \mathtt{nt} | qld | sa | tas | vic | wa |
|-------------|-----|-----|---------------|-----|----|-----|-----|----|
| 35+ thru 45 | 1 | 1 | 0 | 1 | 0 | 0 | 1 | 0 |
| 45+ thru 55 | 1 | 1 | 1 | 1 | 2 | 0 | 1 | 3 |
| 55+ thru 65 | 0 | 3 | 1 | 3 | 2 | 2 | 2 | 1 |
| 65+ thru 75 | 0 | 1 | 0 | 0 | 0 | 0 | 1 | 0 |

Extension to higher way frequency tables is immediate.

6 Lists, data frames, and their uses

6.1 Lists

An R list is an object consisting of an ordered collection of objects known as its components.

There is no particular need for the components to be of the same mode or type, and, for example, a list could consist of a numeric vector, a logical value, a matrix, a complex vector, a character array, a function, and so on. Here is a simple example of how to make a list:

> Lst \leftarrow list(name="Fred", wife="Mary", no.children=3, child.ages=c(4,7,9))

Components are always numbered and may always be referred to as such. Thus if Lst is the name of a list with four components, these may be individually referred to as Lst[[1]], Lst[[2]], Lst[[3]] and Lst[[4]]. If, further, Lst[[4]] is a vector subscripted array then Lst[[4]][1] is its first entry.

If Lst is a list, then the function length(Lst) gives the number of (top level) components it has.

Components of lists may also be *named*, and in this case the component may be referred to either by giving the component name as a character string in place of the number in double square brackets, or, more conveniently, by giving an expression of the form

> name\$component_name

for the same thing.

This is a very useful convention as it makes it easier to get the right component if you forget the number.

So in the simple example given above:

Lst\$name is the same as Lst[[1]] and is the string "Fred",

Lst\$wife is the same as Lst[[2]] and is the string "Mary",

Lst\$child.ages[1] is the same as Lst[[4]][1] and is the number 4.

Additionally, one can also use the names of the list components in double square brackets, i.e., Lst[["name"]] is the same as Lst\$name. This is especially useful, when the name of the component to be extracted is stored in another variable as in

> $x \leftarrow$ "name"; Lst[[x]]

It is very important to distinguish Lst[[1]] from Lst[1]. "[[...]]" is the operator used to select a single element, whereas "[...]" is a general subscripting operator. Thus the former is the first object in the list Lst, and if it is a named list the name is not included. The latter is a sublist of the list Lst consisting of the first entry only. If it is a named list, the name is transferred to the sublist.

The names of components may be abbreviated down to the minimum number of letters needed to identify them uniquely. Thus Lst\$coefficients may be minimally specified as Lst\$coe and Lst\$covariance as Lst\$cov.

The vector of names is in fact simply an attribute of the list like any other and may be handled as such. Other structures besides lists may, of course, similarly be given a *names* attribute also.

6.2 Constructing and modifying lists

New lists may be formed from existing objects by the function list(). An assignment of the form

6.3 Some functions returning a list result

> Lst \leftarrow list(name₁=object₁, name₂=object₂, ..., name_m=object_m)

sets up a list Lst of m components using $object_1, \ldots, object_m$ for the components and giving them names as specified by the argument names, (which can be freely chosen). If these names are omitted, the components are numbered only. The components used to form the list are copied when forming the new list and the originals are not affected.

Lists, like any subscripted object, can be extended by specifying additional components. For example

> Lst[5] \leftarrow list(matrix=Mat)

6.2.1 Concatenating lists

When the concatenation function c() is given list arguments, the result is an object of mode list also, whose components are those of the argument lists joined together in sequence.

> list.ABC \leftarrow c(list.A, list.B, list.C)

Recall that with vector objects as arguments the concatenation function similarly joined together all arguments into a single vector structure. In this case all other attributes, such as dim attributes, are discarded.

6.3 Some functions returning a list result

Functions and expressions in R must return a single object as their result; in cases where the result has several component parts, the usual form is that of a list with named components.

6.3.1 Eigenvalues and eigenvectors

The function eigen(Sm) calculates the eigenvalues and eigenvectors of a symmetric matrix Sm. The result of this function is a list of two components named values and vectors. The assignment

> ev \leftarrow eigen(Sm)

will assign this list to ev. Then ev\$val is the vector of eigenvalues of Sm and ev\$vec is the matrix of corresponding eigenvectors. Had we only needed the eigenvalues we could have used the assignment:

```
> evals \leftarrow eigen(Sm)$values
```

evals now holds the vector of eigenvalues and the second component is discarded. If the expression

> eigen(Sm)

is used by itself as a command the two components are printed, with their names, at the terminal.

6.3.2 Singular value decomposition and determinants

The function svd(M) takes an arbitrary matrix argument, M, and calculates the singular value decomposition of M. This consists of a matrix of orthonormal columns U with the same column space as M, a second matrix of orthonormal columns V whose column space is the row space of M and a diagonal matrix of positive entries D such that M = U % % D % % t(V). D is actually returned as a vector of the diagonal elements. The result of svd(M) is actually a list of three components named d, u and v, with evident meanings.

If M is in fact square, then, it is not hard to see that

```
> absdetM \leftarrow prod(svd(M)$d)
```

calculates the absolute value of the determinant of M. If this calculation were needed often with a variety of matrices it could be defined as an R function

```
> absdet \leftarrow function(M) prod(svd(M)$d)
```

after which we could use absdet() as just another R function. As a further trivial but potentially useful example, you might like to consider writing a function, say tr(), to calculate the trace of a square matrix. [Hint: You will not need to use an explicit loop. Look again at the diag() function.]

Functions will be discussed formally later in these notes.

6.3.3 Least squares fitting and the QR decomposition

The function lsfit() returns a list giving results of a least squares fitting procedure. An assignment such as

> ans \leftarrow lsfit(X, y)

gives the results of a least squares fit where y is the vector of observations and X is the design matrix. See the help facility for more details, and also for the follow-up function ls.diag() for, among other things, regression diagnostics. Note that a grand mean term is automatically included and need not be included explicitly as a column of X.

Another closely related function is qr() and its allies. Consider the following assignments

```
> Xplus \leftarrow qr(X)
```

```
> b \leftarrow qr.coef(Xplus, y)
```

```
> fit \leftarrow qr.fitted(Xplus, y)
```

```
> res \leftarrow qr.resid(Xplus, y)
```

These compute the orthogonal projection of y onto the range of X in fit, the projection onto the orthogonal complement in **res** and the coefficient vector for the projection in **b**, that is, **b** is essentially the result of the MATLAB 'backslash' operator.

It is not assumed that X has full column rank. Redundancies will be discovered and removed as they are found.

This alternative is the older, low level way to perform least squares calculations. Although still useful in some contexts, it would now generally be replaced by the statistical models features, as will be discussed in §10.

6.4 Data frames

A data frame is a list with class data.frame. There are restrictions on lists that may be made into data frames, namely

- The components must be vectors (numeric, character, or logical), factors, numeric matrices, lists, or other data frames.
- Matrices, lists, and data frames provide as many variables to the new data frame as they have columns, elements, or variables, respectively.
- Numeric vectors and factors are included as is, and non-numeric vectors are coerced to be factors, whose levels are the unique values appearing in the vector.

6.4 Data frames

• Vector structures appearing as variables of the data frame must all have the same length, and matrix structures must all have the same row size.

Data frames may in many ways be regarded as a matrix with columns possibly of differing modes and attributes. It may be displayed in matrix form, and its rows and columns extracted using matrix indexing conventions.

6.4.1 Making data frames

Objects satisfying the restrictions placed on the columns (components) of a data frame may be used to form one using the function data.frame:

A list whose components conform to the restrictions of a data frame may be *coerced* into a data frame using the function as.data.frame()

The simplest way to construct a data frame from scratch is to use the **read.table()** function to read an entire data frame from an external file. This is discussed further in §7.

6.4.2 attach() and detach()

The \$ notation, such as accountants\$statef, for list components is not always very convenient. A useful facility would be somehow to make the components of a list or data frame temporarily visible as variables under their component name, without the need to quote the list name explicitly each time.

The attach() function, as well as having a directory name as its argument, may also have a data frame. Thus suppose lentils is a data frame with three variables lentils\$u, lentils\$v, lentils\$v. The attach

```
> attach(lentils)
```

places the data frame in the search list at position 2, and provided there are no variables u, v or w in position 1, u, v and w are available as variables from the data frame in their own right. At this point an assignment such as

> u \leftarrow v+w

does not replace the component u of the data frame, but rather masks it with another variable u in the working directory at position 1 on the search list. To make a permanent change to the data frame itself, the simplest way is to resort once again to the \$ notation:

```
> lentilsu \leftarrow v + w
```

However the new value of component **u** is not visible until the data frame is detached and attached again.

To detach a data frame, use the function

> detach()

More precisely, this statement detaches from the search list the entity currently at position 2. Thus in the present context the variables u, v and w would be no longer visible, except under the list notation as lentilsu and so on.

NOTE: With the current release of R the search list can contain at most 20 items. Avoid attaching the same data frame more than once. Always detach the data frame as soon as you have finished using its variables.

NOTE: With the current release of R lists and dataframes can only be attached at position 2 or above. It is not possible to directly assign into an attached list or data frame (thus, to some extent they are static). This is likely to change in the next year or so.

6.4.3 Working with data frames

A useful convention that allows you to work with many different problems comfortably together in the same working directory is

- gather together all variables for any well defined and separate problem in a data frame under a suitably informative name;
- when working with a problem attach the appropriate data frame at position 2, and use the working directory at level 1 for operational quantities and temporary variables;
- before leaving a problem, add any variables you wish to keep for future reference to the data frame using the \$ form of assignment, and then detach();
- finally remove all unwanted variables from the working directory and keep it as clean of left-over temporary variables as possible.

In this way it is quite simple to work with many problems in the same directory, all of which have variables named x, y and z, for example.

6.4.4 Attaching arbitrary lists

attach() is a generic function that allows not only directories and data frames to be attached to the search list, but other classes of object as well. In particular any object of mode list may be attached in the same way:

> attach(any.old.list)

7 Reading data from files

Large data objects will usually be read as values from external files rather than entered during an R session at the keyboard. R input facilities are simple and their requirements are fairly strict and even rather inflexible. There is a clear presumption by the designers of R that you will be able to modify your input files using other tools, such file editors or $per1^9$ fit in with the requirements of R. Generally this is very simple.

There is, however, a function make.fields() that can be used to convert a file with fixed width, non separated, input fields into a file with separated fields. There is also a facility count.fields() that will count the number of fields on each line of such a file. Occasionally for very simple conversion and checking problems these may be adequate to the task, but in most cases it is better to do the preliminary spade work before the R session begins.

If variables are to be held mainly in data frames, as we strongly suggest, they should be, an entire data frame can be read directly with the **read.table()** function. There is also a more primitive input function, **scan()**, that can be called directly.

7.1 The read.table() function

To read an entire data frame directly, the external file will normally have a special form.

- The first line of the file should have a name for each variable in the data frame.
- Each additional line of the file has its first item a row label and the values for each variable.

If the file has one fewer item in its first line than in its second, this arrangement is presumed to be in force. So the first few lines of a file to be read as a data frame might look as in Figure 2. By default numeric items (except row labels) are read as numeric variables and non-numeric

| | Price | Floor | Area | Rooms | Age | Cent.heat |
|-------|-------|-------|------|-------|-----|-----------|
| 01 | 52.00 | 111.0 | 830 | 5 | 6.2 | no |
| 02 | 54.75 | 128.0 | 710 | 5 | 7.5 | no |
| 03 | 57.50 | 101.0 | 1000 | 5 | 4.2 | no |
| 04 | 57.50 | 131.0 | 690 | 6 | 8.8 | no |
| 05 | 59.75 | 93.0 | 900 | 5 | 1.9 | yes |
| • • • | | | | | | |

Figure 2: Input file form with names and row labels

variables, such as Cent.heat in the example, as factors. This can be changed if necessary.

The function read.table() can then be used to read the data frame directly

```
> HousePrice <- read.table("houses.data")
```

Often you will want to omit including the row labels directly and use the default labels. In this case the file may omit the row label column as in Figure 3. The data frame may then be read as

> HousePrice <-- read.table("houses.data", header=T)

where the **heading=T** option specifies that the first line is a line of headings, and hence, by implication from the form of the file, that no explicit row labels are given.

⁹Under UNIX, the utilities sed or awk can be used.

| Floor | Area | Rooms | Age | Cent.heat | |
|-------|----------------------------------|--|--|--|--|
| 111.0 | 830 | 5 | 6.2 | no | |
| 128.0 | 710 | 5 | 7.5 | no | |
| 101.0 | 1000 | 5 | 4.2 | no | |
| 131.0 | 690 | 6 | 8.8 | no | |
| 93.0 | 900 | 5 | 1.9 | yes | |
| | 111.0 128.0 101.0 131.0 | 111.0 830 128.0 710 101.0 1000 131.0 690 | 111.0 830 5 128.0 710 5 101.0 1000 5 131.0 690 6 | 111.0 830 5 6.2 128.0 710 5 7.5 101.0 1000 5 4.2 131.0 690 6 8.8 | 111.0 830 5 6.2 no 128.0 710 5 7.5 no 101.0 1000 5 4.2 no 131.0 690 6 8.8 no |

. . .

| Figure 3: | Input | file | form | without | row | labels |
|-----------|-------|------|------|---------|-----|--------|
| | | | | | | |

7.2 The scan() function

Suppose the data vectors are of equal length and are to be read in in parallel. Further suppose that there are three vectors, the first of mode character and the remaining two of mode numeric, and the file is input.dat. The first step is to use scan() to read in the three vectors as a list, as follows

> in \leftarrow scan("input.dat", list("",0,0))

The second argument is a dummy list structure that establishes the mode of the three vectors to be read. The result, held in in, is a list whose components are the three vectors read in. To separate the data items into three separate vectors, use assignments like

> label \leftarrow in[[1]]; x \leftarrow in[[2]]; y \leftarrow in[[3]]

More conveniently, the dummy list can have named components, in which case the names can be used to access the vectors read in. For example

> in \leftarrow scan("input.dat", list(id="", x=0, y=0))

If you wish to access the variables separately they may either be re-assigned to variables in the working frame:

```
> label \leftarrow in$id; x \leftarrow in$x; y \leftarrow in$y
```

or the list may be attached at position 2 of the search list, (see $\S6.4.4$).

If the second argument is a single value and not a list, a single vector is read in, all components of which must be of the same mode as the dummy value.

> X <-- matrix(scan("light.dat", 0), ncol=5, byrow=T)

There are more elaborate input facilities available and these are detailed in the manual.

7.3 Other facilities; editing data

Once a data set has been read, there is a window based facility in ${\sf R}$ for making small changes. The command

```
> xnew \leftarrow data.entry(xold)
```

will allow you to edit your data set xold using a spreadsheet-like environment in a separate editing window, and on completion the changed object is assigned to xnew. xold, and hence xnew, can be any matrix, vector, data frame, or atomic data object.

Calling data.entry() with no arguments,

```
> xnew \leftarrow data.entry()
```

lets you enter new data via the spreadsheet interface.

8 More language features. Loops and conditional execution

8.1 Grouped expressions

R is an expression language in the sense that its only command type is a function or expression which returns a result. Even an assignment is an expression whose result is the value assigned, and it may be used wherever any expression may be used; in particular multiple assignments are possible.

Commands may be grouped together in braces, $\{expr_1; expr_2; \ldots; expr_m\}$, in which case the value of the group is the result of the last expression in the group evaluated. Since such a group is also an expression it may, for example, be itself included in parentheses and used a part of an even larger expression, and so on.

8.2 Control statements

8.2.1 Conditional execution: if statements

The language has available a conditional construction of the form

```
> if (expr_1) expr_2 else expr_3
```

where $expr_1$ must evaluate to a logical value and the result of the entire expression is then evident.

8.2.2 Repetitive execution: for loops, repeat and while

There is also a for-loop construction which has the form

> for (name in expr1) expr2

where name is the loop variable. $expr_1$ is a vector expression, (often a sequence like 1:20), and $expr_2$ is often a grouped expression with its sub-expressions written in terms of the dummy name. $expr_2$ is repeatedly evaluated as name ranges through the values in the vector result of $expr_1$.

As an example, suppose ind is a vector of class indicators and we wish to produce separate plots of y versus x within classes. One possibility here is to use coplot() to be discussed later, which will produce an array of plots corresponding to each level of the factor. Another way to do this, now putting all plots on the one display, is as follows:

```
> yc \leftarrow split(y, ind); xc \leftarrow split(x, ind)
```

> for (i in 1:length(yc)){plot(xc[[i]], yc[[i]]);

```
abline(lsfit(xc[[i]], yc[[i]]))}
```

(Note the function split() which produces a list of vectors got by splitting a larger vector according to the classes specified by a category. This is a useful function, mostly used in connection with boxplots. See the help facility for further details.)

WARNING: The use of for() loops will result in relatively slow evaluation. While for() loops in R tend to be faster than in S they should be avoided if possible. Many functions, such as apply(), tapply(), sapply() and others, are written primarily to avoid using explicit for() loops.

Other looping facilities include the

```
> repeat expr
```

statement and the

> while (condition) expr

 $\operatorname{statement}$.

The break statement can be used to terminate any loop, possibly abnormally. This is the only way to terminate repeat loops.

The next can be used to discontinue one particular cycle and skip to the "next".

Control statements are most often used in connection with functions which are discussed in $\S9$, and where more examples will emerge.

9 Writing your own functions

As we have seen informally along the way, the R language allows the user to create objects of mode *function*. These are true R functions that are stored in a special internal form and may be used in further expressions and so on. In the process, the language gains enormously in power, convenience and elegance, and learning to write useful functions is one of the main ways to make your use of R comfortable and productive.

It should be emphasized that most of the functions supplied as part of the R system, such as mean(), var(), postscript() and so on, are themselves written in R and thus do not differ materially from user written functions.

A function is defined by an assignment of the form

> name \leftarrow function(arg₁, arg₂, ...) expression

The expression is an R expression, (usually a grouped expression), that uses the arguments, arg_i , to calculate a value. The value of the expression is the value returned for the function.

A call to the function then usually takes the form $name(expr_1, expr_2, ...)$ and may occur anywhere a function call is legitimate.

9.1 Simple examples

As a first example, consider a function to calculate the two sample t-statistic, showing "all the steps". This is an artificial example, of course, since there are other, simpler ways of achieving the same end.

The function is defined as follows:

With this function defined, you could perform two sample t-tests using a call such as

As a second example, consider a function to emulate directly the MATLAB backslash command, which returns the coefficients of the orthogonal projection of the vector y onto the column space of the matrix, X. (This is ordinarily called the least squares estimates of the regression coefficients.) This would ordinarily be done with the qr() function; however this is sometimes a bit tricky to use directly and it pays to have a simple function such as the following to use it safely.

Thus given a vector $y^{n \times 1}$ and a matrix $X^{n \times p}$ then

$$X \setminus y \stackrel{\text{def}}{=} (X'X)^- X'y$$

where $(X'X)^{-}$ is a generalised inverse of X'X.

After this object is created it is permanent, like all objects, and may be used in statements such as

> regcoeff <- bslash(Xmat, yvar)

and so on.

The classical R function lsfit() does this job quite well, and more¹⁰. It in turn uses the functions qr() and qr.coef() in the slightly counterintuitive way above to do this part of the calculation. Hence there is probably some value in having just this part isolated in a simple to use function if it is going to be in frequent use. If so, we may wish to make it a matrix binary operator for even more convenient use.

9.2 Defining new binary operators.

Had we given the bslash() function a different name, namely one of the form

%anything%

it could have been used as a *binary operator* in expressions rather than in function form. Suppose, for example, we choose ! for the internal character. The function definition would then start as

> "%!%" \leftarrow function(X, y) {...}

(Note the use of quote marks.) The function could then be used as $X \ "!" y$. (The backslash symbol itself is not a convenient choice as it presents special problems in this context.)

The matrix multiplication operator, %*%, and the outer product matrix operator %0% are other examples of binary operators defined in this way.

9.3 Named arguments and defaults. "..."

As first noted in §2.3 if arguments to called functions are given in the "name=object" form, they may be given in any order. Furthermore the argument sequence may begin in the unnamed, positional form, and specify named arguments after the positional arguments.

Thus if there is a function fun1 defined by

> fun1 \leftarrow function(data, data.frame, graph, limit) {[function body omitted] }

Then the function may be invoked in several ways, for example

```
> ans ← fun1(d, df, 20, T)
> ans ← fun1(d, df, graph=T, limit=20)
> ans ← fun1(data=d, limit=20, graph=T, data.frame=df)
```

are all equivalent.

In many cases arguments can be given commonly appropriate default values, in which case they may be omitted altogether from the call when the defaults are appropriate. For example, if fun1 were defined as

```
> fun1 \leftarrow function(data, data.frame, graph=T, limit=20) {...<sup>10</sup>}
```

it could be called as

> ans \leftarrow fun1(d, df)

which is now equivalent to the three cases above, or as

> ans \leftarrow fun1(d, df, limit=10)

 $^{^{10}\}mathrm{See}$ also the methods described in $\S10$

9.4 Assignments within functions are local. Frames.

which changes one of the defaults.

It is important to note that defaults may be arbitrary expressions, even involving other arguments to the same function; they are not restricted to be constants as in our simple example here.

Another frequent requirement is to allow one function to pass on argument settings to another. For example many graphics functions use the function par() and functions like plot() allow the user to pass on graphical parameters to par() to control the graphical output. (See §11.4.1 for more details on the par() function.) This can be done by including an extra argument, literally "...", of the function, which may then be passed on. An outline example is given in Figure 4.

```
fun1 ← function(data, data.frame, graph=T, limit=20, ...) {
    [omitted statements]
    if (graph)
        par(pch="*", ...)
        [more omissions]
    }
```

Figure 4: Use of the ellipsis argument, "..."

9.4 Assignments within functions are local. Frames.

Note that any ordinary assignments done within the function are local and temporary and are lost after exit from the function. Thus the assignment $X \leftarrow qr(X)$ does not affect the value of the argument in the calling program.

To understand completely the rules governing the scope of R assignments the reader needs to be familiar with the notion of an evaluation *frame*. This is a somewhat advanced, though hardly difficult, topic and is not covered further in these notes.

If global and permanent assignments are intended within a function, then either the 'superassignment' operator, '<<-' or the function <code>assign()</code> can be used. See the <code>help</code> document for details. S-PLUS users should be aware that <<- has different semantics in R. These are discussed further in §9.6.

9.5 More advanced examples

9.5.1 Efficiency factors in block designs

As a more complete, if a little pedestrian, example of a function, consider finding the efficiency factors for a block design. (Some aspects of this problem have already been discussed in §5.3.)

A block design is defined by two factors, say blocks (b levels) and varieties, (v levels). If $R^{v \times v}$ and $K^{b \times b}$ are the *replications* and *block size* matrices, and $N^{b \times v}$ is the incidence matrix, then the efficiency factors are defined as the eigenvalues of the matrix

$$E = I_v - R^{-1/2} N' K^{-1} N R^{-1/2} = I_v - A' A$$

where $A = K^{-1/2} N R^{-1/2}$. One way to write the function is as in Figure 5.

It is numerically slightly better to work with the singular value decomposition on this occasion rather than the eigenvalue routines.

```
> bdeff \leftarrow function(blocks, varieties) {
           blocks \leftarrow as.factor(blocks)
                                                             # minor safety move
           b \leftarrow length(levels(blocks))
           varieties \leftarrow as.factor(varieties)
                                                             # minor safety move
           v \leftarrow length(levels(varieties))
           K \leftarrow as.vector(table(blocks))
                                                               remove dim attr
           R \leftarrow as.vector(table(varieties))
                                                             # remove dim attr
           \mathbb{N} \leftarrow \text{table(blocks, varieties)}
           A \leftarrow 1/sqrt(K) * N * rep(1/sqrt(R), rep(b, v))
           sv \leftarrow svd(A)
           list(eff=1 - sv$d^2, blockcv=sv$u, varietycv=sv$v)
  }
                        Figure 5: A function for block design efficiencies
```

The result of the function is a list giving not only the efficiency factors as the first component, but also the block and variety canonical contrasts, since sometimes these give additional useful qualitative information.

9.5.2 Dropping all names in a printed array

For printing purposes with large matrices or arrays, it is often useful to print them in close block form without the array names or numbers. Removing the dimnames attribute will not achieve this effect, but rather the array must be given a dimnames attribute consisting of empty strings. For example to print a matrix, X

```
> temp ~ X
> dimnames(temp) ~ list(rep("", nrow(X)), rep("", ncol(X))
> temp; rm(temp)
```

This can be much more conveniently done using a function, no.dimnames(), shown in Figure 6, as a "wrap around" to achieve the same result. It also illustrates how some effective and useful user functions can be quite short. With this function defined, an array may be printed in close

Figure 6: A function for printing arrays in compact form

format using

This is particularly useful for large integer arrays, where patterns are the real interest rather than the values.

9.5.3 Recursive numerical integration

Functions may be recursive, and may themselves define functions within themselves. Note, however, that such functions, or indeed variables, are not inherited by called functions in higher evaluation frames as they would be if they were on the search list.

The example in Figure 7 shows a naive way of performing one dimensional numerical integration. The integrand is evaluated at the end points of the range and in the middle. If the one-panel trapezium rule answer is close enough to the two panel, then the latter is returned as the value. Otherwise the same process is recursively applied to each panel. The result is an adaptive integration process that concentrates function evaluations in regions where the integrand is farthest from linear. There is, however, a heavy overhead, and the function is only competitive with other algorithms when the integrand is both smooth and very difficult to evaluate.

The example is also given partly as a little puzzle in R programming.

```
area \leftarrow function(f, a, b, eps = 1.0e-06, lim = 10)
{
   fun1 \leftarrow function(f, a, b, fa, fb, a0, eps, lim, fun)
   { ## function 'fun1' is only visible inside 'area'
       d \leftarrow (a + b)/2
       h \leftarrow (b - a)/4
       fd \leftarrow f(d)
       a1 \leftarrow h * (fa + fd)
       a2 \leftarrow h * (fd + fb)
       if(abs(a0 - a1 - a2) < eps || lim == 0)
          return(a1 + a2)
       else {
          return(fun(f, a, d, fa, fd, a1, eps, lim - 1, fun) +
                   fun(f, d, b, fd, fb, a2, eps, lim - 1, fun))
       }
   }
   fa \leftarrow f(a)
   fb \leftarrow f(b)
   a0 \leftarrow ((fa + fb) * (b - a))/2
   fun1(f, a, b, fa, fb, a0, eps, lim, fun1)
}
```

Figure 7: A recursive function within a function

9.6 Scope

The discussion in this section is somewhat more technical than in other parts of this document. However, it details one of the major differences between S-PLUS and R.

The symbols which occur in the body of a function can be divided into three classes; formal parameters, local variables and free variables. The formal parameters of a function are those occurring in the argument list of the function. Their values are determined by the process of *binding* the actual function arguments to the formal parameters. Local variables are those whose values are determined by the evaluation of expressions in the body of the functions. Variables

which are not formal parameters or local variables are called free variables. Free variables become local variables if they are assigned to. Consider the following function definition.

```
f \leftarrow function(x) \left\{ \begin{array}{c} y \leftarrow 2*x \\ print(x) \\ print(y) \\ print(z) \end{array} \right\}
```

In this function, \mathbf{x} is a formal parameter, \mathbf{y} is a local variable and \mathbf{z} is a free variable.

In R the free variable bindings are resolved by first looking in the environment in which the function was created. First we define a function called **cube**.

```
cube \leftarrow function(n) {
    sq \leftarrow function() n*n
    n*sq()
}
```

The variable n in the function sq is not an argument to that function. Therefore it is a free variable and the scoping rules must be used to ascertain the value that is to be associated with it. Under static scope the value is that associated with a global variable named n. Under lexical scope it is the parameter to the function cube since that is the active binding for the variable n at the time the function sq was defined. The difference between evaluation in R and evaluation in S-PLUS is that S-PLUS looks for a global variable called n while R first looks for a variable called n in the environment created when cube was invoked.

```
# first evaluation in S
S> cube(2)
Error in sq(): Object "n" not found
Dumped
S> n ~ 3
S> cube(2)
[1] 18
# then the same function evaluated in R
R> cube(2)
[1] 8
```

Lexical scope can also be used to give functions *mutable state*. In the following example we show how R can be used to mimic a bank account. A functioning bank account needs to have a balance or total, a function for making withdrawals, a function for making deposits and a function for stating the current balance. We achieve this by creating the three functions within account and then returning a list containing them. When account is invoked it takes a numerical argument total and returns a list containing the three functions. Because these functions are defined in an environment which contains total, they will have access to its value.

The special assignment operator, <<-, is used to change the value associated with total. This operator looks back in enclosing environments for an environment that contains the symbol total and when it finds such an environment it replaces the value, in that environment, with the value of right hand side. If the global or top-level environment is reached without finding the symbol total then that variable is created and assigned to there. For most users <<- creates a global variable and assigns the value of the right hand side to it¹¹. Only when <<- has been used in a function that was returned as the value of another function will the special behaviour described here occur.

 $^{^{11}}$ In some sense this mimics the behaviour in S-PLUS since in S-PLUS this operator always creates or assigns to a global variable.

```
open.account \leftarrow function(total) {
  list(
    deposit = function(amount) {
        if(amount <= 0)
             stop("Deposits must be positive!\n")
          total \ll - total + amount
          cat(amount, "deposited. Your balance is", total, "nn")
    },
    withdraw = function(amount) {
        if(amount > total)
             stop("You don't have that much money!\n")
        total \ll - total - amount
        cat(amount, "withdrawn. Your balance is", total, "n^{n})
    },
    balance = function() {
        cat("Your balance is", total, "\n\n")
    }
  )
}
ross \leftarrow open.account(100)
robert \leftarrow open.account(200)
ross$withdraw(30)
ross$balance()
robert$balance()
ross$deposit(50)
ross$balance()
ross$withdraw(500)
```

Figure 8: A function that uses lexical scope.

9.7 Customising the environment.

Users can customize their environment in several different ways. There is a system initialization file and every directory can have its own special initialization file. Finally the special functions .First and .Last can be used.

The system initialization file is called **Rprofile** and it is found in the R home subdirectory **library**. This file should contain the commands that you want to execute every time R is started under your system. A second, personal, profile file named .**Rprofile**¹² can be placed in any directory. If R is invoked in that directory then that file will be sourced. This file gives individual users control over their workspace and allows for different start-up procedures in different working directories. If no .**Rprofile** file is found in the startup directory, than R looks for a .**Rprofile** file in the users home directory and uses that (if it exists).

Any function named .First() in either of the two profile files or in the .RData image has a special status. It is automatically performed at the beginning of an R session and may be used to initialise the environment. For example, the definition in Figure 9 alters the prompt to \$ and sets up various other useful things that can then be taken for granted in the rest of the session.

Thus, the sequence in which files are executed is, Rprofile, .Rprofile, .RData and then

¹²So it is hidden under UNIX.

.First(). A definitions in later files will mask definitions in earlier files. Similarly a func-

Figure 9: An example of a .First() function

tion .Last(), if defined, is executed at the very end of the session. An example is given in Figure 10.

Figure 10: An example of a .Last() function

9.8 Classes, generic functions and object orientation

The class of an object determines how it will be treated by what are known as generic functions. Put the other way round, a generic function performs a task or action on its arguments specific to the class of the argument itself. If the argument lacks any class attribute, or has a class not catered for specifically by the generic function in question, there is always a default action provided.

An example makes things clearer. The class mechanism offers the user the facility of designing and writing generic functions for special purposes. Among the other generic functions are plot() for displaying objects graphically, summary() for summarising analyses of various types, and anova() for comparing statistical models.

The number of generic functions that can treat a class in a specific way can be quite large. For example, the functions that can accommodate in some fashion objects of class data.frame include

```
[, [[<-, any, as.matrix,
[<-, model, plot, summary,</pre>
```

A currently complete list can be got by using the methods() function:

```
> methods(class="data.frame")
```

Conversely the number of classes a generic function can handle can also be quite large. For example the plot() function has variants for classes of object

data.frame, default, density, factor,

and more. A complete list can be got again by using the methods() function:

> methods(plot)

The reader is referred to the official references for a complete discussion of this mechanism.

10 Statistical models in R

This section presumes the reader has some familiarity with statistical methodology, in particular with regression analysis and the analysis of variance. Later we make some rather more ambitious presumptions, namely that something is known about generalized linear models and nonlinear regression.

The requirements for fitting statistical models are sufficiently well defined to make it possible to construct general tools that apply in a broad spectrum of problems. R provides an interlocking suite of facilities that make fitting statistical models very simple. However these are not at the same high level as those in, say, Genstat, especially in the form of the output which in keeping with general R policy is rather minimal.

10.1 Defining statistical models; formulæ

The template for a statistical model is a linear regression model with independent, homoscedastic errors

$$y_i = \sum_{j=0}^{p} \beta_j x_{ij} + e_i, \qquad e_i \sim \text{NID}(0, \sigma^2), \qquad i = 1, 2, \dots, n$$

In matrix terms this would be written

 $y = \mathbf{X}eta + e$

where the y is the response vector, \mathbf{X} is the model matrix or design matrix and has columns x_0 , x_1, \ldots, x_p , the determining variables. Very often x_0 will be a column of 1s defining an intercept term.

Examples.

Before giving a formal specification, a few examples may usefully set the picture.

Suppose y, x, x0, x1, x2, \ldots are numeric variables, X is a matrix and A, B, C, \ldots are factors. The following formulæ on the left side below specify statistical models as described on the right.

| y~x y~1+x | Both imply the same simple linear regression model of y on x . The first has an implicit intercept term, and the second an explicit one. |
|-------------------------------------|--|
| y ~ -1 + x y ~ x - 1 | Simple linear regression of y on x through the origin, (that is, without an intercept term). |
| log(y) ~ x1 + x2 | Multiple regression of the transformed variable, $\log(y)$, on x_1 and x_2 (with an implicit intercept term). |
| y ~ poly(x,2) y ~ 1 + x + I(x^2) | Polynomial regression of y on x of degree 2. The first form uses orthogonal polynomials, and the second uses explicit powers, as basis. |
| y ~ X + poly(x,2) | Multiple regression y with model matrix consisting of the matrix X as well as polynomial terms in x to degree 2. |
| у ~ А | Single classification analysis of variance model of y , with classes determined by A . |
| y ~ A + x | Single classification analysis of covariance model of y , with classes determined by A , and with covariate x . |

| у У | ~ A*B ~ A + B + A:B ~ B %in% A ~ A/B | Two factor non-additive model of y on A and B . The first two specify the same crossed classification and the second two specify the same nested classification. In abstract terms all four specify the same model subspace. |
|--------|---|--|
| - | ~ (A + B + C)^2 ~ A*B*C - A:B:C | Three factor experiment but with a model containing main effects and two factor interactions only. Both formulæ specify the same model. |
| | | |
| у | ~ A * x ~ A/x ~ A/(1 + x) - 1 | Separate simple linear regression models of y on x within the levels of A , with different codings. The last form produces explicit estimates of as many different intercepts and slopes as there are levels in A . |

The operator ~ is used to define a model formula in R. The form, for an ordinary linear model, is

response ~ $[\pm]$ term₁ ± term₂ ± term₃ ± · · ·

- **response** is a vector or matrix, (or expression evaluating to a vector or matrix) defining the response variable(s).
- \pm is an operator, either + or -, implying the inclusion or exclusion of a term in the model, (the first is optional).

term is either

- a vector or matrix expression, or 1,
- a factor, or
- a formula expression consisting of factors, vectors or matrices connected by formula operators.

In all cases each term defines a collection of columns either to be added to or removed from the model matrix. A 1 stands for an intercept column and is by default included in the model matrix unless explicitly removed.

The formula operators are similar in effect to the Wilkinson and Rogers notation used by such programs a Glim and Genstat. One inevitable change is that the operator "." becomes ":" since the period is a valid name character in R. The notation is summarised as in the Table 1 (based on Chambers & Hastie, p. 29).

Note that inside the parentheses that usually enclose function arguments all operators have their normal arithmetic meaning. The function

I() is an identity function used only to allow terms in model formulæ to be defined using arithmetic operators.

Note particularly that the model formulæ specify the *columns of the model matrix*, specification of the parameters is implicit. This is not the case in other contexts, for example in fitting nonlinear models.

10.2 Regression models; fitted model objects

The basic function for fitting ordinary multiple models is lm(), and a streamlined version of the call is as follows:

| Form | Meaning |
|------------------|--|
| $Y \sim M$ | Y is modelled as M |
| M_1 + M_2 | Include M_1 and M_2 |
| M_1 - M_2 | Include M_1 leaving out terms of M_2 |
| $M_1: M_2$ | The tensor product of M_1 and M_2 . If both terms factors, then the "subclasses" factor. |
| M_1 %in% M_2 | Similar to $M_1: M_2$, but with a different coding. |
| $M_1 * M_2$ | $M_1 + M_2 + M_1: M_2$ |
| M_{1}/M_{2} | M_1 + M_2 %in% M_1 |
| M^n | All terms in M together with "interactions" up to order n |
| I(<i>M</i>) | Insulate M . Inside M all operators have their normal arithmetic meaning, and that term appears in the model matrix. |

Table 1: Summary of model operator semantics

> fitted.model \leftarrow lm(formula, data=data.frame)

For example

> fm2 \leftarrow lm(y ~ x1 + x2, data=production)

would fit a multiple regression model of y on x_1 and x_2 (with implicit intercept term).

The important but technically optional parameter data=production specifies that any variables needed to construct the model should come first from the production data frame. This is the case regardless of whether data frame production has been attached to the search list or not.

10.3 Generic functions for extracting information

The value of lm() is fitted model object; technically a list of results of class lm. Information about the fitted model can then be displayed, extracted, plotted and so on by using generic functions that orient themselves to objects of class lm. A full list of these at the present time is

add1 residuals coef effects kappa predict labels print alias deviance family summary anova drop1 formula plot proj

A brief description of the most commonly used ones is given in Table 2.

10.4 Analysis of variance; comparing models

The model fitting function aov(formula, data= data.frame) operates at the simplest level in a very similar way to the function lm(), and most of the generic functions listed in Table 2 apply.

It should be noted that in addition aov() allows an analysis of models with multiple error strata such as split plot experiments, or balanced incomplete block designs with recovery of inter-block information. The model formula

| Function | Value or Effect |
|--|--|
| $	ext{anova}(object_1, object_2)$ | Compare a submodel with an outer model and product an analysis of variance table. |
| <pre>coefficients(object)</pre> | Extract the regression coefficient (matrix). Short form: coef(object). |
| <pre>deviance(object)</pre> | Residual sum of squares, weighted if appropriate. |
| <pre>formula(object)</pre> | Extract the model formula. |
| <pre>plot(object)</pre> | Product two plots, one of the observations against the fitted values, the other of the absolute residuals against the fitted values. |
| <pre>predict(object, newdata=data.frame) predict.gam(object, newdata=data.frame)</pre> | The data frame supplied must have variables specified with the same labels as the original. The value is a vec- tor or matrix of predicted values corresponding to the determining variable values in <i>data.frame</i> . predict.gam() is a safe alternative to predict() that can be used for lm, glm and gam fitted objects. It must be used, for example, in cases where orthogonal polyno- mials are used as the original basis functions, and the addition of new data implies different basis functions to the original. |
| <pre>print(object)</pre> | Print a concise version of the object. Most often used implicitly. |
| residuals(object) | Extract the (matrix of) residuals, weighted as appropri- ate. Short form: resid(object). |
| <pre>summary(object)</pre> | Print a comprehensive summary of the results of the regression analysis. |

| | 1 | | c | | 1 | - 1 • . |
|--------------------------------------|-------|---------|-----------|----|-------|------------|
| Table 2: Commonly | 11000 | CONORIC | tunctions | n | Clace | Im objects |
| $\pm a D C \Delta_i = O O m m O m y$ | uscu | generie | runcuons | on | CIGOO | |

specifies a multi-stratum experiment with error strata defined by the *strata.formula*. In the simplest case, *strata.formula* is simply a factor, when it defines a two strata experiment, namely between and within the levels of the factor.

For example, with all determining variables factors, a model formula such as that in:

> fm \leftarrow aov(yield ~ v + n*p*k + Error(farms/blocks), data=farm.data)

would typically be used to describe an experiment with mean model v + n*p*k and three error strata, namely "between farms", "within farms, between blocks" and "within blocks".

10.4.1 ANOVA tables

Note also that the analysis of variance table (or tables) are for a sequence of fitted models. The sums of squares shown are the decrease in the residual sums of squares resulting from an inclusion of *that term* in the model at *that place* in the sequence. Hence only for orthogonal experiments will the order of inclusion be inconsequential.

For multistratum experiments the procedure is first to project the response onto the error strata, again in sequence, and to fit the mean model to each projection. For further details, see Chambers and Hastie, §5.

A more flexible alternative to the default full ANOVA table is to compare two or more models directly using the **anova()** function.

> anova(fitted.model.1, fitted.model.2, ...)

The display is then an ANOVA table showing the differences between the fitted models when fitted in sequence. The fitted models being compared would usually be an hierarchical sequence, of course. This does not give different information to the default, but rather makes it easier to comprehend and control.

10.5 Updating fitted models. The ditto name "."

The update() function is largely a convenience function that allows a model to be fitted that differs from one previously fitted usually by just a few additional or removed terms. Its form is

```
> new.model <- update(old.model, new.formula)
```

In the *new.formula* the special name consisting of a period, ".", only, can be used to stand for "the corresponding part of the old model formula". For example

```
> fm05 \leftarrow lm(y ~ x1 + x2 + x3 + x4 + x5, data=production)
> fm6 \leftarrow update(fm05, . ~ . + x6)
> smf6 \leftarrow update(fm6, sqrt(.) ~ .)
```

would fit a five variate multiple regression with variables (presumably) from the data frame **production**, fit an additional model including a sixth regressor variable, and fit a variant on the model where the response had a square root transform applied.

Note especially that if the data= argument is specified on the original call to the model fitting function, this information is passed on through the fitted model object to update() and its allies.

The name "." can also be used in other contexts, but with slightly different meaning. For example

```
> fmfull \leftarrow lm(y ~ . , data=production)
```

would fit a model with response y and regressor variables all other variables in the data frame production.

Other functions for exploring incremental sequences of models are add1(), drop1(), step() and stepwise(). The names of these give a good clue to their purpose, but for full details see the help document.

10.6 Generalized linear models; families

Generalized linear modelling is a development of linear models to accommodate both non-normal response distributions and transformations to linearity in a clean and straightforward way. A generalized linear model may be described in terms of the following sequence of assumptions:

- There is a response, y, of interest and stimulus variables x_1, x_2, \ldots whose values influence the distribution of the response.
- The stimulus variables influence the distribution of y through a single linear function, only. This linear function is called the *linear predictor*, and is usually written

$$\eta = \beta_1 x_1 + \beta_2 x_2 + \dots + \beta_p x_p$$

hence x_i has no influence on the distribution of y if and only if $\beta_i = 0$.

• The distribution of y is of the form

$$f_Y(y;\mu,arphi) = \exp\left[rac{A}{arphi}\left\{y\lambda(\mu) - \gamma\left(\lambda(\mu)
ight)
ight\} + au(y,arphi)
ight]$$

where φ is a *scale parameter*, (possibly known), and is constant for all observations, A represents a prior weight, assumed known but possibly varying with the observations, and

 μ is the mean of y. So it is assumed that the distribution of y is determined by its mean and possibly a scale parameter as well.

• The mean, μ , is a smooth invertible function of the linear predictor:

 $\mu = m(\eta), \qquad \eta = m^{-1}(\mu) = \ell(\mu)$

and this inverse function, $\ell(.)$ is called the *link function*.

These assumptions are loose enough to encompass a wide class of models useful in statistical practice, but tight enough to allow the development of a unified methodology of estimation and inference, at least approximately. The reader is referred to any of the current reference works on the subject for full details, such as

Generalized linear models by Peter McCullagh and John A Nelder, 2nd edition, Chapman and Hall, 1989, or

An introduction to generalized linear models by Annette J Dobson, Chapman and Hall, 1990.

10.6.1 Families

The class of generalized linear models handled by facilities supplied in R includes gaussian, binomial, poisson, inverse gaussian and gamma response distributions and also quasi-likelihood models where the response distribution is not explicitly specified. In the latter case the variance function must be specified as a function of the mean, but in other cases this function is implied by the response distribution.

Each response distribution admits a variety of link functions to connect the mean with the linear predictor. Those automatically available are as in Table 3.

| | | | Fa | mily Name | | |
|---------------|----------|----------|-------|------------------|---------|-------|
| Link Function | binomial | gaussian | Gamma | inverse.gaussian | poisson | quasi |
| logit | * | | | | | * |
| probit | * | | | | | * |
| cloglog | * | | | | | * |
| identity | | * | * | | * | * |
| inverse | | | * | | | * |
| log | | | * | | * | * |
| 1/mu^2 | | | | * | | * |
| sqrt | | | | | * | * |

Table 3: Families and the link functions available to them

The combination of a response distribution, a link function and various other pieces of information that are needed to carry out the modelling exercise is called the *family* of the generalized linear model.

10.6.2 The glm() function

Since the distribution of the response depends on the stimulus variables through a single linear function *only*, the same mechanism as was used for linear models can still be used to specify the linear part of a generalized model. The family has to be specified in a different way.

The R function to fit a generalized linear model is glm() which uses the form

> fitted.model <- glm(formula, family = family.generator, data=data.frame)

The only new feature is the *family.generator*, which is the instrument by which the family is described. It is the name of a function that generates a list of functions and expressions that together define and control the model and estimation process. Although this may seem a little complicated at first sight, its use is quite simple.

The names of the standard, supplied family generators are given under "Family Name" in Table 3. Where there is a choice of links, the name of the link may also be supplied with the family name, in parentheses as a parameter. In the case of the **quasi** family, the variance function may also be specified in this way.

Some examples make the process clear.

The gaussian family

A call such as

> fm \leftarrow glm(y ~ x1+x2, family=gaussian, data=sales)

achieves the same result as

> fm \leftarrow lm(y ~ x1+x2, data=sales)

but much less efficiently. Note how the gaussian family is not automatically provided with a choice of links, so no parameter is allowed. If a problem requires a gaussian family with a nonstandard link, this can usually be achieved through the **quasi** family, as we shall see later.

The binomial family

Consider a small, artificial example.

On the Greek island of Kalythos the male inhabitants suffer from a congenital eye disease, the effects of which become more marked with increasing age. Samples of islander males of various ages were tested for blindness and the results recorded. The data is shown in Table 4.

| Age: | 20 | 35 | 45 | 55 | 70 |
|-------------|----|----|----|----|----|
| No. tested: | 50 | 50 | 50 | 50 | 50 |
| No. blind: | 6 | 17 | 26 | 37 | 44 |

| Table | e 4: | The | Kalythos | blindness | data |
|-------|------|-----|----------|-----------|------|
|-------|------|-----|----------|-----------|------|

The problem we consider is to fit both logistic and probit models to this data, and to estimate for each model the LD50, that is the age at which the chance of blindness for a male inhabitant is 50%.

If y is the number of blind at age x and n the number tested, both models have the form

$$y \sim B(n, F(\beta_0 + \beta_1 x))$$

where for the probit case, $F(z) = \Phi(z)$ is the standard normal distribution function, and in the logit case, (the default), $F(z) = e^{z}/(1 + e^{z})$. In both cases the LD50 is

$$LD50 = -\beta_0 / \beta_1$$

that is, the point at which the argument of the distribution function is zero.

The first step is to set the data up as a data frame

> kalythos \leftarrow data.frame(x=c(20,35,45,55,70), n=rep(50,5),

$$y=c(6, 17, 26, 37, 44))$$

To fit a binomial model using glm() there are two possibilities for the response:

- If the response is a *vector* it is assumed to hold *binary* data, and so must be a 0, 1 vector.
- If the response is a *two column matrix* it is assumed that the first column holds the number of successes for the trial and the second holds the number of failures.

Here we need the second of these conventions, so we add a matrix to our data frame:

> kalythos\$Ymat <- cbind(kalythos\$y, kalythos\$n - kalythos\$y)

To fit the models we use

```
> fml \leftarrow glm( Ymat<sup>~</sup>x, family=binomial, data=kalythos)
```

Since the logit link is the default the parameter may be omitted on the second call. To see the results of each fit we could use

```
> summary(fmp)
```

```
> summary(fml)
```

Both models fit (all too) well. To find the LD50 estimate we can use a simple function:

- > $1d50 \leftarrow function(b) -b[1]/b[2]$
- > ldp \leftarrow ld50(coef(fmp)); ldl \leftarrow ld50(coef(fmp)); c(ldp, ldl)

The actual estimates from this data are 43.663 years and 43.601 years respectively.

Poisson models

With the poisson family the default link is the log, and in practice the major use of this family is to fit surrogate poisson log-linear models to frequency data, whose actual distribution is often multinomial. This is a large and important subject we will not discuss further here. It even forms a major part of the use of non-gaussian generalized models overall.

Occasionally genuinely poisson data arises in practice and in the past it was often analysed as gaussian data after either a log or a square-root transformation. As a graceful alternative to the latter, a poisson generalized linear model may be fitted as in the following example:

> fmod <-- glm(y ~ A+B + x, family=poisson(link=sqrt), data=worm.counts)

Quasi-likelihood models

For all families the variance of the response will depend on the mean and will have the scale parameter as a multiplier. The form of dependence of the variance on the mean is a characteristic of the response distribution; for example for the poisson distribution $Var[y] = \mu$.

For quasi-likelihood estimation and inference the precise response distribution is not specified, but rather only a link function and the form of the variance function as it depends on the mean. Since quasi-likelihood estimation uses formally identical techniques to those for the gaussian distribution, this family provides a way of fitting gaussian models with non-standard link functions or variance functions, incidently.

For example, consider fitting the non-linear regression

$$y = \frac{\theta_1 z_1}{z_2 - \theta_2} + e \tag{1}$$

10.7 Nonlinear least squares and maximum likelihood models

this may be written alternatively as

$$y = \frac{1}{\beta_1 x_1 + \beta_2 x_2} + e$$

where $x_1 = z_2/z_1$, $x_2 = -1/x_1$, $\beta_1 = 1/\theta_1$ and $\beta_2 = \theta_2/\theta_1$. Supposing a suitable data frame to be set up we could fit this non-linear regression as

```
> nlfit \leftarrow glm(y<sup>x</sup>1+x2-1,family=
```

quasi(link=inverse,variance=constant), data=biochem)

The reader is referred to the manual and the help document for further information, as needed.

10.7 Nonlinear least squares and maximum likelihood models

Certain forms of nonlinear model can be fitted by Generalized Linear Models (glm()). But in the majority of cases we have to approach the nonlinear curve fitting problem as one of nonlinear optimization. R's nonlinear optimization routine is nlm(), which takes the place of S-PLUS's ms(). We seek the parameter values that minimize some index of lack-of-fit, and nlm() does that by trying out various parameter values iteratively. Unlike linear regression for example, there is no guarantee that the procedure will converge on satisfactory estimates. nlm() requires initial guesses about what parameter values to try, and convergence depends critically upon the quality of the initial guesses.

10.7.1 Least squares

One way to fit a nonlinear model is by minimizing the sum of the squared errors (SSE) or residuals. This method makes sense if the observed errors could have plausibly arisen from a normal distribution.

Here is an example from (Bates and Watts, 1988, p. 51). The data are:

> x \leftarrow c(0.02, 0.02, 0.06, 0.06, 0.11, 0.11, 0.22, 0.22, 0.56, 0.56, 1.10, 1.10) > y \leftarrow c(76, 47, 97, 107, 123, 139, 159, 152, 191, 201, 207, 200)

The model to be fitted is:

> fn \leftarrow function(p) sum((y - (p[1] * x)/(p[2] + x))^2)

In order to do the fit we need initial estimates of the parameters. One way to find sensible starting values is to plot the data, guess some parameter values, and superimpose the model curve using those values.

> plot(x,y)

- > xfit \leftarrow seq(.02,1.1,.05)
- > yfit \leftarrow 200*xfit/(.1+xfit)
- > lines(spline(xfit,yfit))

We could do better, but these starting values of 200 and .1 seem adequate. Now do the fit:

> out \leftarrow nlm(fn,p=c(200,.1),hessian=T)

After the fitting, out\$minimum is the SSE, and out\$estimates are the least squares estimates of the parameters. To obtain the approximate standard errors (SE) of the estimates we do:

> sqrt(diag(2*out\$minimum/(length(y)-2)*solve(out\$hessian)))

The 2 in the line above represents the number of parameters. A 95% confidence interval would be the parameter estimate ± 1.96 SE. We can superimpose the least squares fit on a new plot:

> plot(x,y)

- > xfit \leftarrow seq(.02,1.1,.05)
- > yfit <- 212.68384222*xfit/(0.06412146+xfit)
- > lines(spline(xfit,yfit))

10.7.2 Maximum likelihood

Maximum likelihood is a method of nonlinear model fitting that applies even if the errors are not normal. The method finds the parameter values which maximize the log likelihood, or equivalently which minimize the -log likelihood. Here is an example from (Dobson, 1991, pp. 108-11). This example fits a logistic model to dose-response data, which clearly could also be fit by glm(). The data are:

> x ← c(1.6907,1.7242,1.7552,1.7842,1.8113,1.8369,1.8610,1.8839)

> y \leftarrow c(6,13,18,28,52,53,61,60)

> n \leftarrow c(59,60,62,56,63,59,62,60)

The -log likelihood to minimize is:

> fn \leftarrow function(p)

sum(- (y*(p[1]+p[2]*x) - n*log(1+exp(p[1]+p[2]*x)) + log(choose(n,y))))

We pick sensible starting values and do the fit:

> out \leftarrow nlm(fn,p=c(-50,20),hessian=T)

After the fitting, out\$minimum is the -log likelihood, and out\$estimates are the maximum likelihood estimates of the parameters. To obtain the approximate SEs of the estimates we do:

> sqrt(diag(solve(out\$hessian)))

A 95% confidence interval would be the parameter estimate ± 1.96 SE.

10.8 Some non-standard models

Note that only some of these features have been implemented.

We conclude this section with just a brief mention of some of the other facilities available in R for special regression and data analysis problems.

- Local approximating regressions. The loess() function fits a nonparametric regression by using a locally weighted regression. Such regressions are useful for highlighting a trend in messy data or for data reduction to give some insight into a large data set.
- **Robust regression** There are several functions available for fitting regression models in a way resistant to the influence of extreme outliers in the data. The most sophisticated of these is rreg(), but others include lmsfit() for least median squares regression and llfit() for regression using the L_1 -norm. However these do not as yet have the facility of using formulæ to specify the model function, for example, and conform to an older protocol, which makes them sometimes rather tedious to use. There is also a robust() facility to change a glm family object into a robust version for use with the glm() model fitting function.
- Generalized additive models. This technique aims to construct a regression function from smooth additive functions of the determining variables, usually one for each determining variable. The function gam() is in many ways similar to the other model fitting functions outlined above. In addition there are other model fitting functions that do a similar job. These include avas() and ace(). On the other hand ppreg() is available for projection

48

pursuit regression, but this technique is still very much in need of a complete theoretical treatment and further practical experience. These latter functions are again conforming to an older protocol for model fitting functions and lack the convenience of the newer functions.

Tree based models Rather than seek an explicit global linear model for prediction or interpretation, tree based models seek to bifurcate the data, recursively, at critical points of the determining variables in order to partition the data ultimately into groups that are as homogeneous as possible within, and as heterogeneous as possible between. The results often lead to insights that other data analysis methods tend not to yield.

Models are again specified in the ordinary linear model form. The model fitting function is tree(), but many other generic functions such as plot() and text() are well adapted to displaying the results of a tree-based model fit in a graphical way.

11 Graphical procedures

Graphical facilities are an important and extremely versatile component of the R environment. It is possible to use the facilities to display a wide variety of statistical graphs and also to build entirely new types of graph.

The graphics facilities can be used in both interactive modes, but in most cases, interactive use is more productive. Interactive use is also easy because at startup time R initiates a graphics *device driver* which opens a special *graphics window* for the display of interactive graphics. Although this is done automatically, it is useful to know that the command used is X11() under UNIX, Windows () under Windows 95 and Windows NT, and Macintosh() on a Macintosh.

Once the device driver is running, R plotting commands can be used to produce a variety of graphical displays and to create entirely new kinds of display.

Plotting commands are divided into three basic groups:

- High-level plotting functions create a new plot on the graphics device, possibly with axes, labels, titles and so on.
- Low-level plotting functions add more information to an existing plot, such as extra points, lines and labels.
- **Interactive** graphics functions allow you interactively add information to, or extract information from, an existing plot, using a pointing device such as a mouse.

In addition, R maintains a list of *graphical parameters* which can be manipulated to customise your plots.

11.1 High-level plotting commands

High-level plotting functions are designed to generate a complete plot of the data passed as arguments to the function. Where appropriate, axes, labels and titles are automatically generated (unless you request otherwise.) High-level plotting commands always start a new plot, erasing the current plot if necessary.

11.1.1 The plot() function

One of the most frequently used plotting functions in R is the plot() function. This is a *generic* function: the type of plot produced is dependent on the type or *class* of the first argument.

| plot(x,y) plot(xy) | If x and y are vectors, $plot(x,y)$ produces a scatterplot of y against x. The same effect can be produced by supplying one argument (second form) as either a list containing two elements x and y or a two-column matrix. |
|--|--|
| plot(x) | If x is a time series, this produces a time-series plot, if x is a numeric vector, it produce a plot of the values in the vector against their index in the vector, and if x is a complex vector, it produces a plot of imaginary versus real parts of the vector elements. |
| plot(f) plot(f,y) | f is a factor object, y is a numeric vector. The first form generates a bar plot of f ; the second form produces boxplots of y for each level of f . |
| plot(df) plot(~ expr) plot(y ~ expr) | df is a data frame, y is any object, $expr$ is a list of object names separated by '+' (e.g. $a + b + c$). The first two forms produce distributional plots of the variables in a data frame (first form) or of a number of named objects (second form). The third form plots y against every object named in expr. |

11.1.2 Displaying multivariate data

R provides two very useful functions for representing multivariate data. If ${\tt X}$ is a numeric matrix or data frame, the command

> pairs(X)

produces a pairwise scatterplot matrix of the variables defined by the columns of X, that is, every column of X is plotted against every other column of X and the resulting n(n-1) plots are arranged in a matrix with plot scales constant over the rows and columns of the matrix.

When three or four variables are involved a *coplot* may be more enlightening. If a and b are numeric vectors and c is a numeric vector or factor object (all of the same length), then the command

> coplot(a \sim b | c)

produces a number of scatterplots of a against b for given values of c. If c is a factor, this simply means that a is plotted against b for every level of c. When c is numeric, it is divided into a number of *conditioning intervals* and for each interval a is plotted against b for values of c within the interval. The number and position of intervals can be controlled with given.values= argument to coplot() — the function co.intervals() is useful for selecting intervals. You can also use two given variables with a command like

> coplot(a \sim b | c + d)

which produces scatterplots of a against b for every joint conditioning interval of c and d.

The coplot() and pairs() function both take an argument panel= which can be used to customise the type of plot which appears in each panel. The default is points() to produce a scatterplot but by supplying some other low-level graphics function of two vectors x and y as the value of panel= you can produce any type of plot you wish. An example panel function useful for coplots is panel.smooth().

11.1.3 Display graphics

Other high-level graphics functions produce different types of plots. Some examples are:

| tsplot(x1,x2,) | Plots any number of time series on the same scale. This automatic simul- taneous scaling feature is also useful when the x_i 's are ordinary numeric vectors, in which case they are plotted against the numbers $1, 2, 3, \ldots$ |
|--|--|
| qqnorm(x) qqline(x) qqplot(x,y) | Distribution-comparison plots. The first form plots the numeric vector \mathbf{x} against the expected Normal order scores (a normal scores plot) and the second adds a straight line to such a plot by drawing a line throught the distribution and data quartiles. The third form plots the quantiles of \mathbf{x} against those of \mathbf{y} to compare their respective distributions. |
| <pre>hist(x) hist(x,nclass=n) hist(x, breaks=)</pre> | Produces a histogram of the numeric vector x. A sensible number of classes is usually chosen, but a recommendation can be given with the nclass= argument. Alternatively, the breakpoints can be specified exactly with the breaks= argument. If the probability=T argument is given, the bars represent relative frequencies instead of counts. |

dotchart(x,...) Constructs a dotchart of the data in x. In a dotchart the y-axis gives a labelling of the data in x and the x-axis gives its value. For example it allows easy visual selection of all data entries with values lying in specified ranges.

11.1.4 Arguments to high-level plotting functions

There are a number of arguments which may be passed to high-level graphics functions, as follows:

| add=T | Forces the function to act as a low-level graphics function, superimposing the plot on the current plot (some functions only). |
|--------------------------------|---|
| axes=F | Suppresses generation of axes — useful for adding your own custom axes with the axis() function. The default, axes=T, means include axes. |
| log="x" log="y" log="xy" | Causes the x, y or both axes to be logarithmic. This will work for many, but not all, types of plot. |
| type= | The type= argument controls the type of plot produced, as follows: |
| type="p" | Plot individual points (the default) |
| type="l" | Plot lines |
| type="b" | Plot points connected by lines (both) |
| type="o" | Plot points overlaid by lines |
| type="h" | Plot vertical lines from points to the zero axis (high-density) |
| type="s" type="S" | Step-function plots. In the first form, the top of the vertical defines the point; in the second, the bottom. |
| type="n" | No plotting at all. However axes are still drawn (by default) and the coordinate system is set up according to the data. Ideal for creating plots with subsequent low-level graphics functions. |
| xlab="string" ylab="string" | Axis labels for the x and y axes. Use these arguments to change the default labels, usually the names of the objects used in the call to the high-level plotting function. |
| main="string" | Figure title, placed at the top of the plot in a large font. |
| sub="string" | Sub-title, placed just below the x -axis in a smaller font. |

11.2 Low-level plotting commands

Sometimes the high-level plotting functions don't produce exactly the kind of plot you desire. In this case, low-level plotting commands can be used to add extra information (such as points, lines or text) to the current plot.

Some of the more useful low-level plotting functions are:

| <pre>points(x,y) lines(x,y)</pre> | Adds points or connected lines to the current plot. plot()'s type= ar- gument can also be passed to these functions (and defaults to "p" for points() and "l" for lines().) | | | | |
|---|---|--|--|--|--|
| <pre>text(x, y, labels,)</pre> | Add text to a plot at points given by x, y. Normally labels is an integer or character vector in which case labels[i] is plotted at point (x[i], y[i]). The default is 1:length(x). | | | | |
| | Note: This function is often used in the sequence quad > plot(x, y, type="n"); text(x, y, names) The graphics parameter type="n" suppresses the points but sets up the axes, and the text() function supplies special characters, as specified by the character vector names for the points. | | | | |
| abline(a, b) abline(h=y) abline(v=x) abline(<i>lm.obj</i>) | Adds a line of slope b and intercept a to the current plot. h=y may be used to specify y -coordinates for the heights of horizontal lines to go across a plot, and v=x similarly for the x -coordinates for vertical lines. Also <i>lm.obj</i> may be list with a \$coefficients component of length 2 (such as the result of model-fitting functions,) which are taken as an intercept and slope, in that order. | | | | |
| <pre>polygon(x, y,</pre> | Draws a polygon defined by the ordered vertices in (x,y) . and (optionally) shade it in with hatch lines, or fill it if the graphics device allows the filling of figures. | | | | |
| <pre>legend(x,y, legend,)</pre> | Adds a legend to the current plot at the specified position. Plotting characters, line styles, colours etc. are identified with the labels in the character vector legend. At least one other argument \mathbf{v} (a vector the same length as legend) with the corresponding values of the plotting unit must also be given, as follows: | | | | |
| <pre>legend(,angle=v)</pre> | Shading angles | | | | |
| <pre>legend(, density=v)</pre> | Shading densities | | | | |
| <pre>legend(,fill=v)</pre> | Colours for filled boxes | | | | |
| legend(,col=v) | Colours in which points or lines will be drawn | | | | |
| legend(,lty=v) | Line styles | | | | |
| legend(,pch=v) | Plotting characters (character vector) | | | | |
| <pre>legend(,marks=v)</pre> | Plotting symbols, as obtained when using a numeric argument to pch= (numeric vector). | | | | |
| title(main,sub) | Adds a title main to the top of the current plot in a large font and (op- tionally) a sub-title sub at the bottom in a smaller font. | | | | |
| axis(side,) | Adds an axis to the current plot on the side given by the first argument (1 to 4, counting clockwise from the bottom.) Other arguments control the positioning of the axis within or beside the plot, and tick positions and labels. Useful for adding custom axes after calling plot() with the axes=F argument. | | | | |

Low-level plotting functions usually require some positioning information (e.g. x and y coordinates) to determine where to place the new plot elements. Coordinates are given in terms of *user coordinates* which are defined by the previous high-level graphics command and are chosen based on the supplied data.

Where x and y arguments are required, it is also sufficient to supply a single argument being a list with elements named x and y. Similarly a matrix with two columns is also valid input. In this way functions such as locator() (see below) may be used to specify positions on a plot interactively.

11.3 Interactive graphics functions

R also provides functions which allow users to extract or add information to a plot using a mouse. The simplest of these is the locator() function:

locator(n,type) Waits for the user to select locations on the current plot using the left mouse button. This continues until n (default 500) points have been selected, or the middle mouse button is pressed. The type argument allows for plotting at the selected points and has the same effect as for high-level graphics commands; the default is no plotting. locator() returns the locations of the points selected as a list with two components x and y.

locator () is usually called with no arguments. It is particularly useful for interactively selecting positions for graphic elements such as legends or labels when it is difficult to calculate in advance where the graphic should be placed. For example, to place some informative text near an outlying point, the command

```
> text(locator(1), "Outlier", adj=0)
```

may be useful. locator() will still work if the current device does not support a mouse; in this case the user will be prompted for x and y coordinates.

| identify(x,y, | Allow the user to highlight any of the points defined by x and y (using the |
|---------------|---|
| labels) | left mouse button) by plotting the corresponding component of labels |
| | nearby (or the index number of the point if labels is absent). Returns |
| | the indices of the selected points when the middle button is pressed. |

Sometimes we want to identify particular *points* on a plot, rather than their positions. For example, we may wish the user to select some observation of interest from a graphical display and then manipulate that observation in some way. Given a number of (x, y) coordinates in two numeric vectors x and y, we could use the identify() function as follows:

> plot(x,y)

> identify(x,y)

The identify() functions performs no plotting itself, but simply allows the user to move the mouse pointer and click the left mouse button near a point. The point nearest the mouse pointer will be highlighted with its index number (that is, its position in the x/y vectors) plotted nearby. Alternatively, you could use some informative string (such as a case name) as a highlight by using the labels argument to identify(), or disable highlighting altogether with the plot=F

argument. When the middle button is pressed, identify() returns the indices of the selected points; you can use these indices to extract the selected points from the original vectors x and y.

11.4 Using graphics parameters

When creating graphics, particularly for presentation or publication purposes, R does not always produce exactly that which is required. You can, however, customise almost every aspect of the display using *graphics parameters*. R maintains a list of a large number of graphics parameters which control things such as line style, colours, figure arrangement and text justification among many others. Every graphics parameter has a name (such as 'col', which controls colours,) and a value (a colour number, for example.)

A separate list of graphics parameters is maintained for each active device, and each device has a default set of parameters when initialised. Graphics parameters can be set in two ways: either permanently, affecting all graphics functions which access the current device; or temporarily, affecting only a single graphics function call.

11.4.1 Permanent changes: The par() function

The par() function is used to access and modify the list of graphics parameters for the current graphics device.

| par() | Without arguments, returns a list of all graphics parameters and their values for the current device. |
|-------------------------|---|
| par(c("col", "lty")) | With a character vector argument, returns only the named graphics parameters (again, as a list.) |
| par(col=4,lty=2) | With named arguments (or a single list argument) , sets the values of the named graphics parameters, and returns the original values of the parameters as a list. |

Setting graphics parameters with the par() function changes the value of the parameters *permanently*, in the sense that all future calls to graphics functions (on the current device) will be affected by the new value. You can think of setting graphics parameters in this way as setting 'default' values for the parameters, which will be used by all graphics functions unless an alternative value is given.

Note that calls to par() always affect the global values of graphics parameters, even when par() is called from within a function. This is often undesirable behaviour — usually we want to set some graphics parameters, do some plotting, and then restore the original values so as not to affect the user's R session. You can restore the initial values by saving the result of par() when making changes, and restoring the initial values when plotting is complete.

> oldpar \leftarrow par(col=4,lty=2)

... plotting commands ...

> par(oldpar)

11.4.2 Temporary changes: Arguments to graphics functions

Graphics parameters may also be passed to (almost) any graphics function as named arguments. This has the same effect as passing the arguments to the **par()** function, except that the changes only last for the duration of the function call. For example: > plot(x,y,pch="+")

produces a scatterplot using a plus sign as the plotting character, without changing the default plotting character for future plots.

11.5 Graphics parameters list

The following sections detail many of the commonly-used graphical parameters. The R help documentation for the par() function provides a more concise summary; this is provided as a somewhat more detailed alternative.

Graphics parameters will be presented in the following form:

name=valueA description of the parameter's effect. name is the name of the parameter,
that is, the argument name to use in calls to par() or a graphics function.
value is a typical value you might use when setting the parameter.

11.5.1 Graphical elements

R plots are made up of points, lines, text and polygons (filled regions.) Graphical parameters exist which control how these *graphical elements* are drawn, as follows:

| pch="+" | Character to be used for plotting points. The default varies with graphics drivers, but it is usually 'o'. Plotted points tend to appear slightly above or below the appropriate position unless you use "." as the plotting character, which produces centred points. |
|---|--|
| pch=4 | When pch is given as an integer between 0 and 18 inclusive, a specialised plotting symbol is produced. To see what the symbols are, use the command |
| | <pre>> legend(locator(1),as.character(0:18),marks=0:18)</pre> |
| lty=2 | Line types. Alternative line styles are not supported on all graphics devices (and vary on those that do) but line type 1 is always a solid line, and line types 2 and onwards are dotted or dashed lines, or some combination of both. |
| lwd=2 | Line widths. Desired width of lines, in multiples of the 'standard' line width. Affects axis lines as well as lines drawn with lines(), etc. |
| col=2 | Colours to be used for points, lines, text, filled regions and images. Each of these graphic elements has a list of possible colours, and the value of this parameter is an index to that list. Obviously, this parameter applies only to a limited range of devices. |
| font=2 | An integer which specifies which font to use for text. If possible, device drivers arrange so that 1 corresponds to plain text, 2 to bold face , 3 to <i>italic</i> and 4 to <i>bold italic</i> . |
| font.axis, font.lab, font.main, font.sub | The font to be used for axis annotation, x and y labels, main and sub-titles, respectively. |

| adj=-0.1 | Justification of text relative to the plotting position. 0 means left justify, 1 means right justify and 0.5 means to centre horizontally about the plotting position. The actual value is the proportion of text that appears to the left of the plotting position, so a value of -0.1 leaves a gap of 10% of the text width between the text and the plotting position. |
|----------|---|
| cex=1.5 | Character expansion. The value is the desired size of text characters (in- cluding plotting characters) relative to the default text size. |

11.5.2 Axes and tick marks

Many of R's high-level plots have axes, and you can construct axes yourself with the low-level axis() graphics function. Axes have three main components: the *axis line* (line style controlled by the lty graphics parameter), the *tick marks* (which mark off unit divisions along the axis line) and the *tick labels* (which mark the units.) These components can be customised with the following graphics parameters.

| lab=c(5,7,12) | The first two numbers are the desired number of tick intervals on the x and y axes respectively. The third number is the desired length of axis labels, in characters (including the decimal point.) Choosing a too-small value for this parameter may result in all tick labels being rounded to the same number! | |
|----------------------|--|--|
| las=1 | Orientation of axis labels. 0 means always parallel to axis, 1 means always horizontal, and 2 mean always perpendicular to the axis. | |
| mgp=c(3,1,0) | Positions of axis components. The first component is the distance fr the axis label to the axis position, in text lines. The second compon- is the distance to the tick labels, and the final component is the distan- from the axis position to the axis line (usually zero). Positive numb- measure outside the plot region, negative numbers inside. | |
| to m | Length of tick marks, as a fraction of the size of the plotting region. W tck is small (less than 0.5) the tick marks on the x and y axes are for to be the same size. A value of 1 gives grid lines. Negative values give marks outside the plotting region. Use tck=0.01 and mgp=c(1,-1.5 for internal tick marks. | |
| xaxs="s" yaxs="d" | Axis styles for the x and y axes, respectively. With styles "s" (standard) and "e" (extended) the smallest and largest tick marks always lie outside the range of the data. Extended axes may be widened slightly if any points are very near the edge. This style of axis can sometimes leave large blank gaps near the edges. With styles "i" (internal) and "r" (the default) tick marks always fall within the range of the data, however style "r" leaves a small amount of space at the edges. | |
| | Setting this parameter to "d" (direct axis) <i>locks in</i> the current axis and uses it for all future plots (or until the parameter is set to one of the other values above, at least.) Useful for generating series of fixed-scale plots. | |

11.5.3 Figure margins

A single plot in R is known as a **figure** and comprises a *plot region* surrounded by margins (possibly containing axis labels, titles, etc.) and (usually) bounded by the axes themselves. A typical figure appears in Figure 11. Graphics parameters controlling figure layout include:

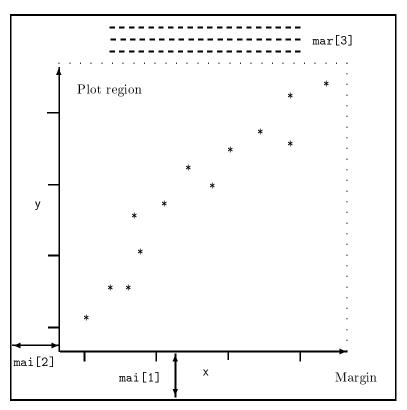


Figure 11: Anatomy of an R figure

mar=c(4,2,2,1) Similar to mai, except the measurement unit is text lines.

mar and mai are equivalent in the sense that setting one changes the value of the other. The default values chosen for this parameter are often too large; the right-hand margin is rarely needed, and neither is the top margin if no title is being used. The bottom and left margins must be large enough to accommodate the axis and tick labels. Furthermore, the default is chosen without regard to the size of the device surface: for example, using the postscript() driver with the height=4 argument will result in a plot which is about 50% margin unless mar or mai are set explicitly. When multiple figures are in use (see below) the margins are reduced by half, however this may not be enough when many figures share the same page.

11.5.4 Multiple figure environment

R allows you to create an $n \times m$ array of figures on a single page. Each figure has its own margins, and the array of figures is optionally surrounded by an *outer margin* as shown in Figure 12.

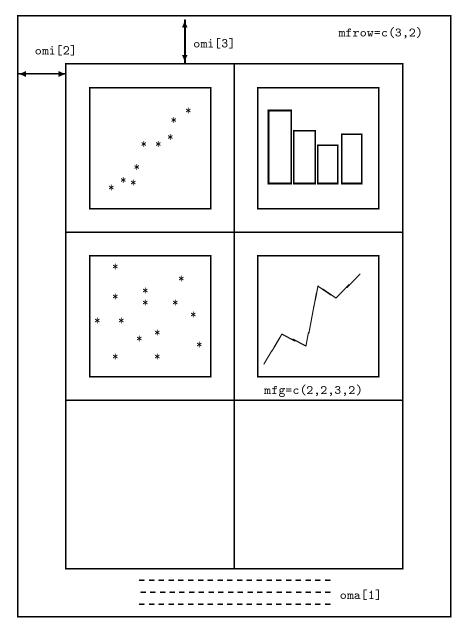


Figure 12: Page layout in multiple figure mode

The graphical parameters relating to multiple figures are as follows:

mfcol=c(3,2)mfrow=c(2,4) Set size of multiple figure array. The first value is the number of rows; the second is the number of columns. The only difference between these two parameters is that setting mfcol causes figures to be filled by column; mfrow fills by rows. The arrangement in Figure 12 would have been created by setting mfrow=c(3,2); the figure shows the page after four plots have been drawn.

| mfg=c(2,2,3,2) | Position of current figure in a multiple figure environment. The first two numbers are the row and column of the current figure; the last two are the number of rows and columns in the multiple figure array. Set this parameter to jump between figures in the array. You can even use different values for the last two numbers than the <i>true</i> values for unequally-sized figures on the same page. |
|------------------------------------|---|
| fig=c(4,9,1,4)/10 | Position of the current figure on the page. Values are the positions of the left, right, bottom and top edges respectively, as a percentage of the page measured from the bottom left corner. The example value would be for a figure in the bottom right of the page. Set this parameter for arbitrary positioning of figures within a page. |
| oma=c(2,0,3,0) omi=c(0,0,0.8,0) | Size of outer margins. Like mar and mai, the first measures in text lines and the second in inches, starting with the bottom margin and working clockwise. |

Outer margins are particularly useful for page-wise titles, etc. Text can be added to the outer margins with the mtext() function with argument outer=T. There are no outer margins by default, however, so you must create them explicitly using oma or omi.

11.6 Device drivers

R can generate graphics (of varying levels of quality) on almost any type of display or printing device. Before this can begin, however, R needs to be informed what type of device it is dealing with. This is done by starting a *device driver*. The purpose of a device driver is to convert graphical instructions from R ('draw a line,' for example) into a form that the particular device can understand.

Device drivers are started by calling a device driver function. There is one such function for every device driver: type help(Devices) for a list of them all. For example, issuing the command

> postscript()

causes all future graphics output to be sent to the printer in PostScript format. Some commonly-used device drivers are:

| X11() | For use with the X11 window system |
|--------------|---|
| postscript() | For printing on PostScript printers, or creating PostScript graphics files. |

pictex() Produces a LAT_EX file

When you have finished with a device, be sure to terminate the device driver by issuing the command

> dev.off()

This ensures that the device finishes cleanly; for example in the case of hardcopy devices this ensures that every page is completed and has been sent to the printer.

11.6.1 **PostScript** diagrams for typeset documents.

By passing the file argument to the postscript() device driver function, you may store the graphics in PostScript format in a file of your choice. The plot will be in landscape orientation unless the horizontal=FALSE argument is given, and you can control the size of the graphic with the width and height arguments (the plot will be scaled as appropriate to fit these dimensions.) For example, the command

> postscript("file.ps", horizontal=FALSE, height=5)

will produce a file containing PostScript code for a figure five inches high, perhaps for inclusion in a document. ¹³ It is important to note that if the file named in the command already exists, it will be overwritten. This is the case even if the file was only created earlier in the same R session.

11.6.2 Multiple graphics devices

In advanced use of R it is often useful to have several graphics devices in use at the same time. Of course only one graphics device can accept graphics commands at any one time, and this is known as the *current device*. When multiple devices are open, they form a numbered sequence with names giving the kind of device at any position.

The main commands used for operating with multiple devices, and their meanings are as follows:

| X11() postscript() | Each new call to a device driver function opens a new graphics device, thus extending by one the device list. This device becomes the current device, to which graphics output will be sent. |
|-----------------------------|---|
| dev.list() | returns the number and name of all active devices. The device at position 1 on the list is always the <i>null device</i> which does not accept graphics commands at all. |
| dev.next() dev.prev() | returns the number and name of the graphics device next to, or previous to the current device, respectively. |
| dev.set(which=k) | can be used to change the current graphics device to the one at position k of the device list. Returns the number and label of the device. |
| dev.off(k) | Terminate the graphics device at point k of the device list. For some devices, such as postscript devices, this will either print the file immediately or correctly complete the file for later printing, depending on how the device was initiated. |
| <pre>dev.copy(device,</pre> | Make a copy of the device k. Here device is a device function, such as postscript, with extra arguments, if needed, specified by dev.print is similar, but the copied device is immediately closed, so that end actions, such as printing hardcopies, are immediately performed. (See also printgraph()). |
| graphics.off() | Terminate all graphics devices on the list, except the null device. |

¹³ Warning: The PostScript code produced by the postscript() device driver is *not* Encapsulated PostScript, and thus including it in a document electronically (as opposed to physical cut-and-paste) can be problematic. It is known to work without problems for IAT_EX , at least.

A R: An introductory session

The following session is intended to introduce to you some features of the R environment by using them. Many features of the system will be unfamiliar and puzzling at first, but this will soon disappear. This is written for the UNIX user. Those using Macintosh and Windows will have to adapt the discussion appropriately.

| login: | Login, start your windowing system. You should also have the file morley.data in your working directory. If not, seek the local expert. If you have, proceed. |
|---|--|
| \$ R | Start R. |
| | The ${\sf R}$ program begins, with a banner. |
| | (Within R the prompt on the left hand side will not be shown to avoid confusion.) $% \left({\left({{{\rm{A}}_{{\rm{A}}}} \right)_{{\rm{A}}}} \right)_{{\rm{A}}}} \right)$ |
| help.start() | Start the HTML interface to online help (using a web browser available at your machine). You should briefly explore the fea- tures of this facility with the mouse. |
| | Iconify the help window and move on to the next part. |
| x11() | Turn on the graphics window. You may need to re-position and re-size to make it convenient to work with both windows. The graphics window should appear automatically on the screen. |
| $x \leftarrow rnorm(50)$ $y \leftarrow rnorm(x)$ | Generate two pseudo random normal vectors of $x-$ and $y-$ co- ordinates. |
| plot(x, y) | Plot the points in the plane. |
| objects() | See which R objects are now in the R image. |
| rm(x,y) | Remove objects no longer needed. (Clean up). |
| x ← 1:20 | Make $x = (1, 2,, 20)$ |
| $w \leftarrow 1 + sqrt(x)/2$ | A 'weight' vector of standard deviations. |
| <pre>dummy ← data.frame(x=x, y= x + rnorm(x)*w) dummy</pre> | Make a <i>data frame</i> of two columns, x and y , and look at it. |
| $\texttt{fm} \ \leftarrow \ \texttt{lm}(\texttt{y} \ \texttt{x}, \ \texttt{data=dummy})$ | |
| <pre>summary(fm)</pre> | Fit a simple linear regression of y on x and look at the analysis. |
| <pre>summary(fm) fm1 ← lm(y~x, data=dummy, weight=1/w^2) summary(fm1)</pre> | Fit a simple linear regression of y on x and look at the analysis. Since we know the standard deviations, we can do a weighted regression. |
| $fm1 \leftarrow lm(y^x, data=dummy, weight=1/w^2)$ | Since we know the standard deviations, we can do a weighted |
| <pre>fm1 ← lm(y[~]x, data=dummy, weight=1/w²) summary(fm1)</pre> | Since we know the standard deviations, we can do a weighted regression. |
| <pre>fm1 ← lm(y~x, data=dummy, weight=1/w^2) summary(fm1) attach(dummy)</pre> | Since we know the standard deviations, we can do a weighted regression. Make the columns in the data frame visible as variables. |
| <pre>fm1 ← lm(y~x, data=dummy, weight=1/w^2) summary(fm1) attach(dummy) lrf ← lowess(x, y)</pre> | Since we know the standard deviations, we can do a weighted regression. Make the columns in the data frame visible as variables. Make a nonparametric local regression function. |
| <pre>fm1 ← lm(y~x, data=dummy, weight=1/w^2) summary(fm1) attach(dummy) lrf ← lowess(x, y) plot(x, y)</pre> | Since we know the standard deviations, we can do a weighted regression. Make the columns in the data frame visible as variables. Make a nonparametric local regression function. Standard point plot. |
| $fm1 \leftarrow lm(y^{x}, data=dummy, weight=1/w^{2})$ summary(fm1) attach(dummy) $lrf \leftarrow lowess(x, y)$ plot(x, y) lines(x, lrf\$y) | Since we know the standard deviations, we can do a weighted regression. Make the columns in the data frame visible as variables. Make a nonparametric local regression function. Standard point plot. Add in the local regression. |
| fm1 \leftarrow lm(y [*] x, data=dummy, weight=1/w ²) summary(fm1) attach(dummy) lrf \leftarrow lowess(x, y) plot(x, y) lines(x, lrf\$y) abline(0, 1, lty=3) | Since we know the standard deviations, we can do a weighted regression. Make the columns in the data frame visible as variables. Make a nonparametric local regression function. Standard point plot. Add in the local regression. The true regression line: (intercept 0, slope 1). |

62

| <pre>plot(fitted(fm), resid(fm),</pre> | A standard regression diagnostic plot to check for heteroscedas- ticity. Can you see it? |
|---|--|
| xlab="Fitted values", ylab="Residuals", main= "Residuals vs Fitted") | |
| qqnorm(resid(fm), main= "Residuals Rankit Plot") | A normal scores plot to check for skewness, kurtosis and outliers. (Not very useful here.) |
| rm(fm,fm1,lrf,x,dummy) | Clean up again. |
| | The next section will look at data from the classical experiment of Michaelson and Morley to measure the speed of light. |
| system("more morley.data") | Optional. Temporarily interrupt R and look at the file. The function system is the way to invoke commands under the operating system. This will only work on UNIX. |
| mm ← read.table("morley.data") mm | Read in the Michaelson and Morley data as a data frame, and look at it. There are five experiments (col. Expt) and each has 20 runs (col. Run) and sl is the recorded speed of light, suitably coded. |
| mm\$Expt ← factor(mm\$Expt) | Change Expt and Run into factors. |
| mm\$Run ← factor(mm\$Run) attach(mm) | Make the data frame visible at position 2 (the default). |
| <pre>plot(Expt,Speed, main= "Speed of Light Data", xlab="Experiment No.")</pre> | Compare the five experiments with simple boxplots. |
| <pre>fm ← aov(Speed~Run+Expt,</pre> | Analyse as a randomized block, with 'runs' and 'experiments' as factors. |
| summary(fm) fm0 \leftarrow update(fm, | Fit the sub-model omitting 'runs', and compare using a formal |
| .~Run) | analysis of variance. |
| anova(fm0,fm) detach() | Clean up before moving on. |
| rm(fm, fm0) | |
| | We now look at some more graphical features: contour and image plots. |
| $x \leftarrow seq(-pi, pi, len=50)$ $y \leftarrow x$ | x is a vector of 50 equally spaced values in $-\pi \le x \le \pi$. y is the same. |
| $f \leftarrow outer(x, y, function(x,y) \\ cos(y)/(1+x^2))$ | f is a square matrix, with rows and columns indexed by x and y respectively, of values of the function $\cos(y)/(1+x^2)$. |
| oldpar ← par() par(pty="s") | Save the plotting parameters and set the plotting region to "square". |
| <pre>contour(x, y, f) contour(x, y, f, nlevels=15, add=T)</pre> | Make a contour map of f ; add in more lines for more detail. |
| $fa \leftarrow (f-t(f))/2$ | fa is the "asymmetric part" of f . (t() is transpose). |
| <pre>contour(x, y, fa, nint=15)</pre> | Make a contour, |

| par(oldpar) | \ldots and restore the old graphics parameters. | | |
|---|--|--|--|
| <pre>image(x, y, f) image(x, y, f)</pre> | Make some pretty high density image plots, (of which you can get hardcopies if you wish) | | |
| <pre>image(x, y, fa) </pre> | | | |
| objects(); rm(x,y,f,fa) | and clean up before moving on. | | |
| th \leftarrow seq(-pi, pi, | ${\sf R}$ can do complex arithmetic, also. 11 is used for the complex number i | | |
| len=100) | | | |
| $z \leftarrow \exp(1i*th)$ | | | |
| par(pty="s") plot(z, type="l") | Plotting complex arguments means plot imaginary versus real parts. This should be a circle. | | |
| w ← rnorm(100) + rnorm(100)*1i | Suppose we want to sample points within the unit circle. One method would be to take complex numbers with standard nor- mal real and imaginary parts | | |
| $w \leftarrow ifelse(Mod(w) > 1, 1/w, w)$ | and to map any outside the circle onto their reciprocal. | | |
| <pre>plot(w, xlim=c(-1,1), ylim=c(-1,1), pch="+", xlab="x", ylab="y")</pre> | All points are inside the unit circle, but the distribution is not uniform. | | |
| lines(z) | | | |
| $w \leftarrow sqrt(runif(100))*$ exp(2*pi*runif(100)*1i) | The second method uses the uniform distribution. The points should now look more evenly spaced over the disc. | | |
| <pre>plot(w, xlim=c(-1,1),</pre> | | | |
| <pre>ylim=c(-1,1), pch="+",</pre> | | | |
| <pre>xlab="x", ylab="y") lines(z)</pre> | | | |
| rm(th,w,z) | Clean up again. | | |
| | | | |
| par(oldpar) | Restore standard graphics parameters. | | |
| <pre>butterfly()</pre> | An old favourite. Take a hardcopy if you wish. | | |
| rm(oldpar) | Clean up again. | | |
| q() | Quit the R program | | |
| > | and return to UNIX. | | |

B The Inbuilt Command Line Editor in R

B.1 Preliminaries

When the GNU readline library is available at the time R is compiled (actually configured), an inbuilt command line editor allowing recall, editing and re-submission of prior commands is used.

It can be disabled (useful for usage with ESS^{14}).

When using ${\sf R}$ with <code>readline</code> capacities, the following options are available.

The usual typographical conventions apply: ^M means Hold the Control down while you press the m key, but Esc m means First press the Esc key and then the m key. Note that case is significant after Esc.

B.2 Editing Actions

The R program keeps a history of the commands you type, including the error lines, and commands in your history may be recalled, changed if necessary, and re-submitted as new commands. In emacs style command line editing any straight typing you do while in this editing phase causes the characters to be inserted in the command you are editing, displacing any characters to the right of the cursor. In vi mode character insertion mode is started by Esc i or Esc a, characters are typed and insertion mode is finished by typing a further Esc .

Pressing the Return command at any time causes the command to be re-submitted.

Other editing actions are summarised in the following table.

Unfortunately it does not seem to be possible to bind the motion keys, for example, to the arrow keys, which is something of a nuisance.

B.3 Command Line Editor Summary

| 1. Command recall and vertical motion | emacs $	ext{style}$ |
|---|---------------------|
| Go to the previous command (backwards in the history) | ^P |
| Go to the next command (forwards in the history) | ^N |
| Find the last command with the \texttt{text} string in it | ^R text |

2. Horizontal motion of the cursor

| Go to the beginning of the command | ^A |
|------------------------------------|-------|
| Go to the end of the line | ^E |
| Go back one word | Esc b |
| Go forward one word | Esc f |
| Go back one character | ^В |
| Go forward one character | ^F |

3. Editing and re-submission

| Insert text at the cursor | text |
|---|-----------------------|
| Append text after cursor | ftext |
| Delete the previous character (left of the cursor) | Delete |
| Delete the character under the cursor | ^D |
| Delete rest of the word under the cursor, and 'save' it | Esc d |
| Delete from cursor to end of command, and 'save' it | ſΚ |
| Insert (yank) the last 'saved' text here | Ŷ |
| Transpose the character under the cursor with the next | ^T |
| Change the rest of the word to lower case | Esc l |
| Change the rest of the word to capitals (upper case) | Esc c |
| Re-submit the command to ${\sf R}$ | Return |
| | |

Exercises

C Exercises

C.1 The cloud point data

Source: Draper & Smith, *Applied Regression Analysis*, p. 162 Category: Polynomial regression. Simple plots.

Description

The cloud point of a liquid is a measure of the degree of crystalization in a stock that can be measured by the refractive index. It has been suggested that the percentage of I_8 in the base stock is an excellent predictor of cloud point using the second or third order model:

$$Y = \beta_0 + \beta_1 x + \beta_2 x^2 + \beta_3 x^3 + E, \qquad E \sim N(0, \sigma^2)$$

Data

The following data was collected on stocks with known percentage of I_8 :

| $I_8\%$ | Cloud Point |
|---------|-------------|---------|-------------|---------|-------------|---------|-------------|
| 0 | 21.9 | 2 | 26.1 | 5 | 28.9 | 8 | 31.4 |
| 0 | 22.1 | 3 | 26.8 | 6 | 29.8 | 8 | 31.5 |
| 0 | 22.8 | 3 | 27.3 | 6 | 30.0 | 9 | 31.8 |
| 1 | 24.5 | 4 | 28.2 | 6 | 30.3 | 10 | 33.1 |
| 2 | 26.0 | 4 | 28.5 | 7 | 30.4 | | |

The data may be read from file cloud.data in a form suitable to construct a data frame.

Suggested analysis

Fit polynomial regression models using the lm() function, and choose the degree carefully.

C.2 The Janka hardness data

Source: E. J. Williams: *Regression Analysis*, Wiley, 1959. Category: Polynomial regression. Transformations.

Description

The Janka hardness is an important structural property of Australian timbers, which is difficult to measure. It is, however, related to the density of the timber, which is relatively easy to measure. A low degree polynomial regression is suggested as appropriate.

$$Y = \beta_0 + \beta_1 x + \beta_2 x^2 + \dots + E$$

where Y is the hardness and x the density.

Data

| D | Η | D | Η | D | Η | D | Η | D | Η | D | Н |
|------|-----|------|------|------|------|------|------|------|------|------|------|
| 24.7 | 484 | 30.3 | 587 | 39.4 | 1210 | 42.9 | 1270 | 53.4 | 1880 | 59.8 | 1940 |
| 24.8 | 427 | 32.7 | 704 | 39.9 | 989 | 45.8 | 1180 | 56.0 | 1980 | 66.0 | 3260 |
| 27.3 | 413 | 35.6 | 979 | 40.3 | 1160 | 46.9 | 1400 | 56.5 | 1820 | 67.4 | 2700 |
| 28.4 | 517 | 38.5 | 914 | 40.6 | 1010 | 48.2 | 1760 | 57.3 | 2020 | 68.8 | 2890 |
| 28.4 | 549 | 38.8 | 1070 | 40.7 | 1100 | 51.5 | 1710 | 57.6 | 1980 | 69.1 | 2740 |
| 29.0 | 648 | 39.3 | 1020 | 40.7 | 1130 | 51.5 | 2010 | 59.2 | 2310 | 69.1 | 3140 |

The following data comes from samples of 36 Australian Eucalypt hardwoods.

The data may be read as a data frame from file janka.data.

Suggested analysis

Fit polynomial regression models, choosing the degree carefully. Examine the residuals and see if the data has any obvious outliers or heteroscedasticity. Check to see what effect a square root or log transformation has on the residual pattern when plotted against fitted values.

More advanced: Consider a quasi-likelihood model with variance proportional to the mean and a square root link.

C.3 The Tuggeranong house price data

Source: Dr Ray Correll, Personal communication **Category:** Multiple regression, coplots.

Description

Before buying a house in Tuggeranong in February, 1987, a cautious potential householder collected some data on houses on the market. The data for 20 such houses is shown in the table and is available as the file house.dat. The variables collected are, in order, price, total floor area, block area, number of main rooms, age of house and whether or not the house was centrally heated.

Data

The data is given in Table 5 and is available as the file house.data.

Suggested analysis

Explore the data with coplot() using Age and CentHeat as conditioning variables.

Choose a multiple regression model carefully and check for outliers, (that is, for "bargains" and "rip-offs").

C.4 Yorke Penninsula wheat yield data

Source: K. W. Morris (private communication) **Category:** Multiple regression.

C.5 The lowa wheat yield data

| Price (\$000s) | Floor (m^2) | Block (m^2) | Rooms | Age (years) | Cent. Heat. |
|----------------|---------------|---------------|-------|-------------|----------------|
| 52.00 | 111.0 | 830 | 5 | 6.2 | no |
| 54.75 | 128.0 | 710 | 5 | 7.5 | no |
| 57.50 | 101.0 | 1000 | 5 | 4.2 | no |
| 57.50 | 131.0 | 690 | 6 | 8.8 | no |
| 59.75 | 93.0 | 900 | 5 | 1.9 | yes |
| 62.50 | 112.0 | 640 | 6 | 5.2 | no |
| 64.75 | 137.6 | 700 | 6 | 6.6 | \mathbf{yes} |
| 67.25 | 148.5 | 740 | 6 | 2.3 | no |
| 67.50 | 113.5 | 660 | 6 | 6.1 | no |
| 69.75 | 152.0 | 645 | 7 | 9.2 | no |
| 70.00 | 121.5 | 730 | 5 | 4.3 | yes |
| 75.50 | 141.0 | 730 | 7 | 4.3 | no |
| 77.50 | 124.0 | 670 | 6 | 1.0 | yes |
| 77.50 | 153.5 | 795 | 7 | 7.0 | yes |
| 81.25 | 149.0 | 900 | 6 | 3.6 | yes |
| 82.50 | 135.0 | 810 | 6 | 1.7 | yes |
| 86.25 | 162.0 | 930 | 6 | 1.2 | yes |
| 87.50 | 145.0 | 825 | 6 | 0.0 | yes |
| 88.00 | 172.0 | 950 | 7 | 2.3 | yes |
| 92.00 | 170.5 | 870 | 7 | 0.7 | yes |

Table 5: The Tuggeranong house price data

Description

The annual yield of wheat in a marginal wheat growing district on the Yorke Penninsula, South Australia, together with the rainfall for the three growing months, for the years 1931–1955. The year itself is potentially a surrogate predictor to allow for improvements in varieties and farm practice. Yield is in bushels per acre, and rainfall is in inches.

Data

The data is given in Table 6 and may be read as a data frame from file sawheat.data.

Suggested analysis

Fit a multiple regression model and check the results, via residual plots especially.

C.5 The Iowa wheat yield data

Source: CAED Report, 1964. Quoted in Draper & Smith. Category: Multiple regression; diagnostics.

Description

The data gives the pre-season and three growing months' precipitation, the mean temperatures for the three growing months and harvest month, the year, and the yield of wheat for the USA

| Year | Rain0 | Rain1 | Rain2 | Yield | Year | Rain0 | Rain1 | Rain2 | Yield |
|------|-------|-------|-------|-------|------|-------|-------|-------|-------|
| 1931 | .05 | 1.61 | 3.52 | .31 | 1944 | 3.30 | 4.19 | 2.11 | 4.60 |
| 1932 | 1.15 | .60 | 3.46 | .00 | 1945 | .44 | 3.41 | 1.55 | .35 |
| 1933 | 2.22 | 4.94 | 3.06 | 5.47 | 1946 | .50 | 3.26 | 1.20 | .00 |
| 1934 | 1.19 | 11.26 | 4.91 | 16.73 | 1947 | .18 | 1.52 | 1.80 | .00 |
| 1935 | 1.40 | 10.95 | 4.23 | 10.54 | 1948 | .80 | 3.25 | 3.55 | 2.98 |
| 1936 | 2.96 | 4.96 | .11 | 5.89 | 1949 | 7.08 | 5.93 | .93 | 11.89 |
| 1937 | 2.68 | .67 | 2.17 | .03 | 1950 | 2.54 | 4.71 | 2.51 | 6.56 |
| 1938 | 3.66 | 8.49 | 11.95 | 16.03 | 1951 | 1.08 | 3.37 | 4.02 | 1.30 |
| 1939 | 5.15 | 3.60 | 2.18 | 6.57 | 1952 | .22 | 3.24 | 4.93 | .03 |
| 1940 | 6.44 | 2.69 | 1.37 | 8.43 | 1953 | .55 | 1.78 | 1.97 | .00 |
| 1941 | 2.01 | 6.88 | .92 | 8.68 | 1954 | 1.65 | 3.22 | 1.65 | 3.09 |
| 1942 | .73 | 3.30 | 3.97 | 2.49 | 1955 | .72 | 3.42 | 3.31 | 2.72 |
| 1943 | 2.52 | 1.93 | 1.16 | .98 | | | | | |

Table 6: Yorke Penninsula wheat yield data

state of Iowa, for the years 1930–1962.

Data

The data is given in Table 7 and may be read as a data frame from file iowheat.data.

Suggested analysis

Fit a multiple regression model and select carefully the predictors. Work either by backward elimination of forward selection. Examine the residuals by plotting them in turn against each predictor variable.

Consider the effect of adding quadratic terms in the predictors.

It is interesting to compare this set of data with the Yorke Penninsula data for a similar period.

C.6 The gasoline yield data

 Source: Estimate gasoline yields from crudes by Nilon H. Prater, Petroleum Refiner, 35, #5.
 Category: Analysis of variance, covariance, and multiple regression. Modern regression.

Description

The data gives the gasoline yield as a percent of crude oil, say y, and four independent variables which may influence yield. These are

- x_1 : The crude oil gravity, in ⁰API,
- x_2 : The crude oil vapour pressure,
- x_3 : The crude oil 10% point, ASTM,
- x_4 : The gasoline end point.

| Year | Rain0 | Temp1 | Rain1 | Temp2 | Rain2 | Temp3 | Rain3 | Temp4 | Yield |
|------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| 1930 | 17.75 | 60.2 | 5.83 | 69.0 | 1.49 | 77.9 | 2.42 | 74.4 | 34.0 |
| 1931 | 14.76 | 57.5 | 3.83 | 75.0 | 2.72 | 77.2 | 3.30 | 72.6 | 32.9 |
| 1932 | 27.99 | 62.3 | 5.17 | 72.0 | 3.12 | 75.8 | 7.10 | 72.2 | 43.0 |
| 1933 | 16.76 | 60.5 | 1.64 | 77.8 | 3.45 | 76.4 | 3.01 | 70.5 | 40.0 |
| 1934 | 11.36 | 69.5 | 3.49 | 77.2 | 3.85 | 79.7 | 2.84 | 73.4 | 23.0 |
| 1935 | 22.71 | 55.0 | 7.00 | 65.9 | 3.35 | 79.4 | 2.42 | 73.6 | 38.4 |
| 1936 | 17.91 | 66.2 | 2.85 | 70.1 | 0.51 | 83.4 | 3.48 | 79.2 | 20.0 |
| 1937 | 23.31 | 61.8 | 3.80 | 69.0 | 2.63 | 75.9 | 3.99 | 77.8 | 44.6 |
| 1938 | 18.53 | 59.5 | 4.67 | 69.2 | 4.24 | 76.5 | 3.82 | 75.7 | 46.3 |
| 1939 | 18.56 | 66.4 | 5.32 | 71.4 | 3.15 | 76.2 | 4.72 | 70.7 | 52.2 |
| 1940 | 12.45 | 58.4 | 3.56 | 71.3 | 4.57 | 76.7 | 6.44 | 70.7 | 52.3 |
| 1941 | 16.05 | 66.0 | 6.20 | 70.0 | 2.24 | 75.1 | 1.94 | 75.1 | 51.0 |
| 1942 | 27.10 | 59.3 | 5.93 | 69.7 | 4.89 | 74.3 | 3.17 | 72.2 | 59.9 |
| 1943 | 19.05 | 57.5 | 6.16 | 71.6 | 4.56 | 75.4 | 5.07 | 74.0 | 54.7 |
| 1944 | 20.79 | 64.6 | 5.88 | 71.7 | 3.73 | 72.6 | 5.88 | 71.8 | 52.0 |
| 1945 | 21.88 | 55.1 | 4.70 | 64.1 | 2.96 | 72.1 | 3.43 | 72.5 | 43.5 |
| 1946 | 20.02 | 56.5 | 6.41 | 69.8 | 2.45 | 73.8 | 3.56 | 68.9 | 56.7 |
| 1947 | 23.17 | 55.6 | 10.39 | 66.3 | 1.72 | 72.8 | 1.49 | 80.6 | 30.5 |
| 1948 | 19.15 | 59.2 | 3.42 | 68.6 | 4.14 | 75.0 | 2.54 | 73.9 | 60.5 |
| 1949 | 18.28 | 63.5 | 5.51 | 72.4 | 3.47 | 76.2 | 2.34 | 73.0 | 46.1 |
| 1950 | 18.45 | 59.8 | 5.70 | 68.4 | 4.65 | 69.7 | 2.39 | 67.7 | 48.2 |
| 1951 | 22.00 | 62.2 | 6.11 | 65.2 | 4.45 | 72.1 | 6.21 | 70.5 | 43.1 |
| 1952 | 19.05 | 59.6 | 5.40 | 74.2 | 3.84 | 74.7 | 4.78 | 70.0 | 62.2 |
| 1953 | 15.67 | 60.0 | 5.31 | 73.2 | 3.28 | 74.6 | 2.33 | 73.2 | 52.9 |
| 1954 | 15.92 | 55.6 | 6.36 | 72.9 | 1.79 | 77.4 | 7.10 | 72.1 | 53.9 |
| 1955 | 16.75 | 63.6 | 3.07 | 67.2 | 3.29 | 79.8 | 1.79 | 77.2 | 48.4 |
| 1956 | 12.34 | 62.4 | 2.56 | 74.7 | 4.51 | 72.7 | 4.42 | 73.0 | 52.8 |
| 1957 | 15.82 | 59.0 | 4.84 | 68.9 | 3.54 | 77.9 | 3.76 | 72.9 | 62.1 |
| 1958 | 15.24 | 62.5 | 3.80 | 66.4 | 7.55 | 70.5 | 2.55 | 73.0 | 66.0 |
| 1959 | 21.72 | 62.8 | 4.11 | 71.5 | 2.29 | 72.3 | 4.92 | 76.3 | 64.2 |
| 1960 | 25.08 | 59.7 | 4.43 | 67.4 | 2.76 | 72.6 | 5.36 | 73.2 | 63.2 |
| 1961 | 17.79 | 57.4 | 3.36 | 69.4 | 5.51 | 72.6 | 3.04 | 72.4 | 75.4 |
| 1962 | 26.61 | 66.6 | 3.12 | 69.1 | 6.27 | 71.6 | 4.31 | 72.5 | 76.0 |

Table 7: The Iowa historical wheat yield data

The data comes as 10 separate samples, and within each sample the values for x_1 , x_2 , and x_3 are constant.

Data

The data is shown in Table 8, and is available as the file oil.data in a form suitable for constructing a data frame.

Suggested analysis

Using EndPt as a covariate, check to see if differences between samples can be accounted for by regression models on the other predictors.

| Sample | x_1 | x_2 | x_3 | x_4 | y | Sample | x_1 | x_2 | x_3 | x_4 | y |
|--------|-------|-------|-------|-------|------|--------|-------|-------|-------|-------|------|
| 1 | 31.8 | 0.2 | 316 | 365 | 8.5 | 6 | 40.0 | 6.1 | 217 | 212 | 7.4 |
| 1 | 31.8 | 0.2 | 316 | 379 | 14.7 | 6 | 40.0 | 6.1 | 217 | 272 | 18.2 |
| 1 | 31.8 | 0.2 | 316 | 428 | 18.0 | 6 | 40.0 | 6.1 | 217 | 340 | 30.4 |
| 2 | 32.2 | 2.4 | 284 | 351 | 14.0 | 7 | 40.3 | 4.8 | 231 | 307 | 14.4 |
| 2 | 32.2 | 2.4 | 284 | 424 | 23.2 | 7 | 40.3 | 4.8 | 231 | 367 | 26.8 |
| | | | | | | 7 | 40.3 | 4.8 | 231 | 395 | 34.9 |
| 3 | 32.2 | 5.2 | 236 | 267 | 10.0 | 8 | 40.8 | 3.5 | 210 | 218 | 8.0 |
| 3 | 32.2 | 5.2 | 236 | 360 | 24.8 | 8 | 40.8 | 3.5 | 210 | 273 | 13.1 |
| 3 | 32.2 | 5.2 | 236 | 402 | 31.7 | 8 | 40.8 | 3.5 | 210 | 347 | 26.6 |
| 4 | 38.1 | 1.2 | 274 | 285 | 5.0 | 9 | 41.3 | 1.8 | 267 | 235 | 2.8 |
| 4 | 38.1 | 1.2 | 274 | 365 | 17.6 | 9 | 41.3 | 1.8 | 267 | 275 | 6.4 |
| 4 | 38.1 | 1.2 | 274 | 444 | 32.1 | 9 | 41.3 | 1.8 | 267 | 358 | 16.1 |
| | | | | | | 9 | 41.3 | 1.8 | 267 | 416 | 27.8 |
| 5 | 38.4 | 6.1 | 220 | 235 | 6.9 | 10 | 50.8 | 8.6 | 190 | 205 | 12.2 |
| 5 | 38.4 | 6.1 | 220 | 300 | 15.2 | 10 | 50.8 | 8.6 | 190 | 275 | 22.3 |
| 5 | 38.4 | 6.1 | 220 | 365 | 26.0 | 10 | 50.8 | 8.6 | 190 | 345 | 34.7 |
| 5 | 38.4 | 6.1 | 220 | 410 | 33.6 | 10 | 50.8 | 8.6 | 190 | 407 | 45.7 |

Table 8: The gasoline recovery data

More advanced: Fit a two stratum ANOVA model using between and within samples as the two strata.

C.7 The Michaelson and Morley speed of light data

Source: Weekes: A Genstat Primer. Category: Analysis of Variance.

Description

The classical data of Michaelson and Morley on the speed of light. The data consists of five experiments, each consisting of 20 consecutive "runs". The response is the speed of light measurement, suitably coded. The data is here viewed as a randomized block experiment with *experiment* and *run* as the factors. *run* may also be considered a quantitative variate to account for linear (or polynomial) changes in the measurement over the course of a single experiment.

Data

The data is given in Table 9 and may be read as a data frame from file morley.data in a form suitable for constructing a data frame.

Suggested analysis

Using an single classification ANOVA model check for differences between experiments and summarise your conclusions.

| Runs 1–10 | | | | | |
|-----------------|-----------------|-----------------|------------------|-----------------|--|
| \mathcal{E}_1 | \mathcal{E}_2 | \mathcal{E}_3 | ${\mathcal E}_4$ | \mathcal{E}_5 | |
| 850 | 960 | 880 | 890 | 890 | |
| 740 | 940 | 880 | 810 | 840 | |
| 900 | 960 | 880 | 810 | 780 | |
| 1070 | 940 | 860 | 820 | 810 | |
| 930 | 880 | 720 | 800 | 760 | |
| 850 | 800 | 720 | 770 | 810 | |
| 950 | 850 | 620 | 760 | 790 | |
| 980 | 880 | 860 | 740 | 810 | |
| 980 | 900 | 970 | 750 | 820 | |
| 880 | 840 | 950 | 760 | 850 | |

Table 9: The Michaelson and Morley speed of light data

C.8 The rat genotype data

Source: Quoted in Scheffe, H.: *The Analysis of Variance* **Category:** Unbalanced double classification.

Description

Data from a foster feeding experiment with rat mothers and litters of four different genotypes: A, F, I and J. The measurement is the litter weight gain after a trial feeding period.

Data

The data is given in Table 10 and may be read as a data frame from file genotype.data.

Suggested analysis

Fit a double classification model. Check for interaction using both a formal analysis and graphically using interaction.plot(). Test the main effects and summarise.

C.9 Fisher's sugar beet data

Source: R. A. Fisher, *Design of Experiments.* **Category:** Analysis of variance and covariance.

Description

A classical 3×2^3 randomized block experiment in four blocks of size 24. The response is the total weight of sugarbeet roots off the plot, but this is accompanied by the number of roots measured. The suggestion is that number of roots should be a covariate to allow for varying plot size.

The factors are Variety. (3 levels, a, b and c), and N, P and K each at 2 levels, present or absent.

| Litter's | Mo | other's | Genoty | vpe |
|----------|------|---------|--------|------|
| Genotype | A | F | Ι | J |
| A | 61.5 | 55.0 | 52.5 | 42.0 |
| | 68.2 | 42.0 | 61.8 | 54.0 |
| | 64.0 | 60.2 | 49.5 | 61.0 |
| | 65.0 | | 52.7 | 48.2 |
| | 59.7 | | | 39.6 |
| F | 60.3 | 50.8 | 56.5 | 51.3 |
| | 51.7 | 64.7 | 59.0 | 40.5 |
| | 49.3 | 61.7 | 47.2 | |
| | 48.0 | 64.0 | 53.0 | |
| | | 62.0 | | |
| Ι | 37.0 | 56.3 | 39.7 | 50.0 |
| | 36.3 | 69.8 | 46.0 | 43.8 |
| | 68.0 | 67.0 | 61.3 | 54.5 |
| | | | | 55.3 |
| | | | | 55.7 |
| J | 59.0 | 59.5 | 45.2 | 44.8 |
| | 57.4 | 52.8 | 57.0 | 51.5 |
| | 54.0 | 56.0 | 61.4 | 53.0 |
| | 47.0 | | | 42.0 |
| | | | | 54.0 |

Table 10: The rat genotype data

Data

The data is given in Table 11 and may be read from the file sugar.data in a form suitable to construct a data frame.

Suggested analysis

Analyse the data as a randomised block experiment with Wt as the response and No as a covariate. Prune the model of all unnecessary interaction terms and summarise.

C.10 A barley split plot field trial

Source: Unknown. Traditional data. Category: Multistratum analysis of variance.

Description

An experiment involving barley varieties and manure (nitrogen) was conducted in 6 blocks of 3 whole plots.

Each whole plot was divided into 4 subplots. Three varieties of barley were used in the experiment with one variety being sown in each whole plot, while the four levels of manure (0, 0.01, 0.02, and 0.04 tons per acre) were used, one level in each of the four subplots of each whole plot. In the above table V_i denotes the *i*th variety and N_j denotes the *j*th level of nitrogen.

| | | | | Blo | ck 1 | Blo | ck 2 | Blo | ck 3 | Blo | ck 4 |
|---|---|---|---|-----|------|-----|------|-----|------|-----|------|
| V | Ν | Р | Κ | No | Wt | No | Wt | No | Wt | No | Wt |
| a | _ | _ | _ | 124 | 162 | 133 | 162 | 114 | 127 | 127 | 158 |
| a | _ | _ | k | 131 | 152 | 161 | 164 | 130 | 141 | 145 | 188 |
| a | _ | p | — | 115 | 173 | 134 | 175 | 134 | 142 | 109 | 162 |
| a | _ | p | k | 126 | 140 | 133 | 158 | 106 | 148 | 132 | 160 |
| a | n | — | — | 136 | 184 | 134 | 178 | 127 | 168 | 139 | 199 |
| a | n | — | k | 134 | 112 | 156 | 193 | 101 | 171 | 138 | 191 |
| a | n | p | — | 132 | 190 | 104 | 166 | 119 | 157 | 132 | 193 |
| a | n | p | k | 120 | 175 | 147 | 155 | 107 | 139 | 148 | 192 |
| b | _ | - | — | 145 | 133 | 147 | 130 | 139 | 138 | 127 | 128 |
| b | _ | - | k | 156 | 117 | 152 | 137 | 107 | 121 | 147 | 147 |
| b | — | p | — | 152 | 140 | 138 | 101 | 125 | 124 | 120 | 143 |
| b | — | p | k | 137 | 127 | 145 | 132 | 125 | 132 | 143 | 139 |
| b | n | — | — | 124 | 163 | 138 | 159 | 140 | 166 | 159 | 174 |
| b | n | — | k | 136 | 143 | 142 | 144 | 133 | 142 | 148 | 159 |
| b | n | p | _ | 140 | 168 | 142 | 150 | 133 | 118 | 138 | 157 |
| b | n | p | k | 146 | 144 | 135 | 160 | 138 | 155 | 140 | 153 |
| c | _ | _ | _ | 113 | 122 | 138 | 132 | 119 | 123 | 127 | 146 |
| c | _ | _ | k | 91 | 107 | 149 | 171 | 118 | 142 | 129 | 151 |
| c | _ | p | _ | 123 | 118 | 139 | 142 | 127 | 120 | 124 | 138 |
| c | _ | p | k | 129 | 140 | 126 | 115 | 129 | 130 | 142 | 152 |
| c | n | _ | — | 121 | 118 | 141 | 152 | 127 | 149 | 127 | 165 |
| c | n | — | k | 126 | 148 | 128 | 152 | 107 | 147 | 110 | 136 |
| c | n | p | — | 103 | 112 | 144 | 175 | 102 | 152 | 143 | 173 |
| c | n | p | k | 120 | 162 | 125 | 160 | 129 | 173 | 137 | 185 |

Table 11: Fisher's sugar beet data

Data

| Block | Variety | N_1 | N_2 | N_3 | N_4 | Block | Variety | N_1 | N_2 | N_3 | N_4 |
|-------|---------|-------|-------|-------|-------|-------|---------|-------|-------|-------|-------|
| | V_1 | 111 | 130 | 157 | 174 | | V_1 | 74 | 89 | 81 | 122 |
| Ι | V_2 | 117 | 114 | 161 | 141 | IV | V_2 | 64 | 103 | 132 | 133 |
| | V_3 | 105 | 140 | 118 | 156 | | V_3 | 70 | 89 | 104 | 117 |
| | V_1 | 61 | 91 | 97 | 100 | | V_1 | 62 | 90 | 100 | 116 |
| II | V_2 | 70 | 108 | 126 | 149 | V | V_2 | 80 | 82 | 94 | 126 |
| | V_3 | 96 | 124 | 121 | 144 | | V_3 | 63 | 70 | 109 | 99 |
| | V_1 | 68 | 64 | 112 | 86 | | V_1 | 53 | 74 | 118 | 113 |
| III | V_2 | 60 | 102 | 89 | 96 | VI | V_2 | 89 | 82 | 86 | 104 |
| | V_3 | 89 | 129 | 132 | 124 | | V_3 | 97 | 99 | 119 | 121 |

Table 12: A split plot barley field trial

The data is given in Table 12 and may be read as a data frame from file barley.data.

Suggested analysis

Analyse as a split plot field experiment and summarise.

C.11 The snail mortality data

Source: Zoology Department, The University of Adelaide. **Category:** Generalized Linear Modelling.

Description

Groups of 20 snails were held for periods of 1, 2, 3 or 4 weeks (exposure) in carefully controlled conditions of temperature (3 levels) and relative humidity (4 levels). There were two species of snail, A and B, and the experiment was designed as a $4 \times 3 \times 4 \times 2$ completely randomized design. At the end of the exposure time the snails were tested to see if they had survived; this process itself is fatal for the animals. The object of the exercise was to model the probability of survival in terms of the stimulus variables, and in particular to test for differences between species.

The data is unusual in that in most cases fatalities during the experiment were fairly small.

| | | | | | | Rela | ative | Humi | dity | | | | |
|---------|----------|-----|-------|-----------------------|-----|-------|-----------------------|------|-------|-----------------------|-----|-------|-----------------------|
| | | | 60.0% | ,) | | 65.8% | Ó | | 70.5% | , D | | 75.8% | ó |
| | | Ten | npera | ture | Ten | npera | ture | Ten | npera | ture | Ten | npera | ture |
| Species | Exposure | 10 | 15 | 20 | 10 | 15 | 20 | 10 | 15 | 20 | 10 | 15 | 20 |
| А | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| | 2 | 0 | 1 | 1 | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| | 3 | 1 | 4 | 5 | 0 | 2 | 4 | 0 | 2 | 3 | 0 | 1 | 2 |
| | 4 | 7 | 7 | 7 | 4 | 4 | 7 | 3 | 3 | 5 | 2 | 3 | 3 |
| В | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| | 2 | 0 | 3 | 2 | 0 | 2 | 1 | 0 | 0 | 1 | 1 | 0 | 1 |
| | 3 | 7 | 11 | 11 | 4 | 5 | 9 | 2 | 4 | 6 | 2 | 3 | 5 |
| | 4 | 12 | 14 | 16 | 10 | 12 | 12 | 5 | 7 | 9 | 4 | 5 | 7 |

Data

Table 13: The snail mortality data

The data is given in Table 13 and may be read as a data frame from file snails.data.

Suggested analysis

The data is intersting in that although it has many extremely small cell counts there is every indication that some of the likelihood ratio large sample theory is quite safe.

Fit Binomial models to the data with either a logit or a probit link. Show that a model with parallel regressions on Temp, Humid, Exposure and Exposure² for each species (in the logit/probit scale) is reasonable, and summarise.

C.12 The Kalythos blindness data

Source: S. D. Silvey: *Statistical Inference*. (Fictitious?) Category: Generalized linear modelling

Description

On the Greek island of Kalythos the male inhabitants suffer from a congenital eye disease, the effects of which become more marked with increasing age. Samples of islander males of various ages were tested for blindness and the results recorded.

Data

| Age: | 20 | 35 | 45 | 55 | 70 |
|-------------|----|----|----|----|----|
| No. tested: | 50 | 50 | 50 | 50 | 50 |
| No. blind: | 6 | 17 | 26 | 37 | 44 |

Table 14: The Kalythos blindness data

The data is given in Table 14 and may be read as a data frame from file kalythos.data.

Suggested analysis

Using an logit or probit model estimate the LD50, that is, the age at which the probability of blindness is $p = \frac{1}{2}$, together the standard error. Check how different the logit and probit models are in this respect.

C.13 The Stormer viscometer calibration data

Source: E. J. Williams: *Regression Analysis*, Wiley, 1959 Category: Nonlinear regression, special regression.

Description

The stormer viscometer measures the viscosity of a fluid by measuring the time taken for an inner cylinder in the mechanism to perform a fixed number of revolutions in response to an actuating weight. The viscometer is calibrated by measuring the time taken with varying weights while the mechanism is suspended in fluids of accurately known viscosity. The data comes from such a calibration, and theoretical considerations suggest a nonlinear relationship between time, weight and viscosity of the form

$$T_i = \frac{\beta v_i}{w_i - \theta} + E_i$$

where β and θ are unknown parameters to be estimated.

Data

The data is given in Table 15 and may be read as a data frame from file stormer.data.

| | | Weight | | | | | | | |
|-----------|-------|--------|------|--|--|--|--|--|--|
| Viscosity | 20 | 50 | 100 | | | | | | |
| 14.7 | 35.6 | 17.6 | | | | | | | |
| 27.5 | 54.3 | 24.3 | | | | | | | |
| 42.0 | 75.6 | 31.4 | | | | | | | |
| 75.7 | 121.2 | 47.2 | 24.6 | | | | | | |
| 89.7 | 150.8 | 58.3 | 30.0 | | | | | | |
| 146.6 | 229.0 | 85.6 | 41.7 | | | | | | |
| 158.3 | 270.0 | 101.1 | 50.3 | | | | | | |
| 161.1 | | 92.2 | 45.1 | | | | | | |
| 298.3 | | 187.2 | 89.0 | | | | | | |
| | | | 86.5 | | | | | | |

Table 15: The Stormer viscometer calibration data

Suggested analysis

Estimate the nonlinear regression model using the nlr() software. A suitable initial value may be obtained by writing the regression model in the form

$$w_i T_i = \beta v_i + \theta T_i + (w_i - \theta) E_i$$

and regressing $w_i T_i$ on v_i and T_i using ordinary linear regression.

C.14 The chlorine availability data

Source: Draper & Smith, *Applied Regression Analysis*, (adapted). **Category:** Nonlinear regression

Description

The following set of industrial chemical data shows the amount of chlorine available in a certain product at various times of testing after manufacture. A nonlinear regression model for the chlorine decay of the form

$$Y = \beta_0 + \beta_1 \exp(-\theta x)$$

has been suggested on theoretical grounds, with Y the amount remaining at time x.

| Data |
|------|
|------|

| Weeks | Percent available | Weeks | Percent available | Weeks | Percent available |
|-------|-------------------|-------|-------------------|-------|-------------------|
| 8 | 49, 49 | 20 | 42, 43, 42 | 32 | 40, 41 |
| 10 | 47, 47, 48, 48 | 22 | 40, 41, 41 | 34 | 40 |
| 12 | 43, 45, 46, 46 | 24 | 40, 40, 42 | 36 | 38, 41 |
| 14 | 43, 43, 45 | 26 | 40, 41, 41 | 38 | 40, 40 |
| 16 | 43, 43, 44 | 28 | 40, 41 | 40 | 39 |
| 18 | 45, 46 | 30 | 38, 40, 40 | 42 | 39 |

Table 16: The chlorine availability data.

The data is given in Table 16 and may be read as a data frame from file chlorine.data.

Suggested analysis

Fit the nonlinear regression model using the nlr() function. A simple way to find an initial value is to guess a value for θ , say $\theta = 1$ and plot Y against $\exp(-\theta x)$. Now repeatedly either double or halve θ until the plot is near to linear. (This can be done very simply with the inbuilt line editor.) Once an initial value for θ is available, initial values for the others can be got by linear regression.

Check the fitted model for suspicious data points.

C.15 The saturated steam pressure data

Source: Quoted in Draper & Smith: *Applied Regression Analysis...* **Category:** Nonlinear regression.

Description

The data gives the temperature (^{0}C) and pressure (Pascals) in a saturated steam driven experimental device. The relationship between pressure, Y, and temperature, x, in saturated steam can be written as

$$Y = \alpha \exp\left\{\frac{\beta x}{\gamma + x}\right\} + E$$

However a more realistic model may have the experimental errors multiplicative rather than additive, in which case an analysis in the log scale using the model

$$\log Y = \log \alpha + \left\{\frac{\beta x}{\gamma + x}\right\} + E$$

may be more appropriate.

Data

| Temp | Press | Temp | \mathbf{Press} | Temp | \mathbf{Press} |
|------|-------|------|------------------|------|------------------|
| 0 | 4.14 | 50 | 98.76 | 90 | 522.78 |
| 10 | 8.52 | 60 | 151.13 | 95 | 674.32 |
| 20 | 16.31 | 70 | 224.74 | 100 | 782.04 |
| 30 | 32.18 | 80 | 341.35 | 105 | 920.01 |
| 40 | 64.62 | 85 | 423.36 | | |

Table 17: Temperature and pressure in saturated steam

The data is given in Table 17 and may be read as a data frame from file steam.data.

Suggested analysis

Fit both models and compare. Initial values may be got by a similar method to that employed for the Chlorine data, since again there is only one nonlinear parameter.

C.16 Count Rumford's friction data

Source: Bates & Watts: Nonlinear Regression Analysis... Category: Nonlinear regression

Description

Data on the amount of heat generated by friction was obtained by Lord Rumford in 1798. A bore was fitted into a stationary cylinder and pressed against the bottom by a screw. The bore was turned by a team of horses for 30 minutes, after which Lord Rumford "suffered the thermometer to remain in its place nearly three quarters of an hour, observing and noting down, at small intervals of time, the temperature indicated by it".

Newton's law of cooling suggests a nonlinear regression model of the form

$$Y = \beta_0 + \beta_1 \exp(-\theta x)$$

where Y is the temperature and x is the time in minutes.

Data

| Time | Temp | Time | Temp |
|-----------|-----------|-----------|-----------|
| $(\min.)$ | (^{0}F) | $(\min.)$ | (^{0}F) |
| 4.0 | 126 | 24.0 | 115 |
| 5.0 | 125 | 28.0 | 114 |
| 7.0 | 123 | 31.0 | 113 |
| 12.0 | 120 | 34.0 | 112 |
| 14.0 | 119 | 37.5 | 111 |
| 16.0 | 118 | 41.0 | 110 |
| 20.0 | 116 | | |

Table 18: The Rumford friction cooling data

The data is given in Table 18 and may be read as a data frame from file rumford.data.

Suggested analysis

This data is mainly of historical interest. Handle similarly to the Chlorine data above.

C.17 The jellyfish data

Source: *Interactive Statistics*, Ed. Don McNeil. **Category:** Bivariate, two sample data.

Description

Two samples of jellyfish, from Danger Island and Salamander Bay respectively, were measured for length and width.

80

| | Danger | ' Island | | | Salamar | ıder Bay | |
|-------|-------------------------|------------------------|-------------------------|------------------------|-------------------------|------------------------|-------------------------|
| Width | Length | Width | Length | Width | Length | Width | Length |
| 6.0 | 9.0 | 11.0 | 13.0 | 12.0 | 14.0 | 16.0 | 20.0 |
| 6.5 | 8.0 | 11.0 | 14.0 | 13.0 | 17.0 | 16.0 | 20.0 |
| 6.5 | 9.0 | 11.0 | 14.0 | 14.0 | 16.5 | 16.0 | 21.0 |
| 7.0 | 9.0 | 12.0 | 13.0 | 14.0 | 19.0 | 16.5 | 19.0 |
| 7.0 | 10.0 | 13.0 | 14.0 | 15.0 | 16.0 | 17.0 | 20.0 |
| 7.0 | 11.0 | 14.0 | 16.0 | 15.0 | 17.0 | 18.0 | 19.0 |
| 8.0 | 9.5 | 15.0 | 16.0 | 15.0 | 18.0 | 18.0 | 19.0 |
| 8.0 | 10.0 | 15.0 | 16.0 | 15.0 | 18.0 | 18.0 | 20.0 |
| 8.0 | 10.0 | 15.0 | 19.0 | 15.0 | 19.0 | 19.0 | 20.0 |
| 8.0 | 11.0 | 16.0 | 16.0 | 15.0 | 21.0 | 19.0 | 22.0 |
| 9.0 | 11.0 | | | 16.0 | 18.0 | 20.0 | 22.0 |
| 10.0 | 13.0 | | | 16.0 | 19.0 | 21.0 | 21.0 |

Table 19: The jellyfish data – Danger Island and Salamander Bay

Data

The data is given in Table 19 and may be read as a data frame from file jellyfish.data.

Suggested analysis

Plot the two samples and mark in their convex hulls. Test for differences using Hotelling's T^2 . (A simple way of conducting the analysis is to regress a dummy variable for *Location* on *Length* and *width* and to test the significance of both regression coefficients simultaneously.

C.18 The Archæological pottery data

Source: Tubb, A. *et al.* Archæometry, **22**, 153–171, (1980) Category: Multivariate analysis

Description

The data arises from a chemical analysis of 26 samples of pottery found at Romano-British kiln sites in Wales, Gwent and the New Forest. The variables describe the composition, in terms of various metals, and are expressed as percentages of the oxides of the metals.

The metals are aluminium, iron, magnesium, calcium and sodium and the sites are

L: Llanederyn, C: Caldicot I: Island Thorns A: Ashley Rails

Data

The data is given in Table 20 and may be read as a data frame from file pottery.data.

Suggested analysis

Investigate both numerically and graphically using a simple discriminant analysis. Exhibit the four samples using the first two discriminant functions as coordinate axes. Summarise.

| Site | Al | Fe | Mg | Ca | Na | Site | Al | Fe | Mg | Ca | Na |
|------|------|------|------|------|------|------|------|------|------|------|------|
| L | 14.4 | 7.00 | 4.30 | 0.15 | 0.51 | С | 11.8 | 5.44 | 3.94 | 0.30 | 0.04 |
| L | 13.8 | 7.08 | 3.43 | 0.12 | 0.17 | С | 11.6 | 5.39 | 3.77 | 0.29 | 0.06 |
| L | 14.6 | 7.09 | 3.88 | 0.13 | 0.20 | Ι | 18.3 | 1.28 | 0.67 | 0.03 | 0.03 |
| L | 11.5 | 6.37 | 5.64 | 0.16 | 0.14 | Ι | 15.8 | 2.39 | 0.63 | 0.01 | 0.04 |
| L | 13.8 | 7.06 | 5.34 | 0.20 | 0.20 | Ι | 18.0 | 1.50 | 0.67 | 0.01 | 0.06 |
| L | 10.9 | 6.26 | 3.47 | 0.17 | 0.22 | Ι | 18.0 | 1.88 | 0.68 | 0.01 | 0.04 |
| L | 10.1 | 4.26 | 4.26 | 0.20 | 0.18 | Ι | 20.8 | 1.51 | 0.72 | 0.07 | 0.10 |
| L | 11.6 | 5.78 | 5.91 | 0.18 | 0.16 | Α | 17.7 | 1.12 | 0.56 | 0.06 | 0.06 |
| L | 11.1 | 5.49 | 4.52 | 0.29 | 0.30 | Α | 18.3 | 1.14 | 0.67 | 0.06 | 0.05 |
| L | 13.4 | 6.92 | 7.23 | 0.28 | 0.20 | Α | 16.7 | 0.92 | 0.53 | 0.01 | 0.05 |
| L | 12.4 | 6.13 | 5.69 | 0.22 | 0.54 | Α | 14.8 | 2.74 | 0.67 | 0.03 | 0.05 |
| L | 13.1 | 6.64 | 5.51 | 0.31 | 0.24 | Α | 19.1 | 1.64 | 0.60 | 0.10 | 0.03 |
| L | 12.7 | 6.69 | 4.45 | 0.20 | 0.22 | | | | | | |
| L | 12.5 | 6.44 | 3.94 | 0.22 | 0.23 | | | | | | |

Table 20: The pottery composition data

C.19 The Beaujolais quality data

Source: Quoted in Weekes: A Genstat Primer Category: Multivariate analysis

Description

Quality measurements for some identified samples of young Beaujolais. Extracted from Table 1 in M. G. Jackson, *et al*: Red wine quality: correlations between colour, aroma and flavour and pigment and other parameters of young Beaujolais, *Journal of Science of Food and Agriculture*, **29**, 715–727, (1978).

Data

| Label | OQ | AC | pH | TSO | Label | OQ | AC | $_{\mathrm{pH}}$ | TSO |
|-------|-------|------|---------------|------|--------------|-------|------|------------------|------|
| А | 13.54 | 1.51 | 3.36 | 13.8 | Ι | 12.25 | 1.32 | 3.38 | 1.4 |
| В | 12.58 | 1.35 | 3.15 | 5.2 | J | 14.04 | 1.52 | 3.61 | 4.5 |
| С | 11.83 | 1.09 | 3.30 | 10.6 | Κ | 12.67 | 1.62 | 3.38 | 0.4 |
| D | 12.83 | 1.15 | 3.41 | 2.2 | \mathbf{L} | 13.54 | 1.57 | 3.55 | 7.9 |
| Е | 12.83 | 1.32 | 3.44 | 2.3 | Μ | 13.75 | 1.63 | 3.34 | 6.3 |
| F | 12.12 | 1.23 | 3.31 | 10.5 | Ν | 9.63 | 0.78 | 3.19 | 40.4 |
| G | 11.29 | 1.14 | 3.49 | 2.5 | 0 | 12.42 | 1.14 | 3.31 | 3.1 |
| Н | 12.79 | 1.22 | 3.56 | 16.7 | | | | | |

Table 21: Quality measurements on young Beaujolais wine samples

The data is given in Table 21 and may be read as a data frame from file beaujolais.data.

Suggested analysis

Look at ways of exhibiting the data graphically. Consider a principal component analysis using the correlation matrix and look for any wild outliers.

C.20 The painters data of de Piles

Source: Weekes: A Genstat Primer. Category: Multivariate Analysis: Discriminant Analysis.

Description

The data shows the subjective assessment, on a 0–20 integer scale, of 54 classical painters. The painters were assessed on four characteristics: composition, drawing, colour and expression. The data is due to the Eighteenth century art critic, de Piles.

The School to which a painter belongs is indicated by a letter code as follows:

| Α | Renaissance | Е | Lombard |
|---|-------------|--------------|---------------------|
| В | Mannerist | \mathbf{F} | Sixteenth Century |
| C | Seicento | G | Seventeenth Century |
| D | Venetian | Η | French |

Data

The data is given in Table 22 and may be read as a data frame from file painters.data.

Suggested analysis

Using a multivariate analysis of variance check for differences between schools. Use the likelihood ratio test. Also find the canonical F-statistics and discriminant functions.

Plot the painters on the first two discriminant function axes and use the school symbol as a plotting character. Mark in the convex hulls of the schools. Using identify() find interactively some of the painers that appear to lie towards the extremes of the plot, or who deviate considerably from their school mean.

| | Composition | Drawing | Colour | Expression | School |
|----------------------------|-------------|---------|--------|------------|--------------|
| Da Udine | 10 | 8 | 16 | 3 | A |
| Da Vinci | 15 | 16 | 4 | 14 | А |
| Del Piombo | 8 | 13 | 16 | 7 | А |
| Del Sarto | 12 | 16 | 9 | 8 | А |
| Fr. Penni | 0 | 15 | 8 | 0 | А |
| Guilio Romano | 15 | 16 | 4 | 14 | А |
| Michelangelo | 8 | 17 | 4 | 8 | А |
| Perino del Vaga | 15 | 16 | 7 | 6 | А |
| Perugino | 4 | 12 | 10 | 4 | А |
| Raphael | 17 | 18 | 12 | 18 | А |
| F. Zucarro | 10 | 13 | 8 | 8 | В |
| Fr. Salviata | 13 | 15 | 8 | 8 | В |
| Parmigiano | 10 | 15 | 6 | 6 | В |
| Primaticcio | 15 | 14 | 7 | 10 | В |
| T. Zucarro | 13 | 14 | 10 | 9 | В |
| Volterra | 12 | 15 | 5 | 8 | В |
| Barocci | 14 | 15 | 6 | 10 | С |
| Cortona | 16 | 14 | 12 | 6 | С |
| Josepin | 10 | 10 | 6 | 2 | С |
| L. Jordaens | 13 | 12 | 9 | 6 | С |
| Testa | 11 | 15 | 0 | 6 | С |
| Vanius | 15 | 15 | 12 | 13 | С |
| Bassano | 6 | 8 | 17 | 0 | D |
| Bellini | 4 | 6 | 14 | 0 | D |
| Giorgione | 8 | 9 | 18 | 4 | D |
| Murillo | 6 | 8 | 15 | 4 | D |
| Palma Giovane | 12 | 9 | 14 | 6 | D |
| Palma Vecchio | 5 | 6 | 16 | 0 | D |
| Pordenone | 8 | 14 | 17 | 5 | D |
| Tintoretto | 15 | 14 | 16 | 4 | D |
| Titian | 12 | 15 | 18 | 6 | D |
| Veronese | 15 | 10 | 16 | 3 | D |
| Albani | 14 | 14 | 10 | 6 | E |
| Caravaggio | 6 | 6 | 16 | 0 | \mathbf{E} |
| Corregio | 13 | 13 | 15 | 12 | \mathbf{E} |
| Domenichino | 15 | 17 | 9 | 17 | \mathbf{E} |
| Guercino | 18 | 10 | 10 | 4 | \mathbf{E} |
| Lanfranco | 14 | 13 | 10 | 5 | \mathbf{E} |
| The Carraci | 15 | 17 | 13 | 13 | \mathbf{E} |
| Durer | 8 | 10 | 10 | 8 | F |
| Holbein | 9 | 10 | 16 | 13 | \mathbf{F} |
| Pourbus | 4 | 15 | 6 | 6 | \mathbf{F} |
| Van Leyden | 8 | 6 | 6 | 4 | \mathbf{F} |
| Diepenbeck | 11 | 10 | 14 | 6 | G |
| J. Jordaens | 10 | 8 | 16 | 6 | G |
| Otho Venius | 13 | 14 | 10 | 10 | G |
| $\operatorname{Rembrandt}$ | 15 | 6 | 17 | 12 | G |
| Rubens | 18 | 13 | 17 | 17 | G |
| Teniers | 15 | 12 | 13 | 6 | G |
| Van Dyck | 15 | 10 | 17 | 13 | G |
| Bourdon | 10 | 8 | 8 | 4 | Н |
| Le Brun | 16 | 16 | 8 | 16 | Н |
| Le Suer | 15 | 15 | 4 | 15 | Η |
| Poussin | 15 | 17 | 6 | 15 | Н |

Table 22: The subjective assessment data of de Piles

References

Bates, D. M. and Watts, D. G. (1988). Nonlinear regression analysis and its applications. Wiley. Dobson, A. J. (1991). An Introduction to Generalized Linear Models. Chapman and Hall, London, NY.