Introduction to the R Project for Statistical Computing for use at ITC

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If you are impatient ... Start R (\S 3) and follow the sample R session (\S A).

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1 What is R?

R is an open-source environment for statistical computing and visualisation. It is based on the S language developed at Bell Laboratories in the 1980's [12], and is the product of an active movement among statisticians for a powerful, programmable, portable, and open computing environment, applicable to the most complex and sophsticated problems, as well as "routine" analysis, without any restrictions on access or use. Here is a description from the R Project home page:¹

"R is an **integrated suite of software facilities** for data manipulation, calculation and graphical display. It includes:

- · 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 onscreen 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."

The last point has resulted in another major feature:

Practising statisticians have implemented hundreds of specialised statistical produces for a wide variety of applications as contributed packages, which are also freely-available and which integrate directly into R.

A few examples especially relevant to ITC are the gstat and spatial packages for geostatistical analysis, contributed by Pebesma [17] and Ripley [22], respectively; the spatstat package for spatial point-pattern analysis and simulation; the vegan package of ordination methods for ecology; the circular package for directional statistics; the sp package for a programming interface to spatial data, and the rgdal package for GDAL-standard data access. There are also packages for the most modern statistical techniques such as neural networks (nnet), non-linear mixed-effects models (nlme), recursive partitioning (rpart), and splines (splines), as well as standard sophisticated techniques such as generalized linear models, principal components, factor analysis, bootstrapping, and robust regression.

¹ http://www.r-project.org/

2 Why R for ITC?

ITC is an international institution of post-graduate education located in Enschede, the Netherlands, with a thematic focus on geo-information science and earth observation in support of development. Its mission² is described as follows:

"ITC aims at capacity building and institutional development of professional and academic organizations and individuals specifically in countries that are economically and/or technologically less developed."

Thus the two pillars on which ITC stands are *development-related* and *geo-information*. R supports both of these.

2.1 Advantages

R has several major **advantages** for a typical ITC student or collaborator:

- 1. It is **completely free** and will always be so, since it is issued under the GNU Public License;³
- 2. It is **freely-available over the internet**, via a large network of *mirror* servers; see Appendix B for how to obtain R;
- 3. It runs on almost **all operating systems**: Unix[©] and derivatives including Darwin, Mac OS X, Linux, FreeBSD, and Solaris; most flavours of Microsoft Windows; Apple Macintosh OS; and even some mainframe OS.
- 4. It is the product of **international collaboration** between **top computational statisticians** and computer language designers;
- 5. It allows **statistical analysis** and **visualisation** of **unlimited sophistication**; you are not restricted to a small set of procedures or options, and because of the contributed packages, you are not limited to one method of accomplishing a given computation or graphical presentation;
- 6. It can work on **objects of unlimited size and complexity** with a consistent, logical **expression language**;
- 7. It is supported by comprehensive **technical documentation** and user-contributed tutorials (§9). There are also several good textbooks on statistical methods that use R (or S) for illustration.
- 8. Every computational step is **recorded**, and this history can be saved

² http://www.itc.nl/about_itc/mission_statement.asp

³ http://www.gnu.org/copyleft/gpl.html

for later use or documentation.

- 9. It stimulates **critical thinking** about problem-solving rather than a "push the button" mentality.
- 10. It is **fully programmable**, with its own sophisticated computer language (§4). Repetitive procedures can easily be automated by userwritten **scripts** (§3.9). It is easy to write your own **functions** (§C), and not too difficult to write whole **packages** if you invent some new analysis;
- 11. All **source code** is published, so you can see the exact algorithms being used; also, expert statisticians can make sure the code is correct;
- 12. It can **exchange data** in MS-Excel, text, fixed and delineated formats (e.g. CSV), so that existing datasets are easily imported (§6), and results computed in R are easily exported (§7).
- 13. Most programs written for the commercial **S-PLUS** program will run unchanged, or with minor changes, in R (§2.3.1).

2.2 Disadvantages

R has its **disadvantages** (although some of these may be considered advantages as well):

- 1. The default Windows and Mac OS X **graphical user interface** (GUI) is limited to simple system interaction and does not include statistical procedures. The user must **type commands** to enter data, do analyses, and plot graphs. This has the advantage that you have complete control over the system. The Rcmdr add-on package (§3.10) provides a reasonable GUI for common tasks.
- 2. The user must decide on the sequence of analyses and execute them step-by-step. However, it is easy to create **scripts** with all the steps in an analysis, and run the script from the command line or menus (§3.9).
- 3. The user must learn a **new way of thinking about data**, as **data frames** (§4.7) and **objects** each with its **class**, which in turn supports a set of **methods**. This has the advantage common to object-oriented languages that you can only operate on an object according to methods that make sense⁴ and methods can adapt to the type of object.⁵
- 4. The user must learn the **S language** (§4), both for commands and the notation used to specify statistical models. The S statistical mod-

⁴ For example, the t (transpose) method only can be applied to matrices

⁵ For example, the summary and plot methods give different results depending on the class of object.

elling language is a *lingua franca* among statisticians, and provides a compact way to express models ($\S4.17$).

2.3 Alternatives

There are many ways to do computational statistics; this section discusses them in relation to R. None of these programs are open-source, meaning that you must trust the company to do the computations correctly.

2.3.1 S-PLUS

S-PLUS is a commercial program distributed by the Insightful corporation, and is a popular choice for large-scale commercial statistical computing. Like R, it is a dialect of the original S language developed at Bell Laboratories. S-PLUS has a full graphical user interface (GUI); it may be also used like R, by typing commands at the console or by running scripts. It has a rich interactive graphics environment called Trellis, which has been emulated with the lattice package in R (§5.2). S-PLUS is licensed by local distributors in each country at prices ranging from moderate to high, depending factors such as type of licensee and application, and how many computers it will run on. The important point for ITC R users is that their expertise will be immediately applicable if they later use S-PLUS in a commercial setting.

2.3.2 Statistical packages

There are many statistical packages, including MINITAB, SPSS, Systat, Gen-Stat, and BMDP, which are attractive if you are already familiar with them or if you are required to use them at your workplace. Although these are programmable to varying degrees, it is not intended that specialists develop completely new algorithms. These must be purchased from local distributors in each country, and the purchaser must agree to the license terms. These often have common analyses built-in as menu choices; these can be convenient but it is tempting to use them without fully understanding what choices they are making for you.

SAS is a commercial competitor to S-PLUS, and is used widely in industry. It is fully programmable with a language descended from PL/I (used on IBM mainframe computers).

⁶ http://www.insightful.com/

⁷ There are differences in the language definitions of S, R, and S-PLUS that are important to programmers, but rarely to end-users. There are also differences in how some algorithms are implemented, so the numerical results of an identical method may be somewhat different.

⁸ See the list at http://www.stata.com/links/stat_software.html

2.3.3 Special-purpose statistical programs

Some programs adress specific statistical issues, e.g. geostatistical analysis and interpolation (SURFER, gslib, GEO-EAS), ecological analysis (FRAG-STATS), and ordination (CONOCO). The algorithms in these programs have or can be programmed as an R package; examples are the gstat program for geostatistical analysis⁹ [19], which is now available within R [17], and the vegan package for ecological statistics.

2.3.4 Spreadsheets

Microsoft Excel is useful for data manipulation. It can also calculate some statistics (means, variances, ...) directly in the spreadsheet. This is also an add-on module (menu item \underline{T} ools | \underline{D} ata Analysis...) for some common statistical procedures including random number generation. Be aware that Excel was not designed by statisticians. There are also some commercial add-on packages for Excel that provide more sophisticated statistical analyses.

OpenOffice¹⁰ includes an open-source and free spreadsheet which can replace Excel.

2.3.5 Applied mathematics programs

MATLAB is a widely-used applied mathematics program, especially suited to matrix maniupulation (as is R, see §4.6), which lends itself naturally to programming statistical algorithms. Add-on packages are available for many kinds of statistical computation. Statistical methods are also programmable in Mathematica.

3 Using R for Windows

3.1 R on the ITC network

R has been installed on the ITC Windows NT network at:

\\Itcnt03\Apps\R\bin\RGui.exe

For most ITC accounts drive P: has been mapped to \\Itcnt03\Apps, so R can be accessed using this drive letter instead of the network address:

! → P:\R\bin\RGui.exe

You can copy this to your local desktop as a shortcut.

⁹ http://www.gstat.org/
10 http://www.openoffice.org/

Documentation has been installed at:

P:\R\doc

3.2 Starting R

R is started like any Windows program:

- 1. Open Windows Explorer
- 2. Navigate to the directory where the R executable is located; e.g. on the ITC network, this is P:\R\bin
- 3. Double-click on the icon for RGui.exe

This will start R the directory where it was installed, which is not where you should store your projects. If you are using the copy of R on the ITC network, you do not have write permission to this directory, so you won't be able to save any data or session information there. So, you will probably want to change your workspace, as explained in §3.4. You can also create a desktop shortcut or Start menu item for R, also as explained in §3.4.

3.3 Stopping R

To stop an R session, type q() at the command prompt¹¹, or select the <u>File</u> | Exit menu item in the Windows GUI.

3.4 Setting up a workspace

An important concept in R is the **workspace**, which contains the local data and procedures for a given statistics project. Under Windows this is usually determined by the folder from which R is started.

Under Windows, the easiest way to set up a statistics project is:

- 1. Create a **shortcut** to **RGui.exe** on your desktop;
- 2. Modify its **properties** so that its in your working directory rather than the default (e.g. P:\R\bin).

Now when you double-click on the shortcut, it will start R in the directory of your choice. So, you can set up a different shortcut for each of your projects.

Another way to set up a new statistics project in R is:

1. Start R as just described: double-click the icon for program RGui.exe

¹¹ This is a special case of the q method

in the Windows Explorer;

- 2. Select the File | Change Directory ... menu item in R;
- 3. Select the directory where you want to work;
- 4. Exit R by selecting the File | Exit menu item in R, or typing the q() command; R will ask "Save workspace image?"; Answer y (Yes). This will create two files in your working directory: .Rhistory and .RData.

The next time you want to work on the same project:

- 1. Open Windows Explorer and navigate to the working directory
- 2. **Double-click on the icon** for file .RData

R should open in that directory, with your previous workspace already loaded. (If R does not open, instead Explorer will ask you what programs should open files of type .RData; navigate to the program RGui.exe and select it.)

Revealing hid-Windows

If you don't see the file .RData in your Windows Explorer, this is because Windows considers any file name that begins with "." to be a 'hidden' file. den files in You need to select the Tools | Folder options in Windows Explorer, then the View tab, and click the radio button for Show hidden files and folders. You must also un-check the box for Hide file extensions for known file types.

3.5 The command prompt

You perform most actions in R by typing commands in a console win**dow**, ¹² in response to a **command prompt**, which usually looks like this:

The > is a **prompt symbol** displayed by R, not typed by you. This is R's way of telling you it's ready for you to type a command.

Type your command and press the Enter or Return keys; R will execute your command.

If your entry is not a complete R command, R will prompt you to complete it with the **continuation prompt symbol**:

¹² An alternative for some analyses is the Rcmdr GUI explained in §3.10.

R will accept the command once it is *syntactically complete*; in particular the parentheses must balance. Once the command is complete, R then presents its results in the same console window, directly under your command.

If you want to abort the current command (i.e. not complete it), press the Esc ("escape") key.

For example, to draw 500 samples from a binomial distribution of 20 trials with a 40% chance of success¹³ you would first use the rbinom method and then summarize it with the summary method, as follows:¹⁴

This could also have been entered on several lines:

```
> x <- rbinom(
+ 500,20,.4
+ )</pre>
```

You can use any white space to increase legibility, *except* that the assignment symbol <- must be written together:

```
> x < - rbinom(500, 20, 0.4)
```

R is **case-sensitive**; that is, method rbinom must be written just that way, not as Rbinom or RBINOM (these might be different methods). Variables are also case-sensitive: x and X are different names.

Some methods produce output in a separate graphics window:

```
> hist(x)
```

3.6 On-line help

Both the base R system and contributed package have extensive help.

Individual methods

In Windows, you can use the Help menu and navigate to the method you want to understand. You can also get help on any method with the ? method, typed at the command prompt; this is just a shorthand for the help method:

For example, if you don't know the format of the rbinom method used

¹³ This simulates, for example, the number of women who would be expected, by chance, to present their work at a conference where 20 papers are to be presented, if the women make up 40% of the possible presenters.

¹⁴ Your output will probably be somewhat different; why?

above. Either of these two forms:

- > ?rbinom
 > help(rbinom)
 - will display a text page with the syntax and options for this method. There are **examples** at the end of many help topics, with executable code that you

can experiment with to see just how the method works.

Searching for methods

If you don't know the method name, you can search the help for relevant methods using the help.search method¹⁵:

> help.search("binomial")

will show a window with all the methods that include this word in their description, along with the packages where these methods are found, whether already loaded or not.

In the list shown as a result of the above method, we see the Binomial (stats) topic; we can get more information on it with the ? method; this is written as the ? character *immediately* followed by the method name:

> ?Binomial

This shows the named topic, which explains the rbinom (among other) methods.

Vignettes

Packages have a long list of methods, each of which has its own documentation as explained above. Some packages are documented as a whole by so-called **vignettes**¹⁶; for now most packages do not have one, but more will be added over time.

You can see a list of the vignettes installed on your system with the vignette method with an empty argument:

> vignette()

and then view a specific vignette by naming it:

> vignette("sp")

3.7 Saving your analysis steps

The File | Save to file ... menu command will save the entire console contents, i.e. both your commands and R's response, to a text file, which you can later review and edit with any text editor. This is useful for

¹⁵ also available via the Help | Search help ... menu item

¹⁶ from the OED meaning "a brief verbal description of a person, place, etc.; a short descriptive or evocative episode in a play, etc."

cutting-and-pasting into your reports or thesis, and also for writing scripts to repeat procedures.

3.8 Saving your graphs

In the Windows version of R, you can save any graphical output for insertion into documents or printing. If necessary, bring the graphics window to the front (e.g. click on its title bar), select menu command File | Save as ..., and then one of the formats. Most useful for insertion into MS-Word documents is Metafile; most useful for LATEX is Postscript; most useful for PDFLaTeX and stand-alone printing is PDF. If you want to add other graphical elements, you may want to save as a PNG or JPEG; however in most cases it is cleaner to add annotations within R itself.

You can also write your graphics commands directly to a graphics file in many formats, e.g. PDF or JPEG. You do this by opening a graphics device, writing the commands, and then closing the device. You can get a list of graphics devices (formats) available on your system with ?Devices (note the upper-case D).

For example, to write a PDF file, we open the pdf graphics device:

```
pdf("figure1.pdf", h=6, w=6)
hist(rnorm(100), main="100 random values from N[0,1])")
dev.off()
```

Note the use of the optional height= and width= arguments (here abbreviated h= and w=) to specify the size of the PDF file (in US inches); this affects the font sizes.

3.9 Writing and running scripts

After you have worked out an analysis by typing a sequence of commands, you will probably want to re-run them on edited data, new data, subsets etc. This is easy to do by means of **scripts**, which are simply lists of commands in a file, written exactly as you would type them at the console. They are run with the **source** method. A useful feature of scripts is that you can include comments (lines that begin with the # character) to explain to yourself or others what the script is doing and why.

Here's a step-by-step description of how to create and run a simple script which draws two random samples from a normal distribution and computes their correlation:¹⁷

- 1. Open Notepad or another pure-text editor.
- 2. Type in the following lines:¹⁸

¹⁷ What is the expected value of this correlation cofficient?

¹⁸ You can cut-and-paste from here if you're feeling lazy

```
x <- rnorm(100, 180, 20)
y <- rnorm(100, 180, 20)
plot(x, y)
cor.test(x, y)</pre>
```

- 3. Save the file with the name test.R, in a convenient directory.
- 4. Start R (if it's not already running)
- 5. In R, select menu command File | Source R code ...
- 6. In the file selection dialog, locate the file test.R that you just saved (changing directories if necessary) and select it; R will run the script.
- 7. Examine the output.

You can source the file directly from the command line. Instead of steps 5 and 6 above, just type source("test.R") at the R command prompt (assuming you've switched to the directory where you saved the script).

Appendix C contains an example of a more sophisticated script.

For serious work with R you should consider using a more flexible editor than Notepad. The R for Windows, R for Mac OS X and JGR interfaces include built-in editors; other choices include WinEdit (on Windows only) and, for power users, EMACS with the ESS (Emacs Speaks Statistics) module. The Tinn-R code editor for Windows¹⁹ is tightly integrated with the Windows R GUI.

3.10 Using the Rcmdr GUI

The Rcmdr add-on package, written by John Fox of McMaster University, provides a GUI for common data management and statistical analysis tasks. It is loaded like any other package, with the library method:

```
> library("Rcmdr")
```

As it is loaded, it starts up in another window, with its own menu system. You can run commands from these menus, but you can also continue to type commands at the R prompt. Figure 1 shows an R Commander screen shot.

To use Rcmdr, you first import or activate a dataset using one of the commands on Rcmdr's Data menu; then you can use procedures in the Statistics, Graphs, and Models menus. You can also create and graph probability distributions with the Distributions menu.

¹⁹ http://www.sciviews.org/Tinn-R/

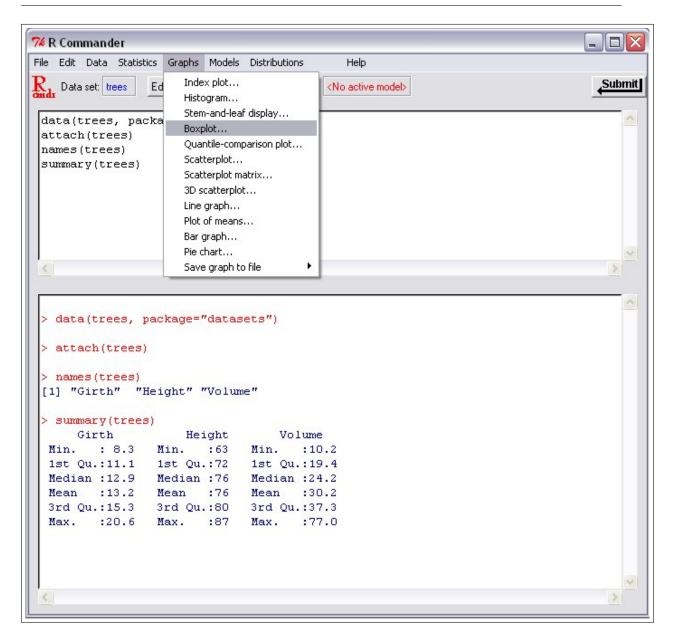


Figure 1: The R Commander screen: Menu bar at the top; a top panel showing commands submitted to R by the menu commands; a bottom panel showing the results after execution by R

When using Rcmdr, observe the commands it formats in response to your menu and dialog box choices. Then you can modify them yourself at the R command line or in a script.

Rcmdr also provides some nice graphics options, including scatterplots (2D and 3D) where observations can be coloured by a classifying factor.

3.11 Loading optional packages

R starts up with a base package, which provides basic statistics and the R language itself. There are a large number of optional packages for specific statistical procedures which can be loaded during a session. Some of these are quite common, e.g. MASS ("Modern Applied Statistics with S" [33]) and lattice (Trellis graphics [29], §5.2). Others are more specialised, e.g. for geostatistics and time-series analysis, such as gstat. Some are loaded by default in the base R distribution (see Table 4).

If you try to run a method from one of these packages before you load it, you will get the error message

Error: object not found

You can see a list of the packages installed on your system with the library method with an empty argument:

> library()

To see what functions a package provides, use the library method with the named argument. For example, to see what's in the geostatistical package qstat:

> library(help=gstat)

To load a package, simply give its name as an argument to the library method, for example:

> library(gstat)

Once it is loaded, you can get help on any method in the package in the usual way. For example, to get help on the variogram method of the gstat package, once this package has been loaded:

> ?variogram

3.12 Sample datasets

R comes with many example datasets (part of the default datasets package) and most add-in packages also include example datasets. Some of the datasets are classics in a particular application field; an example is the iris dataset used extensively by R A Fisher to illustrate multivariate methods.

To see the list of installed datasets, use the data method with an empty argument:

> data()

To see the datasets in a single add-in package, use the package= argument:

> data(package="gstat")

To load one of the datasets, use its name as the argument to the data method:

> data(iris)

The dataframe representing this dataset is now in the workspace.

4 The S language

R is a dialect of the S language, which has a syntax similar to ALGOL-like programming languages such as C, Pascal, and Java. However, S is object-oriented, and makes vector and matrix operations particularly easy; these make it a modern and attractive user and programming environment. In this section we build up from simple to complex commands, and break down their anatomy. A full description of the language is given in the *R* Language Definition [21]²⁰ and a comprehensive introduction is given in the *Introduction to R* [20].²¹ This section reviews the most outstanding features of S.

All the methods, packages and datasets mentioned in this section (as well as the rest of this note) are indexed (§D) for quick reference.

4.1 Command-line calculator and mathematical operators

The simplest way to use R is as an interactive calculator. For example, to compute the number of radians in one Babylonian degree of a circle:

```
> 2*pi/360
[1] 0.0174533
```

As this example shows, S has a few built-in constants, among them pi for the mathematical constant π . The Euler constant e is not built-in, it must be calculated with the exp method as exp(1).

If the assignment operator (explained in the next section) is not present, the *expression* is evaluated and its value is displayed on the console. S has the usual arithmetic operators +, -, *, /, $^{\wedge}$ and some less-common ones like % (modulus) and %/% (integer division). Expressions are evaluated in accordance with the usual *operator precedence*; parentheses may be used to change the precedence or make it explicit:

```
> 3 / 2<sup>2</sup> + 2 * pi
[1] 7.03319
> ((3 / 2)<sup>2</sup> + 2) * pi
[1] 13.3518
```

Spaces may be used freely and do not alter the meaning of any S expression.

Common mathematical functions are provided as *methods* (see §4.3), including log, log10 and log2 methods to compute logarithms; exp for exponentiation; sqrt to extract square roots; abs for absolute value; round, ceiling, floor and trunc for rounding and related operations; trigonometric functions such as sin, and inverse trigonometric functions such as

²⁰ In RGui, menu command <u>H</u>elp | <u>M</u>anuals | R <u>L</u>anguage Manual ²¹ In RGui, menu command <u>H</u>elp | <u>M</u>anuals | R <u>I</u>ntroduction

asin.

```
> log(10); log10(10); log2(10)
[1] 2.3026
[1] 1
[1] 3.3219
> round(log(10))
[1] 2
> sqrt(5)
[1] 2.2361
sin(45 * (pi/180))
[1] 0.7071
> (asin(1)/pi)*180
[1] 90
```

4.2 Creating new objects: the assignment operator

New objects in the workspace are created with the *assignment operator* <-, which may also be written as =:

```
> mu < -180
> mu = 180
```

The symbol on the left side is given the value of the *expression* on the right side, creating a new object (or redefining an existing one), here named mu, in the workspace and *assigning* it the value of the expression, here the scalar value 180, which is stored as a one-element vector. The two-character symbol <- *must* be written as two adjacent characters with no spaces..

Now that mu is defined, it may be printed at the console as an expression:

```
> print(mu)
[1] 180
> mu
[1] 180
```

and it may be used in an expression:

```
> mu/pi
[1] 57.2958
```

More complex objects may be created:

```
> s <- seq(10)
> s
[1] 1 2 3 4 5 6 7 8 9 10
```

This creates a new object named s in the workspace and *assigns* it the vector (1 2 ...10). (The function syntax in seq(10) is explained in the next section.)

Multiple assignments are allowed in the same expression:

```
> (mu <- theta <- pi/2)
[1] 1.5708
```

The final value of the expression, in this case the value of mu, is printed, because the parentheses force the expression to be evaluated as a unit.

Removing objects from the workspace You can remove objects when they are no longer needed with the rm method:

```
> rm(s)
> s
Error: Object "s" not found
```

4.3 Methods and their arguments

In the command $s \leftarrow seq(10)$, seq is an example of an S *method*, often called a *function* by analogy with mathematical functions, which has the form:

```
function.name ( arguments )
```

Some functions do not need arguments, e.g. to list the objects in the workspace use the 1s method with an *empty* argument list:

```
> 1s()
```

Note that the empty argument list, i.e. nothing between the (and) is still needed, otherwise the computer code for the function itself is printed.

Optional arguments Most methods have *optional arguments*, which may be *named* like this:

```
> s <- seq(from=20, to=0, by=-2)
> s
[1] 20 18 16 14 12 10 8 6 4 2 0
```

Named arguments have the form name = value.

In some cases arguments can also be *positional*, that is, their meaning depends on their position in the argument list. The previous command could be written:

```
> s <- seq(20, 0, by=-2); s
[1] 20 18 16 14 12 10 8 6 4 2 0
```

because the **seq** method expects its first un-named argument to be the starting point of the vector and its second to be the end.

The command separator This example shows the use of the ; *command separator*. This allows several commands to be written on one line. In this case the first command computes the sequence and stores it in an object, and the second displays this object. This effect can also be achieved by enclosing the entire expression in parentheses, because then S prints the value of the expression, which in this case is the new object:

```
> (s <- seq(from=20, to=0, by=-2))
[1] 20 18 16 14 12 10 8 6 4 2 0</pre>
```

Named arguments give more flexibility; this could have been written with names:

```
> (s <- seq(to=0, from=20, by=-2))
[1] 20 18 16 14 12 10 8 6 4 2 0
```

but if the arguments are specified only by position the starting value must be before the ending value.

For each method, the list of arguments, both positional and named, and their meaning is given in the on-line help:

```
> ? seq
```

Any element or group of elements in a vector can be accessed by using subscripts, very much like in mathematical notation, with the [] (select array elements) operator:

```
> samp[1]
[1] -1.239197
> samp[1:3]
[1] -1.23919739  0.03765046  2.24047546
> samp[c(1,10)]
[1] -1.239197  9.599777
```

The notation 1:3, using the : *sequence operator*, produces the sequence from 1 to 3.

The catenate method The notation c(1, 10) is an example of the very useful c or *catenate* ("make a chain") method, which makes a *list* out of its arguments, in this case the two integers representing the indices of the first and last elements in the vector.

4.4 Vectorized operations and re-cycling

A very powerful feature of S is that most operations work on vectors or matrices with the same syntax as they work on scalars, so there is rarely any need for explicit looping commands (which are provided, e.g. for). These are called *vectorized* operations.

As an example of vectorized operations, consider simulating a noisy random process:

```
> (sample <- seq(1, 10) + rnorm(10))
[1] -0.1878978  1.6700122  2.2756831  4.1454326
[5]  5.8902614  7.1992164  9.1854318  7.5154372
[9]  8.7372579  8.7256403</pre>
```

This adds a random noise (using the rnorm method) with mean 0 and standard deviation 1 (the default) to each of the 10 numbers 1..10. Note that both vectors have the same length (10), so they are added *element-wise*: the first to the first, the second to the second and so forth

If one vector is shorter than the other, its elements are *re-cycled* as needed:

```
> (samp <- seq(1, 10) + rnorm(5))
[1] -1.23919739  0.03765046  2.24047546  4.89287818
[5]  4.59977712  3.76080261  5.03765046  7.24047546
[9]  9.89287818  9.59977712</pre>
```

This perturbs the first five numbers in the sequence the same as the second five.

A simple example of re-cycling is the computation of sample variance directly from the definition, rather than with the var method:

```
> (sample <- seq(1:8))
[1] 1 2 3 4 5 6 7 8
> (sample - mean(sample))
[1] -3.5 -2.5 -1.5 -0.5 0.5 1.5 2.5 3.5
> (sample - mean(sample))^2
[1] 12.25 6.25 2.25 0.25 0.25 2.25 6.25 12.25
> sum((sample - mean(sample))^2)
[1] 42
> sum((sample - mean(sample))^2)/(length(sample)-1)
[1] 6
> var(sample)
[1] 6
```

In the expression sample - mean(sample), the mean mean(sample) (a scalar) is being subtracted from sample (a vector). The scalar is a one-element vector; it is shorter than the eight-element sample vector, so it is re-cycled: the same mean value is subtracted from each element of the sample vector in turn; the result is a vector of the same length as the sample. Then this entire vector is squared with the ^ operator; this also is applied element-wise.

The sum and length methods are examples of methods that *summarise* a vector and reduce it to a scalar.

Other methods transform one vector into another. Useful examples are sort, which sorts the vector, and rank, which returns a vector with the rank (order) of each element of the original vector:

```
> data(trees)
> trees$Volume
[1] 10.3 10.3 10.2 16.4 18.8 19.7 15.6 18.2 22.6 19.9
[11] 24.2 21.0 21.4 21.3 19.1 22.2 33.8 27.4 25.7 24.9 34.5
[22] 31.7 36.3 38.3 42.6 55.4 55.7 58.3 51.5 51.0 77.0
> sort(trees$Volume)
[1] 10.2 10.3 10.3 15.6 16.4 18.2 18.8 19.1 19.7 19.9
[11] 21.0 21.3 21.4 22.2 22.6 24.2 24.9 25.7 27.4 31.7 33.8
[22] 34.5 36.3 38.3 42.6 51.0 51.5 55.4 55.7 58.3 77.0
> rank(trees$Volume)
[1] 2.5 2.5 1.0 5.0 7.0 9.0 4.0 6.0 15.0 10.0
[11] 16.0 11.0 13.0 12.0 8.0 14.0 21.0 19.0 18.0 17.0 22.0
[22] 20.0 23.0 24.0 25.0 28.0 29.0 30.0 27.0 26.0 31.0
```

Note how rank averages tied ranks by default; this can be changed by the optional ties.method argument.

This example also illustrates the \$ operator for extracting fields from dataframes; see §4.7.

4.5 Vector and list data structures

Many S commands create complicated *data structures*, whose structure must be known in order to use the results in further operations. For example, the sort method sorts a vector; when called with the optional index=TRUE argument it also returns the ordering index vector:

```
> ss <- sort(samp, index=TRUE)
> str(ss)
List of 2
$ x : num [1:10] -1.2392  0.0377  2.2405  3.7608 ...
$ ix: int [1:10] 1 2 3 6 5 4 7 8 10 9
```

This example shows the very important str method, which displays the S *structure* of an object.

Lists In this case the object is a *list*, which in S is an arbitrary collection of other objects. Here the list consists of two objects: a ten-element vector of sorted values ss\$x and a ten-element vector of the indices ss\$ix, which are the positions in the original list where the corresponding sorted value was found. We can display just one element of the list if we want:

```
> ss$ix
[1] 1 2 3 6 5 4 7 8 10 9
```

This shows the syntax for accessing named components of a data frame or list using the \$ operator: object \$ component, where the \$ indicates that the component (or field) is to be found *within* the named object.

We can combine this with the vector indexing operation:

```
> ss$ix[length(ss$ix)]
[1] 9
```

So the largest value in the sample sequence is found in the ninth position. This example shows how *expressions may contain other expressions*, and S evaluates them from the inside-out, just like in mathematics. In this case:

- The innermost expression is ss\$ix, which is the vector of indices in object ss;
- The next enclosing expression is length(...); the length method returns the length of its argument, which is the vector ss\$ix (the innermost expression);
- The next enclosing expression is ss\$ix[...], which converts the result of the expression length(ss\$ix) to a subscript and extracts that element from the vector ss\$ix.

The result is the array position of the maximum element. We could go one step further to get the actual value of this maximum, which is in the vector ss\$x:

```
> samp[ss$ix[length(ss$ix)]]
[1] 9.599777
```

but of course we could have gotten this result much more simply with the max method as max(ss\$x) or even max(samp).

4.6 Arrays and matrices

An *array* is simply a vector with an associated *dimension* attribute, to give its shape. *Vectors* in the mathematical sense are one-dimensional arrays in S; *matrices* are two-dimensional arrays; higher dimensions are possible.

For example, consider the sample confusion matrix of Congalton *et al.* [4], also used as an example by Skidmore [30] and Rossiter [24]:²²

		Reference Class			
		A	В	C	D
	Α	35	14	11	1
Mapped	В	4	11	3	0
Class	C	12	9	38	4
	D	2	5	12	2

This can be entered as a list in *row-major* order:

```
> cm <- c(35,14,11,1,4,11,3,0,12,9,38,4,2,5,12,2) > cm
```

²² This matrix is also used as an example in §6.1

```
[1] 35 14 11 1 4 11 3 0 12 9 38 4 2 5 12 2 > dim(cm)
```

Initially, the list has no dimensions; these may be added with the dim method:

```
> dim(cm) <- c(4, 4)
> cm
     [,1] [,2] [,3] [,4]
[1,]
       35
             4
                 12
                        5
[2,]
            11
                  9
       14
       11
            3
                 38
[3,]
                       12
             0
                   4
[4,]
        1
> dim(cm)
[1] 4 4
> attributes(cm)
$dim
[1] 4 4
> attr(cm, "dim")
[1] 4 4
```

The attributes method shows any object's attributes; in this case the object only has one, its dimension; this can also be read with the attr or dim method.

Note that the list was converted to a matrix in *column-major* order, following the usual mathematical convention that a matrix is made up of column vectors. The t (*transpose*) method must be used to specify row-major order:

```
> cm <- t(cm)
> cm
     [,1] [,2] [,3] [,4]
[1,]
       35
             14
                  11
                         1
[2,]
                   3
                         0
        4
             11
             9
                         4
[3,]
       12
                  38
[4,]
              5
                         2
        2
                  12
```

A new matrix can also be created with the matrix method, which in its simplest form fills a matrix of the specified dimensions (rows, columns) with the value of its first argument:

```
> (m <- matrix(0, 5, 3))
     [,1] [,2] [,3]
        0
              0
                    0
[2,]
        0
              0
                    0
                    0
[3,]
        0
              0
[4,]
              0
                    0
        0
              0
                    0
[5,]
        0
```

This value may also be a vector:

```
> (m <- matrix(1:15, 5, 3, byrow=T))
[,1] [,2] [,3]
```

```
[1,]
               2
                     3
         1
[2,]
         4
               5
                     6
         7
               8
                     9
[3,]
[4,]
        10
              11
                    12
[5,]
        13
              14
                    15
> (m <- matrix(1:5, 5, 3))</pre>
      [,1] [,2] [,3]
[1,]
         1
               1
                     1
[2,]
         2
               2
                     2
         3
               3
                     3
[3,]
[4,]
         4
               4
                     4
         5
                     5
[5,]
               5
```

In this last example the shorter vector 1:5 is *re-cycled* as many times as needed to match the dimensions of the matrix; in effect it fills each column with the same sequence.

A matrix element's rows and column are given by the row and col methods, which are also vectorized and so can be applied to an entire matrix:

```
> col(m)
      [,1] [,2] [,3]
[1,]
                     3
         1
               2
[2,]
         1
               2
                     3
[3,]
         1
               2
                     3
[4,]
         1
               2
                     3
[5,]
               2
                     3
```

The diag method applied to an existing matrix extracts its diagonal as a vector:

```
> (d <- diag(cm))
[1] 35 11 38 2</pre>
```

The diag method applied to a vector creates a square matrix with the vector on the diagonal:

```
(d <- diag(seq(1:4)))
     [,1] [,2] [,3] [,4]
[1,]
        1
              0
                    0
                          0
[2,]
        0
              2
                    0
                          0
[3,]
                          0
        0
              0
                    3
[4,]
        0
              0
                    0
```

And finally diag with a scalar argument creates an indentity matrix of the specified size:

Arithmetic operators such as * operate element-wise on matrices as on

any vector; if matrix multiplication is desired the %*% operator must be used:

```
> Cm*Cm
     [,1] [,2] [,3] [,4]
[1,] 1225
           196
               121
                       1
[2,]
      16
           121
                  9
                       0
[3,]
     144
            81 1444
                      16
[4,]
       4
            25
               144
> cm%*%cm
     [,1] [,2] [,3] [,4]
[1,] 1415
           748
               857
                      81
[2,]
           204
                191
     220
                      16
          629 1651
[3,]
     920
                     172
[4,] 238 201 517
> cm%*%c(1,2,3,4)
     [,1]
[1,]
     100
[2,]
       35
[3,]
     160
[4,]
       56
```

As the last example shows, %*% also multiplies matrices and vectors.

Matrix inversion

A matrix can be *inverted* with the solve method, usually with little accuracy loss; in the following example the round method is used to show that we recover an identity matrix:

```
> solve(cm)
             [,1]
                         [,2]
                                       [,3]
[1,] 0.034811530 -0.03680710 -0.004545455 -0.008314856
[2,] -0.007095344   0.09667406 -0.018181818   0.039911308
[3,] -0.020399113  0.02793792  0.072727273  -0.135254989
[4,] 0.105321508 -0.37250554 -0.386363636 1.220066519
> solve(cm)%*%cm
                            [,2]
              [,1]
[1,] 1.000000e+00 -4.683753e-17 -7.632783e-17 -1.387779e-17
[2,] -1.110223e-16 1.000000e+00 -2.220446e-16 -1.387779e-17
[3,] 1.665335e-16 1.110223e-16 1.000000e+00 5.551115e-17
[4,] -8.881784e-16 -1.332268e-15 -1.776357e-15 1.000000e+00
> round(solve(cm)%*%cm, 10)
     [,1] [,2] [,3] [,4]
[1,]
        1
             0
                  0
                       0
[2,]
        0
             1
                  0
                       0
[3,]
        0
             0
                  1
                       0
[4,]
             0
                  0
                       1
```

Solving linear equations The same solve method applied to a matrix ${\bf A}$ and column vector ${\bf b}$ solves the linear equation ${\bf b}={\bf A}{\bf x}$ for ${\bf x}$:

```
[3,] 3
[4,] 4
```

The apply method *applies* a function to the *margins* of a matrix, i.e. the rows (1) or columns (2). For example, to compute the row and column sums of the confusion matrix, use apply with the sum method as the function to be applied:

```
> (rsum <- apply(cm, 1, sum))
[1] 61 18 63 21
> (csum <- apply(cm, 2, sum))
[1] 53 39 64 7</pre>
```

These can be used, along with the diag method, to compute the producer's and user's classification accuracies, since diag(cm) gives the correctly-classified observations:

```
> (pa <- round(diag(cm)/csum, 2))
[1] 0.66 0.28 0.59 0.29
> (ua <- round(diag(cm)/rsum, 2))
[1] 0.57 0.61 0.60 0.10</pre>
```

There are also methods to compute the determinant (det), eigenvalues and eigenvectors (eigen), the singular value decomposition (svd), the QR decomposition (qr), and the Choleski factorization (chol); these use long-standing numerical codes from LINPACK, LAPACK, and EISPACK.

4.7 Data frames

The fundamental S data structure for statistical modelling is the *data frame*. This can be thought of as a matrix where the *rows* are *cases*, called *observations* by S (whether or not they were field observations), and the *columns* are the *variables*. In standard database terminology, these are *records* and *fields*, respectively. Rows are generally accessed by the row number (although they can have names), and columns by the variable *name* (although they can also be accessed by number). A data frame can also be considerd a *list* whose members are the fields; these can be accessed with the [[]] (list access) operator.

Sample data R comes with many example datasets (§3.12) organized as data frames; let's load one (trees) and examine its structure and several ways to access its components:

The help text tells us that this data set contains measurements of the girth (diameter in inches²³, measured at 4.5 ft²⁴ height), height (feet) and timber volume (cubic feet²⁵) in 31 felled black cherry trees. The data frame has 31 observations (rows, cases, records) each of which has three variables (columns, attributes, fields). Their names can be retrieved or changed by the names method. For example, to name the fields Var.1, Var.2 etc. we could use the paste method to build the names into a list and then assign this list to the names attribute of the data frame:

```
> (saved.names <- names(trees))
[1] "Girth" "Height" "Volume"
> (names(trees) <- paste("Var", 1:dim(trees)[2], sep="."))
[1] "Var.1" "Var.2" "Var.3''
> names(trees)[1] <- "Perimeter"
> names(trees)
[1] "Perimeter" "V.2" "V.3"
> (names(trees) <- saved.names)
[1] "Girth" "Height" "Volume"
> rm(saved.names)
```

Note in the paste method how the shorter vector "Var" was *re-cycled* to match the longer vector 1:dim(trees)[2]. This was just an example of how to name fields; at the end we restore the original names, which we had saved in a variable which, since we no longer need it, we remove from the workspace with the rm method.

The data frame can accessed various ways:

```
> # most common: by field name
> trees$Height
 [1] 70 65 63 72 81 83 66 75 80 75 79 76 76 69
[15] 75 74 85 86 71 64 78 80 74 72 77 81 82 80
[29] 80 80 87
> # the result is a vector, can select elements of it
> trees$Height[1:5]
[1] 70 65 63 72 81
> # but this is also a list element
 trees[[2]]
 [1] 70 65 63 72 81 83 66 75 80 75 79 76 76 69
[15] 75 74 85 86 71 64 78 80 74 72 77 81 82 80
[ 29] 80 80 87
> trees[[2]][1:5]
[1] 70 65 63 72 81
> # as a matrix, first by row....
> trees[1,]
  Girth Height Volume
    8.3
            70
                 10.3
> # ... then by column
> trees[,2]
> trees[[2]]
 [1] 70 65 63 72 81 83 66 75 80 75 79 76 76 69
[15] 75 74 85 86 71 64 78 80 74 72 77 81 82 80
     ^{23} 1 inch = 2.54 cm
     ^{24} 1 \, \text{ft} = 30.48 \, \text{cm}
     ^{25} 1 \text{ ft}^3 = 28.3168 \text{ dm}^3
```

```
[ 29] 80 80 87
> # get one element
> trees[1,2]
[1] 70
> trees[1,"Height"]
[1] 70
> trees[1,]$Height
[1] 70
```

The forms like \$Height use the \$ operator to select a named field within the frame. The forms like [1, 2] show that this is just a matrix with column names, leading to forms like trees[1,"Height"]. The forms like trees[1,]\$Height show that each row (observation, case) can be considered a list with named items. The forms like trees[[2]] show that the data frame is also a list whose elements can be accessed with the [[]] operator.

Attaching data frames to the search path To simplify access to named columns of data frames, S provides an attach method that makes the names visible in the outer namespace:

```
> attach(trees)
> Height[1:5]
[1] 70 65 63 72 81
```

Building a data frame S provides the data.frame method for creating data frames from smaller objects, usually vectors. As a simple example, suppose the number of trees in a plot has been measured at five plots in each of two transects on a regular spacing. We enter the x-coördinate as one list, the y-coördinate as another, and the number of trees in each plot as the third:

```
> x <- rep(seq(182,183, length=5), 2)*1000
> y \leftarrow rep(c(381000, 310300), 5)
> n.trees <- c(10, 12, 22, 4, 12, 15, 7, 18, 2, 16)
> (ds <- data.frame(x, y, n.trees))</pre>
               y n.trees
        Х
1 182000 381000
                       10
  182250 310300
                       12
   182500 381000
                       22
   182750 310300
                        4
   183000 381000
                       12
   182000 310300
                       15
   182250 381000
                        7
  182500 310300
                       18
9 182750 381000
                        2
10 183000 310300
                       16
```

Note the use of the rep method to repeat a sequence. Also note that an arithmetic expression (in this case * 1000) can be applied to an entire vector (in this case rep(seq(182,183, length=5), 2)).

In practice, this data frame would probably be prepared outside R and then imported, see §6.

Adding rows to a data frame The rbind ("row bind") method is used to add rows to a data frame, and to combine two data frames with the same structure. For example, to add one more trees to the data frame:

```
> (ds <- rbind(ds, c(183500, 381000, 15)))</pre>
               y n.trees
        Х
 182000 381000
                       10
  182250 310300
                       12
  182500 381000
                       22
3
  182750 310300
                       4
5
  183000 381000
                       12
  182000 310300
6
                       15
   182250 381000
                       7
  182500 310300
                       18
  182750 381000
                       2
10 183000 310300
                       16
11 183500 381000
                       15
```

This can also be accomplished by directly assigning to the next row:

```
> ds[12,] <- c(183400, 381200, 18)
> ds
              y n.trees
 182000 381000
  182250 310300
                      12
3
 182500 381000
                      22
4 182750 310300
5
 183000 381000
                      12
6 182000 310300
                      15
  182250 381000
7
                      7
8
  182500 310300
                      18
  182750 381000
                       2
10 183000 310300
                      16
11 183500 381000
                      12
12 183400 381200
                      18
```

Adding fields to a data frame A vector with the same number of rows as an existing data frame may be added to it with the cbind ("column bind") method. For example, we could compute a height-to-girth ratio for the trees (a measure of a tree's shape) and add it as a new field to the data frame; we illustrate this with the trees example dataset introduced in §4.7:

```
> attach(trees)
> HG.Ratio <- Height/Girth; str(HG.Ratio)
num [1:31] 8.43 7.56 7.16 6.86 7.57 ...
> trees <- cbind(trees, HG.Ratio); str(trees)
`data.frame': 31 obs. of 4 variables:
$ Girth : num 8.3 8.6 8.8 10.5 10.7 10.8 ...
$ Height : num 70 65 63 72 81 83 66 75 80 75 ...
$ Volume : num 10.3 10.3 10.2 16.4 18.8 19.7 ...</pre>
```

```
$ HG.Ratio: num 8.43 7.56 7.16 6.86 7.57 .. > rm(HG.Ratio)
```

Note that this new field is not visible in an attached frame; the frame must be detached (with the detach method) and re-attached:

```
> summary(HG.Ratio)
Error: Object "HG.Ratio" not found
> detach(trees); attach(trees)
> summary(HG.Ratio)
    Min. 1st Qu. Median Mean 3rd Qu. Max.
    4.22    4.70    6.00    5.99    6.84    8.43
```

Sorting a data frame This is most easily accomplished with the order method, naming the field(s) on which to sort, and then using the returned indices to extract rows of the data frame in sorted order:

```
> trees[order(trees$Height, trees$Girth),]
   Girth Height Volume
     8.8
             63
                  10.2
20 13.8
             64
                  24.9
2
     8.6
             65
                  10.3
4
   10.5
             72
                  16.4
24 16.0
             72
                  38.3
16 12.9
             74
                  22.2
23 14.5
             74
                  36.3
             86
                  27.4
18 13.3
                  77.0
31
   20.6
             87
```

Note that the trees are first sorted by height, then any ties in height are sorted by girth.

4.8 Factors

Some variables are *categorical*: they can take only a defined set of values. In S these are called *factors* and are of two types: *unordered* (nominal) and *ordered* (ordinal). An example of the first is a soil type, of the second soil structure grade, from "none" through "weak" to "strong" and "very strong"; there is a natural order in the second case but not in the first. Many analyses in R depend on factors being correctly identified; some such as table (§4.15) only work with categorical variables.

Factors are defined with the factor and ordered methods. They may be converted from existing character or numeric vectors with the as.factor and as.ordered method; these are often used after data import if the read.table or related methods could not correctly identify factors; see §6.2 for an example. The levels of an existing factor are extracted with the levels method.

For example, suppose we have given three tests to each of three students and we want to rank the students. We might enter the data frame as follows (see also $\S6.1$):

```
> student <- rep(1:3, 3)
> score <- c(9, 6.5, 8, 8, 7.5, 6, 9.5, 8, 7)
> tests <- data.frame(cbind(student, score))
> str(tests)
`data.frame': 9 obs. of 2 variables:
$ student: num 1 2 3 1 2 3 1 2 3
$ score : num 9 6.5 8 8 7.5 6 9.5 8 7
```

We have the data but the student is just listed by a number; the table method won't work and if we try to predict the score from the student using the 1m method (see §4.17) we get nonsense:

The problem is that the student is considered as a continuous variable when in fact it is a factor. We do much better if we make the appropriate conversion:

Factors require special care in statistical models; see §4.17.1.

4.9 Selecting subsets

We often need to examine subsets of our data, for example to perform a separate analysis for several strata defined by some factor, or to exclude outliers defined by some criterion.

Selecting known elements If we know the observation numbers, we simply name them as the first subscript, using the [] (select array elements) operator:

```
> trees[1:3,]
  Girth Height Volume
1  8.3   70  10.3
2  8.6   65  10.3
3  8.8   63  10.2
```

```
> trees[c(1, 3, 5),]
 Girth Height Volume
  8.3
           70
                10.3
   8.8
           63
                10.2
5 10.7
           81
                18.8
> trees[seq(1, 31, by=10),]
  Girth Height Volume
    8.3
            70
                 10.3
11 11.3
            79
                 24.2
21 14.0
            78
                 34.5
31 20.6
            87
                 77.0
```

A *negative* subscript in this syntax *excludes* the named rows and includes all the others:

```
> trees[-(1:27),]
    Girth Height Volume
28  17.9  80  58.3
29  18.0  80  51.5
30  18.0  80  51.0
31  20.6  87  77.0
```

Selecting with a logical expression The simplest way to select subsets is with a *logical expression* on the *row* subscript which gives the criterion. For example, in the trees example dataset introduced in §4.7, there is only one tree with volume greater than 58 cubic feet, and it is substantially larger; we can see these in order with the sort method:

```
> attach(trees)
> sort(Volume)
[1]    10.2    10.3    10.3    15.6    16.4    18.2    18.8    19.1    19.7
[11]    19.9    21.0    21.3    21.4    22.2    22.6    24.2    24.9    25.7
[21]    27.4    31.7    33.8    34.5    36.3    38.3    42.6    51.0    51.5
[31]    55.4    55.7    58.3    77.0
```

To analyze the data without this "unusual" tree, we use a logical expression to select rows (observations), here using the < (less than) *comparaison operator*, and then the [] (select array elements) operator to extract the array elements that are selected:

```
> tr <- trees[Volume < 60,]</pre>
```

Note that there is no condition for the second subscript, so all columns are selected.

To make a list of the observation numbers where a certain condition is met, use the which method:

```
> which(trees$Volume > 60)
[1] 31
> trees[which(trees$Volume > 60),]
    Girth Height Volume
31 20.6 87 77
```

Logical expressions may be combined with *logical operators* such as & (logical AND) and | (logical OR), and their truth sense inverted with! (logical NOT). For example, to select trees with volumes between 20 and 40 cubic feet:

```
> tr <- trees[Volume >=20 & Volume <= 40,]</pre>
```

Note that &, like S arithmetical operators, is *vectorized*, i.e. it operates on each pair of elements of the two logical vectors separately.

Parentheses should be used if you are unclear about operator precedence.

Another way to select elements is to make a *subset*, with the subset method:

```
> (tr.small <- subset(trees, Volume < 18))</pre>
  Girth Height Volume
   8.3
           70
                10.3
   8.6
            65
                 10.3
   8.8
            63
                10.2
4 10.5
            72
                 16.4
  11.0
            66
                 15.6
```

Selecting random elements of an array Random elements of a vector can be selected with the sample method:

```
> trees[sort(sample(1:dim(trees)[1], 5)), ]
  Girth Height Volume
13 11.4
            76
                 21.4
18 13.3
            86
                 27.4
22 14.2
            80
                 31.7
23 14.5
            74
                 36.3
26 17.3
            81
                 55.4
```

Each call to sample will give a different result.

By default sampling is *without* replacement, so the same element can not be selected more than once; for sampling *with* replacement use the replace=T optional argument.

In this example, the command dim(trees) uses the dim method to give the dimensions of the data frame (rows and columns); the first element of this two-element list is the number of rows: dim(trees)[1].

Splitting on a factor Another common operation is to split a dataset into several *strata* defined by some factor. For this, S provides the split method, which we illustrate with the iris dataset which has one factor, the species of Iris:

```
> data(iris); str(iris)
```

```
`data.frame': 150 obs. of 5 variables:
$ Sepal.Length: num 5.1 4.9 4.7 4.6 5 5.4 4.6 5 4.4 4.9 ...
$ Sepal.Width : num 3.5 3 3.2 3.1 3.6 3.9 3.4 3.4 2.9 3.1 ...
$ Petal.Width : num 0.2 0.2 0.2 0.2 0.4 0.3 0.2 0.2 0.1 ...
              : Factor w/ 3 levels "setosa", "versic..", ...: 1 1 ....
> attach(iris)
> ir.s <- split(iris, Species); str(ir.s)</pre>
List of 3
            :`data.frame': 50 obs. of 5 variables:
$ setosa
  ..$ Sepal.Length: num [1:50] 5.1 4.9 4.7 4.6 5 5.4 4.6 5 ...
 ..$ Sepal.Width : num [1:50] 3.5 3 3.2 3.1 3.6 3.9 3.4 3.4 ...
 ..$ Petal.Length: num [1:50] 1.4 1.4 1.3 1.5 1.4 1.7 1.4 ...
 ..$ Petal.Width : num [1:50] 0.2 0.2 0.2 0.2 0.2 0.4 0.3
                 : Factor w/ 3 levels "setosa", "versic..", ...: 1 1 ....
 $ versicolor:`data.frame': 50 obs. of 5 variables:
 ..$ Sepal.Length: num [1:50] 7 6.4 6.9 5.5 6.5 5.7 6.3 4.9 ...
 ..$ Sepal.Width : num [1:50] 3.2 3.2 3.1 2.3 2.8 2.8 3.3 2.4 ...
 ...$ Petal.Length: num [1:50] 4.7 4.5 4.9 4 4.6 4.5 4.7 3.3 ...
 ..$ Petal.Width : num [1:50] 1.4 1.5 1.5 1.3 1.5 1.3 1.6 1 ...
                : Factor w/ 3 levels "setosa", "versic..", ...: 2 2 ....
  ..$ Species
 $ virginica : `data.frame': 50 obs. of 5 variables:
  ..$ Sepal.Length: num [1:50] 6.3 5.8 7.1 6.3 6.5 7.6 4.9 7.3 ...
 ..$ Sepal.Width : num [1:50] 3.3 2.7 3 2.9 3 3 2.5 2.9 2.5 ...
 ..$ Petal.Length: num [1:50] 6 5.1 5.9 5.6 5.8 6.6 4.5 6.3
 ..$ Petal.Width : num [1:50] 2.5 1.9 2.1 1.8 2.2 2.1 1.7 1.8
                 : Factor w/ 3 levels "setosa", "versic..", ...: 3 3 ...
 ..$ Species
```

The split method builds a *list* of data frames named by the level of the factor on which the original data frame was split. Here the original 150 observations have been split into three lists of 50, one for each species. These can be accessed by name:

```
> summary(ir.s$setosa$Petal.Length)
  Min. 1st Qu. Median Mean 3rd Qu. Max.
  1.00  1.40  1.50  1.46  1.58  1.90
```

4.9.1 Simultaneous operations on subsets

We often want to apply some computation to all subsets of a data frame. For example, to compute the mean petal length of the iris data set for each species separately, we could first split the set as shown in the previous section (§4.9), compute each subset's mean, and join them in one vector. This can be accomplished in one step using the by method:

In this example, we applied the mean function to the Petal.Length field in the attached data frame, grouping the petal lengths by the Species categorical factor.

A function can be applied to several fields at the same time, and the results can be saved to the workspace:

```
> iris.m <- by(iris[,1:4], Species, mean)</pre>
> class(iris.m)
[1] "by"
> str(iris.m)
List of 3
             : Named num [1:4] 5.006 3.428 1.462 0.246
 $ setosa
  ..- attr(*, "names")= chr [1:4] "Sepal.Length" "Sepal.Width" ...
 $ versicolor: Named num [1:4] 5.94 2.77 4.26 1.33
 ..- attr(*, "names")= chr [1:4] "Sepal.Length" "Sepal.Width" ...
 $ virginica : Named num [1:4] 6.59 2.97 5.55 2.03
 ..- attr(*, "names")= chr [1:4] "Sepal.Length" "Sepal.Width" ...
 - attr(*, "dim")= int 3
- attr(*, "dimnames")=List of 1
  ..$ Species: chr [1:3] "setosa" "versicolor" "virginica"
 - attr(*, "call")= language by.data.frame(data = iris[, 1:4],
                                    INDICES = Species, FUN = mean)
 - attr(*, "class")= chr "by"
> iris.m$setosa
Sepal.Length Sepal.Width Petal.Length Petal.Width
                                 1.462
       5.006
                    3.428
                                                0.246
> iris.m$setosa[3]
Petal.Length
       1.462
> iris.m$setosa["Petal.Length"]
Petal.Length
       1.462
```

As this example shows, the result is one list for each level of the grouping factor (here, the *Iris* species). Each list is a vector with named elements (the dimnames attribute).

4.10 Rearranging data

As explained above (§4.7), the *data frame* is the object class on which most analysis is performed. Sometimes the same data must be arranged different ways into data frames, depending on what we consider the observations and columns.

A typical re-arrangement is *stacking* and its inverse, *unstacking*. In stacking, several variables are combined into one, coded by the original variable name; unstacking is the reverse.

For example, consider the data from a small plant growth experiment:

```
> data(PlantGrowth); str(PlantGrowth)
`data.frame': 30 obs. of 2 variables:
$ weight: num 4.17 5.58 5.18 6.11 4.5 4.61 5.17 4.53 ...
```

```
$ group : Factor w/ 3 levels "ctrl","trt1",..: 1 1 1 1 1 1 1 ...
```

There were two treatments and one control, and the weights are given in one column. If we want to find the maximum growth in the control group, we could select just the controls and then find the maximum:

```
> max(PlantGrowth$weight[PlantGrowth$group == "ctrl"])
[1] 6.11
```

But we could also *unstack* this two-column frame into a frame with three variables, one for each treatment, and then find the maximum of one (new) column; for this we use the unstack method:

```
> pg <- unstack(PlantGrowth, weight ~ group; str(pg)
`data.frame': 10 obs. of 3 variables:
$ ctrl: num   4.17 5.58 5.18 6.11 4.5 4.61 5.17 4.53 5.33 5.14
$ trt1: num   4.81 4.17 4.41 3.59 5.87 3.83 6.03 4.89 4.32 4.69
$ trt2: num   6.31 5.12 5.54 5.5 5.37 5.29 4.92 6.15 5.8 5.26
> max(pg$ctrl)
[1] 6.11
```

The names of the groups in the unstacked frame become the names of the variables in the stacked frame; the formula weight ~group told the unstack method that group was the column with the new column names.

This process also works in reverse, when we have a frame with several variables to make into one, we use the stack method:

```
> pg.stacked <- stack(pg); str(pg.stacked)
`data.frame': 30 obs. of 2 variables:
$ values: num 4.17 5.58 5.18 6.11 4.5 4.61 5.17 4.53 ...
$ ind : Factor w/ 3 levels "ctrl","trt1",..: 1 1 1 1 1 1 1 ...
> names(pg.stacked) <- c("weight", "group"); str(pg.stacked)
`data.frame': 30 obs. of 2 variables:
$ weight: num 4.17 5.58 5.18 6.11 4.5 4.61 5.17 4.53 ...
$ group : Factor w/ 3 levels "ctrl","trt1",..: 1 1 1 1 1 1 ...</pre>
```

The stacked frame has two columns with default names value (for the variables which were combined) and ind (for their names); these can be changed with the names method.

A more general method for data re-shaping is reshape.

4.11 Random numbers and simulation

R includes methods to evaluate a cumulative distribution function (CDF), the probability density function (PDF) and the quantiles, and to draw random samples, from a large number of distributions including the *uniform* (R name unif), *normal* (R name norm), *Student's t* (R name t), *binomial* (R name binom), *Poisson* (R name pois), and many others; see Chapter 8 of [20] for a complete list.

The names of the methods are built from two parts:

- 1. A *prefix* indicating the type of method: p for the CDF, d for the density, q for the quantile, and r for random samples;
- 2. The *R name* of the distribution, as listed above, e.g. norm for the normal distribution.

So the functions for the normal distribution are:

- p pnorm for the CDF;
- d dnorm for the density;
- q qnorm for the quantiles (inverse probability);
- r rnorm to draw random numbers.

For example, to find the proportion of people in a normally-distributed population with mean height 170 cm and standard deviation 15 cm shorter than 200 cm use pnorm:

```
> pnorm(200, 170, 15)
[1] 0.9772499
```

To plot the bell-shaped normal curve use dnorm:

```
> q <- seq(-3, 3, by=.05)
> plot(q, dnorm(q), type="1", xlab="z", ylab="Prob(z)")
```

To find which normal score corresponds to a list of critical Type I error probabilities use qnorm:

```
> alpha <- c(0.1, 0.05, 0.01, 0.001)
> qnorm(1-alpha/2)
[1] 1.644854 1.959964 2.575829 3.290527
```

Finally, to simulate sampling ten individuals from a normally-distributed population with mean height 170 cm and standard deviation 15 cm, with a measurement precision of 1 cm, use rnorm draw the sample and then round the results to the nearest integer:

```
> sort(round(rnorm(10, 170, 15)))
[1] 147 159 166 169 169 174 176 180 183 185
```

Each time this command is issued it will give different results, because the sample is *random*:

```
> sort(round(rnorm(10, 170, 15)))
[1] 155 167 170 177 181 182 185 186 188 199
```

To start a simulation at the same point (e.g. for testing) use the set.seed method:

```
> set.seed(61921)
> sort(round(rnorm(10, 170, 15)))
[1] 129 157 157 166 168 170 173 175 185 193
> set.seed(61921)
> sort(round(rnorm(10, 170, 15)))
[1] 129 157 157 166 168 170 173 175 185 193
```

Now the results are the same every time.

4.12 Character strings

R can work with *character vectors*, also known as *strings*. These are often used in graphics as labels, titles, and explanatory text. A string is created by the " *quote* operator:

```
> (label <- "A good graph")
[1] "A good graph"</pre>
```

Strings can be built from smaller pieces with the paste method; parts can be extracted or replaced with the substring method; strings can be split into pieces with the strsplit method:

```
> paste(label, ":", 15, "x", 20, "cm")
[1] "A nice graph : 15 x 20 cm"
> (labels <- paste("B", 1:8, sep=""))
[1] "B1" "B2" "B3" "B4" "B5" "B6" "B7" "B8"
> substring(label, 1, 4)
[1] "A go"
> substring(label, 3) <- "nice"; label</pre>
[1] "A nice graph"
> strsplit(label, " ")
[[1]]
[1] "A"
             "nice" "graph'
> unlist(strsplit(label, ""))
            "nice" "graph"
[1] "A"
> unlist(strsplit(label, " "))[3]
[1] "graph
```

Note the use of the unlist method to convert the list (of one element) returned by strsplit into a vector.

Numbers or factors can be converted to strings with the as.character method; however this conversion is performed automatically by many methods, so an explicit conversion is rarely needed.

4.13 Objects and classes

S is an *object-oriented* computer language: everything in S (including variables, results of expressions, results of statistical models, and functions)

is an *object*, each with a *class*, which says what the object is and also controls the way in which it may be manipulated. The class of an object may be inspected with the class method:

```
> class(lm)
[1] "function"
> class(letters)
[1] "character"
> class(seq(1:10))
[1] "integer"
> class(seq(1,10, by=.01))
[1] "numeric"
> class(diag(10))
[1] "matrix"
> class(iris)
[1] "data.frame"
> class(iris$Petal.Length)
[1] "numeric"
> class(iris$Species)
[1] "factor"
> class(iris$Petal.Length > 2)
[1] "logical"
> class(lm(iris$Petal.Width ~ iris$Petal.Length))
[1] "lm''
> class(hist(iris$Petal.Width))
[1] "histogram"
> class(table(iris$Species))
[1] "table"
```

The letters built-in constant in this example is a convenient way to get the 26 lower-case Roman letters; for upper-case use LETTERS.

As the last three examples show, many S methods create their own classes. These then can be used by *generic* methods such as summary to determine appropriate behaviour:

```
> summary(iris$Petal.Length)
                        Mean 3rd Qu.
  Min. 1st Qu. Median
                                         Max.
   1.00
          1.60
                4.35
                          3.76
                               5.10
                                         6.90
> summary(iris$Species)
    setosa versicolor virginica
       50
                             50
                 50
> summary(lm(iris$Petal.Width ~ iris$Petal.Length))
lm(formula = iris$Petal.Width ~ iris$Petal.Length)
Residuals:
  Min
          1Q Median
                        30
                              Max
-0.565 -0.124 -0.019 0.133 0.643
Coefficients:
                 Estimate Std. Error t value Pr(>|t|)
(Intercept)
                 -0.36308 0.03976 -9.13 4.7e-16
iris$Petal.Length 0.41576
                             0.00958
                                      43.39 < 2e-16
```

```
Residual standard error: 0.206 on 148 degrees of freedom Multiple R-Squared: 0.927, Adjusted R-squared: 0.927 F-statistic: 1.88e+03 on 1 and 148 DF, p-value: <2e-16 > summary(table(iris$Species)) Number of cases in table: 150 Number of factors: 1
```

S has methods for testing if an object is in a specific class or mode, and for converting modes or classes, as long as such a conversion makes sense. These have the form is. (test) or as. (convert), followed by the class name. For example:

The is.factor and is.numeric class test methods return a logical value (TRUE or FALSE) depending on the class their argument. The as.factor class conversion method determined the unique values of petal length (22) and then coded each observation; this is not too useful here; in practice you would use the cut method. The as.numeric conversion method extracts the *level number* of the factor for each object; this can be useful if we want to give a numeric argument derived from the factor

4.13.1 The S3 and S4 class systems

S has two class systems, referred to as *S3* (old-style) and *S4* (new-style). Most R methods still use S3 classes, as presented in the previous section, but most new and rewritten packages use the more powerful and modern S4 classes. The difference between the two systems is readily apparent in the output of both the class and str methods.

A good example of S4 classes is the class structure of the sp spatial statistics package [18]:

```
> library(sp)
> data(meuse)
> class(meuse)
[1] "data.frame"
> str(meuse)
`data.frame': 155 obs. of 14 variables:
$ x : num 181072 181025 181165 181298 181307 ...
```

```
$ y : num 333611 333558 333537 333484 333330 ...
$ cadmium: num 11.7 8.6 6.5 2.6 2.8 3 3.2 2.8 2.4 1.6 ...
$ dist.m : num 50 30 150 270 380 470 240 120 240 420 ...
```

The sample data meuse is imported as an S3 class, namely a data.frame. Notice that the coördinates of each point are listed as fields. However, sp has defined some S4 classes to make the spatial nature of the data explicit. It also provides a coordinates method to set the spatial coördinates and thereby create explict spatial data:

```
> coordinates(meuse) <- ~ x + y
     # alternate command format: coordinates(meuse) <- c("x", "y")</pre>
> class(meuse)
[1] "SpatialPointsDataFrame"
attr(,"package")
[1] "sp"
> str(meuse)
Formal class 'SpatialPointsDataFrame' [package "sp"] with 5 slots
  ..@ data :Formal class 'AttributeList' [package "sp"] with 1 slots
  .. .. ..@ att:List of 12
  ..... scadmium: num [1:155] 11.7 8.6 6.5 2.6 2.8 3 3.2 2.8 2.4 1.6 ...
  .....$ dist.m : num [1:155] 50 30 150 270 380 470 240 120 240 420 ...
  ..@ coords.nrs : int [1:2] 1 2
  ..@ coords : num [1:155, 1:2] 181072 181025 181165 181298 181307 ...
  .. ..- attr(*, "dimnames")=List of 2
  .. .. ..$ : NULL
  .. .. ..$ : chr [1:2] "x" "v"
                 : num [1:2, 1:2] 178605 329714 181390 333611
  ....- attr(*, "dimnames")=List of 2
  .. .. ..$ : chr [1:2] "x" "y"
  .. .. ..$ : chr [1:2] "min" "max"
  ..@ proj4string:Formal class 'CRS' [package "sp"] with 1 slots
  .. .. ..@ projargs: chr NA
```

The object meuse has been *promoted* to an S4 class SpatialPointsDataFrame, which is shown as being a *formal class* defined by sp. The S4 class has named *slots*, marked by the @ sign in the output of str; these can also be listed with the slotNames method:

The contents of these slots are explained in the help for the S4 class:

```
> ?"SpatialPointsDataFrame-class"
```

Each slot is either a primitive S object (e.g. slot bbox which is a matrix) or another S4 class (e.g. slot data which is an object of class AttributeList also defined by the sp package):

```
> class(meuse@bbox)
[1] "matrix"
```

```
> class(meuse@data)
[1] "AttributeList"
attr(,"package")
[1] "sp"
```

Slots may be accessed directly with the @ operator, just as fields in data frames are accessed with the \$ operator. For example, to extract the bounding box (limiting coördinates) of this spatial data set:

However, it is better practice to use *access methods*:

```
> bbox(meuse)
    min    max
x 178605 181390
y 329714 333611
```

Each S4 class has a set of *methods* that apply to it; bbox is an example that applies not only to objects of class SpatialPointsDataFrame, but to objects of the generalised class from which class SpatialPointsDataFrame is specialised, namely class SpatialPoints and class Spatial.

To determine the methods that can apply to a class, review the help, using the class?<class name> syntax:

```
class?SpatialPointsDataFrameclass?SpatialPointsclass?Spatial
```

As this example shows, classes may be organised in an *inheritance structure*, so that the behaviour of a more *generalised* class is automatically inherited by a more *specialised* class; these are said to *extend* the base class.

For example class SpatialPointsDataFrame extends class SpatialPoints, which in turn extends the base class Spatial. These have appropriate slots and methods:

Spatial Only has a bounding box (slot bbox and projection (slot proj4string); no spatial objects as such;

SpatialPoints Also has coördinates (slot coords) of each point; at this level of hierarchy there are also class SpatialLines and class SpatialPolygons;

SpatialPointsDataFrame Also has attributes (slot data) for each point;

SpatialGridDataFrame Points are on a regular grid, inherited from class GridTopology as well as class SpatialPointsDataFrame.

The real power of this approach is seen when generic methods are applied to objects of the various classes; each class then specialises the generic method appropriately. For example, the spplot plotting method gives a different kind of plot for each class that inherits from class Spatial; we can see this with the showMethods method:

```
> showMethods(spplot)
Function "spplot":
obj = "SpatialPixelsDataFrame"
obj = "SpatialGridDataFrame"
obj = "SpatialPolygonsDataFrame"
obj = "SpatialLinesDataFrame"
obj = "SpatialPointsDataFrame"
```

For more on the S4 class system, see Chambers [1, Ch. 7 & 8] and Venables & Ripley [32, Ch. 5].

4.14 Descriptive statistics

Numeric vectors can be described by a set of methods with self-evident names, e.g. min, max, median, mean, length:

```
> data(trees); attach(trees)
> min(Volume); max(Volume); median(Volume);
+ mean(Volume); length(Volume)
[1] 10.2
[1] 77
[1] 24.2
[1] 30.17097
[1] 31
```

Another descriptive method is quantile:

```
> quantile(Volume)
    0% 25% 50% 75% 100%
10.2 19.4 24.2 37.3 77.0
> quantile(Volume, .1)
    10%
15.6
> quantile(Volume, seq(0,1,by=.1))
    0% 10% 20% 30% 40% 50% 60% 70% 80% 90% 100%
10.2 15.6 18.8 19.9 21.4 24.2 27.4 34.5 42.6 55.4 77.0
```

The summary method applied to data frames combines several of these descriptive methods:

Some summary methods are *vectorized* and can be applied to an entire data frame:

```
> mean(trees)
  Girth Height
               Volume
13.24839 76.00000 30.17097
> summary(trees)
                          Volume
   Girth
                Height
Min.: 8.30 Min.: 63 Min.: 10.20
Median :12.90 Median :76 Median :24.20
Mean :13.25 Mean :76 Mean :30.17
3rd Qu.:15.25
             3rd Qu.:80 3rd Qu.:37.30
Max. :20.60
             Max. :87 Max. :77.00
```

Others are not, but can be *applied* to margins of a matrix or data frame with the apply method:

```
> apply(trees, 2, median)
Girth Height Volume
12.9 76.0 24.2
```

The margin is specified in the second argument: 1 for rows, 2 for columns (fields in the case of data frames).

4.15 Classification tables

For data items that are classified by one or more *factors*, the table method counts the number of observations at each factor level or combination of levels. We illustrate this with the meuse dataset included with the sp package. This dataset includes four factors:

```
> library(sp); data(meuse); str(meuse)
 data.frame': 155 obs. of 14 variables:
 $ ffreq : Factor w/ 3 levels "1","2","3": 1 1 1 1 1 1 1 1 1 1 ...
 $ soil : Factor w/ 3 levels "1","2","3": 1 1 1 2 2 2 2 1 1 2 ...
$ lime : Factor w/ 2 levels "0","1": 2 2 2 1 1 1 1 1 1 ...
 $ landuse: Factor w/ 15 levels "Aa", "Ab", "Ag", ...: 4 4 4 11 4 11
> attach(meuse)
> table(ffreq)
ffrea
 1 2
84 48 23
> round(100*table(ffreq)/length(ffreq), 1)
ffreq
   1
         2
54.2 31.0 14.8
> table(ffreq, landuse)
     landuse
ffreq Aa Ab Ag Ah Am B Bw DEN Fh Fw Ga SPO STA Tv W
    1 \quad 0 \quad 8 \quad 5 \quad 19 \quad 6 \quad 3 \quad 3 \quad \quad 0 \quad 1 \quad 5 \quad 3 \quad \quad 0 \quad \quad 0 \quad 0 \quad 30
     2 1 0 0 14 11 0 1
                                   1 0 4 0
                                                  1
                                                        2 1 12
        1 0 0 6 5 0 2
                                   0 0 1 0
```

The last example is the *cross-classification* or *contingency table* showing which land uses are associated with which flood frequency classes.

The χ^2 test for conditional independence may be performed with the chisq.test method:

```
> chisq.test(ffreq, lime)
Pearson's Chi-squared test

data: ffreq and lime
X-squared = 26.81, df = 2, p-value = 1.508e-06
```

Both the χ^2 statistic and the probability that a value this large could occur by chance in the null hypothesis of no association is true (the "p-value") are given; the second is from the χ^2 table with the appropriate degrees of freedom ("df"). Here it is highly unlikely, meaning the flood frequency and liming are not independent factors.

4.16 Sets

S has several commands for working with lists (including vectors) as *sets*, i.e. a collection of elements; these include the is.element, union, intersect, setdiff, setequal methods. See the on-line help for details and example(union) for a demonstration.

The unique method removes duplicate elements from a list; the duplicated method returns the indices of the duplicate elements in the original list.

4.17 Statistical models in S

Statistical models in S are specified in *symbolic* form with *model formulae*. These formulae are arguments to many statistical methods, most notably the lm (linear models) and glm (generalised linear models) methods, but also in base graphics (§5.1) methods such as plot and boxplot and trellis graphics (§5.2) methods such as levelplot.

The simplest form is where a (mathematically) *dependent* variable is (mathematically) explained by one (mathematically) *independent* variable; like all model formulae this uses the ~ *formula operator* to separate the left (dependent) from the right (independent) sides of the expression:

This is to be read like a mathematical function, where the left-hand side is the result ("dependent") and the right-hand side is the expression ("independent"). In other words, a formula is read as:

- · a response variable (left-hand side) ...
- · ...is *explained* by (the ~ symbol) ...
- · ... a *formula* including one or more *predictor* variables

In this example, the tree volume is to be explained as a linear function of its height; this is just a first-order linear regression, with the best-fit least-squares line y = -87.12 + 1.54x: for every foot increase in height, the volume increases by 1.54 ft³; also, a zero-height tree would have a negative volume²⁶.

If the data frame has been attached, this can be written more simply:

```
> attach(trees)
> model <- lm(Volume ~ Height)</pre>
```

but even if not, the variable names can be referred to a frame with the data= named argument:

```
> model <- lm(Volume ~ Height, data=trees)</pre>
```

Additive effects More complicated models include *additive effects*, using the + formula operator:

```
> model <- lm(Volume ~ Height + Girth, data=trees)</pre>
```

Note this is *not* an arithmetic addition, but rather a special use in the model notation. Here the tree volume is explained by by both its height and girth, considered as independent predictors.

Interactions The : formula operator is used to indicate *interactions*; usually these are used in addition to additive terms:

```
> model <- lm(Volume ~ Height + Girth + Height:Girth, data=trees)</pre>
```

Here the tree volume is explained by both its height and girth, as well as their interaction, i.e. that the effect of girth is different at different heights.

The * formula operator is shorthand for all linear terms and interactions of the named independent variables, so that the previous example could have been more simply written as:

²⁶ Nicely illustrating the risks of extrapolating outside the range of calibration; this data set only has trees from 63 to 87 feet tall, so the fitted relation says nothing about shorter trees

```
> model <- lm(Volume ~ Height * Girth, data=trees)</pre>
```

The ^ formula operator is used to indicate predictor crossing to the specified degree:

```
> model <- lm(Volume ~ (Height + Girth)^2, data=trees)</pre>
```

Here the ^2 expands to all interactions between the named predictors, since there are only two; this is equivlent to Height + Girth + Height:Girth, which in this two-predictor case is also the same as Height * Girth.

Removing terms Sometimes it is convenient to specify a model and then remove a term from it with the – formula operator. As a somewhat artificial example, to model tree volume by only tree girth and its interaction with height:

```
> model <- lm(Volume ~ Girth * Girth - Height, data=trees)

This is equivalent to:
> model <- lm(Volume ~ Girth + Girth:Height, data=trees)</pre>
```

The – formula operator is often used to remove the intercept; see below.

Nested models The / operator is used to specify that the second-named predictor is *nested* within the first-named predictor, i.e. levels of the nested predictor are not independent factors. Nested models are often used in designed experiments such as split-plot designs or replicated measurements within an experimental unit. This is also used for the analysis of covariance (ANCOVA), where the covariates are nested within the treatment; in this case the intercept should be removed (see next ¶).

No intercept The intercept term (e.g. the mean) is implicit in model formulas. For regression through the origin, it must be explicitly removed with the – formula operator, in this case the implied intercept, with the expression –1. Or, the origin can be named explicitly with the + formula operator, with the expression +0. For example, it's certainly true that a tree with no girth has no height, so if we want to force the regression of height on girth to go through (0,0):

```
> model <- lm(Height ~ Girth - 1, data=trees)
> model <- lm(Height ~ 0 + Girth, data=trees)</pre>
```

Although, in the range of timber trees, this may give a poorer predictive relation than allowing a (physically impossible) intercept.

Arithmetic operations in formulas Since the characters +, *, ^, and / have special meaning in formulas, they must be "quoted" with the I operator if they are to interpreted as arithmetic operators. For example, to model tree volume from the height-to-girth ratio:

```
> model <- lm(Volume ~ I(Height / Girth), data=trees)</pre>
```

To model volume as the square of girth:

```
> model <- lm(Volume ~ I(Girth^2), data=trees)</pre>
```

This is only needed if there is a danger of mis-interpretation; most methods can be used directly in formulas, e.g. the log method to compute natural logarithms. For example, to fit a log-log regression of tree height by width:

```
> model <- lm( log(Height) ~ log(Girth) )</pre>
```

For further description of model formulae, see the help topic:

> ?formula

The design matrix For full control of linear modelling, R offers the ability to extract or build *design matrices* of linear models; this is discussed in most regression texts, for example Christensen [2].

The design matrix of a model is extracted with the model.matrix method:

This matrix contains the values of the predictor variables for each observation. This provides a good check on your understanding of the model structure. The matrix can be used to directly compute the least-squares linear solution:

$$\beta = (X'X)^{-1}X'Y$$

using the t (matrix transpose) and solve (matrix inversion) method, and the %*% (matrix multiplication) operator. For example, to directly compute the regression coefficients for the model of tree volume predicted by height and girth in the trees dataset:

```
> Y <- trees$Volume
> ( beta <- solve( t(X) %*% X ) %*% t(X) %*% Y )</pre>
                 [,1]
(Intercept) -57.98766
Height
              0.33925
Girth
              4.70816
> # check this is the same result as from lm()
> lm(trees$Volume ~ trees$Height + trees$Girth)
Coefficients:
 (Intercept) trees$Height
                             trees$Girth
     -57.988
                     0 339
                                    4 708
```

The direct computation may be numerically unstable and is certainly slow; lm uses more sophisticated numerical methods.

4.17.1 Models with categorical predictors

The lm and glm methods are also used for models with categorical predictors and for mixed models, as well as for models using only continuous predictors. The categorical variables must be ordered or unordered S *factors*; this can be checked with the is.factor method or examined directly with the str method.

Factors are included in the design matrix as *contrasts* which divide the observations according to the classifying factors. This is quite a technical subject, treated thoroughly in standard linear modelling texts such as those by Venables & Ripley [33], Fox [10], Christensen [2] and Draper & Smith [8]. The practical importance of contrasts is mainly the interpretation of the results that is possible with a given contrast, and secondly in the computational stability.

One of R's environment options is the default contrast type for unordered and ordered factors; these can be viewed and changed with the options method. Contrasts for specific factors can be viewed and set with the contrasts method, using the contr.helmert, contr.poly, contr.sum, and contr.treatment methods to build contrast matrices.

Polynomial contrasts assume equal feature-space distance between levels of the ordered predictor; this may not be justified and so you may want to change the contrast type.

For example, the meuse soil pollution dataset includes a factor for flooding frequency; this is an unordered factor but the three levels are naturally ordered from least to most flooding. So we might want to change the data type.

```
> data(meuse)
> str(meuse$ffreq)
 Factor w/ 3 levels "1", "2", "3": 1 1 1 1 1 1 1 ...
> contrasts(meuse$ffreq)
  2 3
1 0 0
2 1 0
3 0 1
> lm(log(meuse$lead) ~ meuse$ffreq))
Coefficients:
(Intercept)
                  ffreq2
                                ffreq3
      5.106
                  -0.666
                               -0.626
> meuse$ffreg <- as.ordered(meuse$ffreg)</pre>
> str(meuse$ffrea)
 Ord.factor w/ 3 levels "1"<"2"<"3": 1 1 1 1 1 1 1 1 1 1 ...
> contrasts(meuse$ffreq)
           .L
                     .Q
1 -7.0711e-01 0.40825
2 -9.0738e-17 -0.81650
3 7.0711e-01 0.40825
> lm(log(meuse$lead) ~ meuse$ffreq))
Coefficients:
  (Intercept) meuse$ffreq.L meuse$ffreq.Q
        4.675
                      -0.443
                                       0.288
```

The unordered factor has treatments contrasts (sometimes called "dummy variables") whereas the ordered factor has orthogonal polynomial contrasts. These result in different fitted coefficients.

4.17.2 Analysis of Variance (ANOVA)

The results of linear models can be expressed in the traditional language of ANOVA (as found in many textbooks) with the aov method; this calls lm and formats its results in a traditional ANOVA table:

Two models on the same dataset may be compared with the anova method; this is one way to test if the more complicated model is significantly better than the simpler one:

```
> model.1 <- aov(Volume ~ Height + Girth, data=trees)
> model.2 <- aov(Volume ~ Height * Girth, data=trees)
> anova(model.1, model.2)
Analysis of Variance Table

Model 1: Volume ~ Height + Girth
Model 2: Volume ~ Height * Girth
```

In this case the interaction term of the more complicated model is highly significant.

4.18 Model output

The result of a lm (linear models) method is a complicated data structure with detailed information about the model, how it was fitted, and its results. It can be viewed directly with the str method, but it is better to access the model with a set of *extractor* methods: coefficients to extract a list with the model coefficients, fitted to extract a vector of the fitted values (what the model predicts for each observation), residuals to extract a vector of the residuals at each observation, and formula to extract the model formula:

```
> model <- lm(Volume ~ Height * Girth, data=trees)</pre>
> coefficients(model)
 (Intercept)
                Height
                             Girth Height:Girth
   69.39632
               -1.29708
                          -5.85585
                                      0.13465
> fitted(model)
     1
                   3
                          4
8.2311 9.9974 10.8010 16.3186 18.3800 ...
> residuals(model)
               2
                        3
      1
> formula(model)
Volume ~ Height * Girth
```

The results are best reviewed with the summary generic method, which for linear models is specialized into summary.lm:

```
> summary(model)
Call:
lm(formula = Volume ~ Height * Girth, data = trees)
Residuals:
  Min
          1Q Median
                         3Q
                              Max
-6.582 -1.067 0.303 1.564 4.665
Coefficients:
            Estimate Std. Error t value Pr(>|t|)
                        23.8358
                                   2.91 0.00713
(Intercept)
             69.3963
Height
              -1.2971
                         0.3098
                                  -4.19 0.00027
Girth
              -5.8558
                         1.9213
                                  -3.05
                                         0.00511
                         0.0244
Height:Girth 0.1347
                                    5.52 7.5e-06
Residual standard error: 2.71 on 27 degrees of freedom
Multiple R-Squared: 0.976, Adjusted R-squared: 0.973
F-statistic: 359 on 3 and 27 DF, p-value: <2e-16
```

This provides the most important information about the model; for more insight consult textbooks which explain linear modelling, e.g. Venables & Ripley [33], Fox [10], Christensen [2] or Draper & Smith [8]:

- The *model formula* with which 1m was called;
- · A summary of the *residuals*; by definition the mean is zero so is not reported;
- · The *model coefficients* (first column);
- The standard error associated with each coefficient (second column);
 these can be used to construct confidence intervals;
- The *significance level* of each coefficient (third column); this is the probability rejecting the *null hypothesis* for the listed coefficient would be a mistake;
- The *residual standard error*, which is defined as the square root of the estimated variance of the random error: $\sigma^2 = (1/(n-p)) * \sum (r_i^2)$ where r_i is one of the n residuals and p is the number of coefficients.
- The *coefficient of determination* R^2 , both the unadjusted fraction of variance explained by the model $R^2 = 1$ (Residual SS/Total SS) and the coefficient adjusted for the number of parameters in the model, $1 [(n-1)/(n-p) * (1-R^2)]$.

The AIC (Akaike's An Information Criterion) method is often used to compare models; the lower AIC is better:

```
> AIC(lm(Volume ~ Height * Girth))
[1] 155.47
> AIC(lm(Volume ~ Height + Girth))
[1] 176.91
> AIC(lm(Volume ~ Girth))
[1] 181.64
> AIC(lm(Volume ~ 1))
[1] 264.53
```

In this example the successively more complicated models have lower AIC, i.e. provide more information.

4.18.1 Model diagnostics

The model summary (§4.18) shows the overall fit of the model and a summary of the residuals, but gives little insight into difficulties with the model (e.g. non-linearity, heteroscedascity of the residuals). A graphical presentation of some common diagnostic plots is given by the plot method applied to the model object:

```
> model <- lm(Volume ~ Height * Girth, data=trees)
> plot(model)
```

This shows four plots: (1) residuals vs. fitted; (2) normal QQ plot of the residuals; (3) scale vs. location of residuals; (4) residuals vs. leverage.

Many other diagnostics are available. There are several methods to directly access these from the model itself: dfbetas, dffits, covratio, cooks.distance and hatvalues; methods rstandard and rstudent return the standardized and Studentized residuals, respectively. These diagnostic measures are explained in regression texts [e.g. 8].

For example, to plot the "hat" values (leverage) for each point, with the number of the most influential observations:

```
> h <- hatvalues(model)
> plot(h, type="h")
> text(h, ifelse(h > 3*mean(h), seq(1:length(h)),""), pos=2)
```

A direct way to access diagnostics is with the influence.measures method applied to the fitted model:

```
> infl <- influence.measures(model)
> str(infl)
List of 3
$ infmat: num [1:31, 1:8]  0.23213  0.06511 -0.15754  0.00173 -0.02461 ...
    ... attr(*, "dimnames")=List of 2
    ....$ : chr [1:31] "1" "2" "3" "4" ...
    ....$ : chr [1:8] "dfb.1_" "dfb.Hght" "dfb.Grth" "dfb.Hg:G" ...
$ is.inf: logi [1:31, 1:8] FALSE FALS
```

The key field here is is.inf, which specifies which observations were especially influential in the fit, using eight different measures of influence, which are listed as attributes of this field.

```
> attr(infl$infmat, "dimnames")[[2]]
[1] "dfb.1_"    "dfb.Hght" "dfb.Grth" "dfb.Hg:G" "dffit"    "cov.r"
[7] "cook.d"    "hat"
```

The most common use here is to list the observations for which any of the influence measures were excessive:

```
> infl$is.inf[ which(apply(infl$is.inf, 1, any)) , ]
  dfb.1_ dfb.Hght dfb.Grth dfb.Hg:G dffit cov.r cook.d
   FALSE
            FALSE
                     FALSE
                              FALSE FALSE TRUE FALSE FALSE
3
   FALSE
            FALSE
                     FALSE
                              FALSE FALSE TRUE FALSE FALSE
                     FALSE
18 FALSE
            FALSE
                              FALSE TRUE
                                          TRUE FALSE FALSE
20 FALSE
31 FALSE
                              FALSE FALSE
            FALSE
                     FALSE
                                          TRUE FALSE FALSE
                     FALSE
                              FALSE FALSE TRUE FALSE TRUE
            FALSE
```

This example illustrates the use of the which method to return the indices in a vector where a logical condition is true, and the any method to perform a logical *or* on a set of logical vectors, in this case the eight diagnostics. In this example, observation 31 has a high leverage, 18 a high DFFITS value, and all five high COVRATIO.

4.18.2 Model-based prediction

The fitted method only gives values for the observations; often we want to predict at other values. For this the predict generic method is used; in the case of linear models this specialises to the predict. Im method. The first argument is the fitted model and the second is a *data frame* in which to look for variables with which to predict; these must have the same names as in the model formula. Both confidence and prediction intervals may be requested, with a user-specified confidence level.

For example, to predict tree volumes for all combinations of heights (in 10 foot increments) and girths (in 5 inch radius increments)²⁷, along with the 99% confidence intervals of this prediction:

```
> model <- lm(Volume ~ Height * Girth, data=trees)</pre>
> new.data <- data.frame(expand.grid(Height = seq(50, 100, by=10),</pre>
     Girth = seq(5, 25, by=5))
> pred <- predict(model, new.data, interval="prediction",
             level=0.99)
> # add the predictor values for easy interpretation
> pred <- cbind(new.data, pred)</pre>
> str(pred)
data.frame': 30 obs. of 5 variables:
 $ Height: num 50 60 70 80 90 100 50 60 70 80 ...
 $ Girth : num 5 5 5 5 5 5 10 10 10 10 ...
                8.93
                       2.69 -3.55 -9.79 -16.03 ...
 $ fit
        : num
                 -7.37 -9.37 -12.74 -18.89 -27.88 ...
 $ lwr
         : num
        : num 25.222 14.743 5.639 -0.685 -4.167 ...
 $ upr
> # fits for trees 50 feet tall
> pred[pred$Height==50,]
       fit
               lwr
                      upr Height Girth
    8.9265 -7.3694 25.222
                              50
7 13.3109 3.0322 23.590
                              50
                                    10
13 17.6952 5.7180 29.672
                              50
                                    15
19 22.0796 2.6126 41.547
                              50
                                    20
25 26.4639 -2.0348 54.963
                              50
                                    25
```

4.19 Advanced statistical modelling

The 1m method is the workhorse of modelling in S, because of the importance of linear models and its versatility. However, R has other interesting methods, including g1m for *generalised* linear models, r1m for *robust* fitting of linear models, n1s for *non-linear* least squares fitting. The 1m method itself can use *weighted* least squares if the weights are specified

²⁷ Some of these combinations would result in strange looking trees!

as an optional argument.

Stepwise regression is a dangerous procedure when applied blindly; the step method can be used to select the best model, based on AIC, using forward or backward selection and a user-specified stopping and starting points.

Principal components of multivariate matrices are computed by the prcomp method; the results can be visualised with the biplot and screeplot methods.

Bootstrapping methods are provided in the boot package.

There are many other modelling methods; see §10.3 for some ideas on how to find the one you want. Especially recommended is the advanced text of Venables & Ripley [33] which has chapters on many sophisticated methods, all with theory, references, and S code.

4.20 Missing values

A common problem in a statistical dataset is that not all variables are recorded for all records. R uses a special *missing value* value for all data types, represented as NA, which stands for 'not available'. Within R, it may be assigned to a variable.

For example, suppose the volume of the first tree in the trees dataset is unknown:

```
> trees$Volume[1] <- NA</pre>
> str(trees)
`data.frame': 31 obs. of 3 variables:
 $ Girth : num 8.3 8.6 8.8 10.5 10.7 10.8 11 11
 $ Height: num 70 65 63 72 81 83 66 75 80 75 ...
 $ Volume: num NA 10.3 10.2 16.4 18.8 19.7 15.6
> summary(trees$Volume)
   Min. 1st Qu. Median
                           Mean 3rd Qu.
                                           Max.
                                                    NA's
   10.2
           19.8
                   24.5
                           30.8
                                   37.8
                                            77.0
                                                     1.0
```

As the example shows, some methods (like summary()) can deal with NA's, but others can't. For example, if we try to compute the Pearson's correlation between tree volume and girth, using the cor method, with the missing value included:

This somewhat cryptic message is explained in the help for cov, where several options are given for dealing with missing values, the most common of which is to include a case in the computation only if no variables are missing:

```
> cor(trees$Volume, trees$Girth, use="complete.obs")
[1] 0.967397
```

S provides a method for removing all cases from a data frame where *any* of the variables are missing:

```
> trees.allvars<-na.omit(trees)
> str(trees.allvars)
`data.frame': 30 obs. of 3 variables:
$ Girth : num    8.6 8.8 10.5 10.7 10.8 11 11 ...
$ Height: num    65 63 72 81 83 66 75 80 75 79 ...
$ Volume: num    10.3 10.2 16.4 18.8 19.7 15.6 ...
```

The first observation, with the missing volume, was removed.

4.21 Control structures and looping

S is a powerful programming language with Algol-like syntax²⁸ and control structures.

Single statements may be grouped between the braces { and }, separated either by new lines or the *command separator*;. The if ...else command allows *conditional execution*, and the for, while, and repeat commands allow *looping*. Note however that because of R's many vectorized methods looping is much less common in R than in compiled languages such as C.

For example, to convert the sample confusion matrix from counts to proportions, you might be tempted to try this:

But you can get the same result with a vectorized operation:

```
> cmp <- cm/sum(cm)</pre>
```

See Chapter 9 of [20] for more details.

²⁸ also used in C and its derivatives such as C++ and Java; of Algol it has been aptly said that it was a great improvement over its successors.

4.22 User-defined functions

An R user can use the function method to define *functions* with *arguments*, including *optional* arguments with *default* values. See the example in §D and a good introduction in Chapter 10 of [20]. These then are objects in the workspace which can be *called*.

For example, here's a function to compute the *harmonic mean* of a vector; this is defined as

$$\bar{v}_h = (\prod_{i=1\dots n} v_i)^{1/n}$$

where n is the length of the vector v, but is more reliably computed by taking logarithms, dividing by the length, and exponentiating:

```
> hm <- function(v) exp(sum(log(v))/length(v))
> hm(1:99)
[1] 37.6231
> mean(1:99)
[1] 50
```

As it stands, this function does not check its arguments; it only makes sense for a vector of positive numbers:

```
> hm(c(-1, -2, 1, 2))
[1] NaN
Warning message:
NaNs produced in: log(x)
```

To correct this behaviour we write a multi-line function with a conditional statement and the return method to leave the function:

```
> hm <- function(v) {</pre>
   if (!is.numeric(v)) {
    print("Argument must be numeric"); return(NULL)
   else if (any(v \le 0)) {
    print("All elements must be positive"); return(NULL)
   else return(exp(sum(log(v))/length(v)))
   }
> class(hm)
[1] "function"
> hm
function(v) {
  }
> hm(letters)
[1] "Argument must be numeric"
NULL
> hm(c(-1, -2, 1, 2))
[1] "All elements must be positive"
NULL
> hm(1:99)
[1] 37.6231
```

Note how simply typing the function name *lists* the function object; to *call* the function you must supply the *argument list*.

4.23 Computing on the language

As explained in the R Language Definition:

"R belongs to a class of programming languages in which subroutines have the ability to modify or construct other subroutines and evaluate the result as an integral part of the language itself." [21, Ch. 6]

This may seem quite exotic, but it has some practical applications even for the non-programmer R user, in addition to the deeper applications explained in the Definition.

For example, consider the problem of summarising a set of variables that are named B1, B2, ...B256 29 . To avoid writing m[1] <- mean(B1), m[2] <- mean(B2) etc. we'd like to loop through the numbers and form the variable name (with the B prefix and a number) and perform the operation. We do this in three steps:

- 1. Build up a syntactically-correct string to be evaluated, using the paste method;
- 2. Parse this into an R language object with the parse method;
- 3. Evaluate it with the eval method.

```
> # demonstrate how the string is built up
> paste("m[", b, "] <- mean(B", b, ")", sep="")</pre>
Error in paste("m[", b, "] <- mean(B", b, ")", sep = "") :</pre>
object "b" not found
> # must define a value for b to see how this works
> paste("m[", b, "] <- mean(B", b, ")", sep="")</pre>
[1] "m[4] <- mean(B4)"</pre>
> # what does this look like as a parse language object?
> parse(text=paste("m[", b, "] <- mean(B", b, ")", sep=""))</pre>
expression(m[4] <- mean(B4))</pre>
> # initialise the results vector
> m <- NULL
> # evaluate this one expression
> eval(parse(text=paste("m[", b, "] <- mean(B", b, ")", sep="")))
Error in mean(B4) : object "B4" not found</pre>
> # must define this variable to compute its mean
> B4 <- 0:100
> eval(parse(text=paste("m[", b, "] <- mean(B", b, ")", sep="")))</pre>
> # result so far
[1] NA NA NA 50
> # apply to all 256 variables; need B1 .. B256 defined
```

²⁹ Perhaps reflectances from a hyperspectral sensor

Note: the for expression does not need to be written on separate lines; it is so written here for clarity.

5 R graphics

R provides a rich environment for statistical visualisation [13]. There are two graphics systems: the *base* system (in the graphics package, loaded by default when R starts) and the *trellis* system (in the lattice package).

R graphics are highly customizable; see each method's help page for details and (for base graphics) the help page for graphics parameters: ?par. Except for casual use, it's best to create a script (§3.9) with the graphics commands; this can then be edited, and it also provides a way to produce the exact same graph later.

Multiple graphs can be placed in the same window for display or printing; see §5.4, and several graphics windows can be opened at the same time; see §5.3.

To get a quick appreciation of R graphics, run the demostration programs:

```
> demo(graphics)
> demo(image)
> demo(lattice)
```

5.1 Base graphics

A technical introduction to base graphics is given in Chapter 12 of [20]. Here we give an example of building up a sophisticated plot step-by-step, starting with the defaults and customizing.

The example is a scatter plot of petal length vs. width from the iris data set. A default scatterplot of two variables is produced by the plot.default method, which is automatically used by the generic plot command if two equal-length vectors are given as arguments:

```
> data(iris)
> str(iris)
`data.frame': 150 obs. of 5 variables:
$ Sepal.Length: num 5.1 4.9 4.7 4.6 5 5.4 4.6 5 4.4 4.9 ...
$ Sepal.Width : num 3.5 3 3.2 3.1 3.6 3.9 3.4 3.4 2.9 3.1 ...
$ Petal.Length: num 1.4 1.4 1.3 1.5 1.4 1.7 1.4 1.5 1.4 1.5 ...
$ Petal.Width : num 0.2 0.2 0.2 0.2 0.2 0.4 0.3 0.2 0.2 0.1 ...
$ Species : Factor w/ 3 levels "setosa", "versicolor", ..: 1 1 1 1 1 1 1 ...
> attach(iris)
> plot(Petal.Length, Petal.Width)
```

In this form, the x- and y-axes are given by the first and second arguments, respectively. The same plot can be produced using a *formula* §4.17 showing the dependence, in which case the y-axis is given as the *dependent* variable on the left-hand side of the formula:

```
> plot(Petal.Width ~ Petal.Length)
```

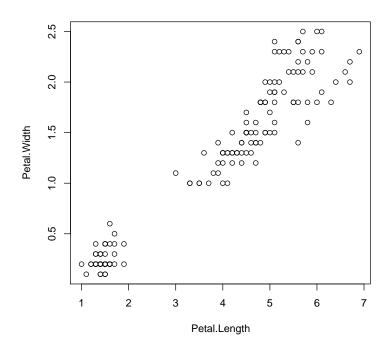


Figure 2: Default scatterplot

This default plot is shown in Figure 2. It is informative but not so attractive. We can customize the plotting symbol (pch argument), its colour and size (col and cex arguments), the axis labels (xlab and ylab arguments), and graph title (main argument).

Plotting symbols can be specified either by a single character (e.g. "*" for an asterisk) or an integer code for one of a set of graphics symbols. Figure 3 shows the symbols and their codes. Note that symbols 21–26 also have a *fill* (background) colour, specified by the bg argument; the main colour specified by the col argument specifies the border.

See §5.5 for details on how to specify colours.

We now produce a customized plot, showing the species:

```
plot(Petal.Length, Petal.Width, pch=20, cex=1.2,
    xlab="Petal length (cm)", ylab="Petal width (cm)",
    main="Anderson Iris data",
    col=c("slateblue", "firebrick", "darkolivegreen")[as.numeric(Species)]
)
```

It's clear that the species are of different sizes (*Setosa* smallest, *Versicolor* in the middle, *Virginica* largest) but that the ratio of petal length to width is about the same in all three.

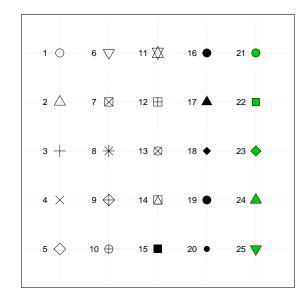


Figure 3: Plotting symbols

Note the use of the as.numeric method to coerce the Species, which is a factor, to the corresponding level number (here, 1, 2 and 3), and then the use of this number to index a list of colours.

The plot generic method is an example of a *high-level* plotting method which begins a new graph. Once the coördinate system is set up by plot, several *mid-level* plotting methods are available to add elements to the graph, such as lines, points, and text; Table 1 lists the principal methods; see the help for each one for more details.

abline	Add a Straight Line
arrows	Add Arrows
axis	Add an Axis
box	Draw a framing Box
grid	Add a Grid
legend	Add Legends
lines	Add Connected Line Segments
mtext	Write Text into the Margins
points	Add Points
polygon	Draw Polygons
rect	Draw Rectangles
rug	Add a Rug
segments	Add Line Segments
symbols	Draw Symbols
text	Add Text
title	Plot Annotation

Table 1: Methods for adding to an existing base graphics plot

For example, to add horizontal and vertical lines at the mean and median centroids, use the abline method:

```
abline(v=mean(Petal.Length), lty=2, col="red")
abline(h=mean(Petal.Width), lty=2, col="red")
abline(v=median(Petal.Length), lty=2, col="blue")
abline(h=median(Petal.Width), lty=2, col="blue")
```

The 1ty argument specifies the *line type* (style). These can be specified as a code (0=blank, 1=solid, 2=dashed, 3=dotted, 4=dotdash, 5=longdash, 6=twodash) or as a descriptive name "blank", "solid", "dashed", "dotted", "dotdash", "longdash", or "twodash").

To add light gray dotted grid lines at the axis ticks, use the grid method:

grid()

To add the mean and median centroids as large filled diamonds, use the points method:

Titles and axis labels can be added with the title method, if they were not already specified as arguments to the plot method:

```
title(sub="Centroids: mean (green) and median (gray)")
```

Text can be added anywhere in the plot with the text method; the first two arguments are the coördinates as shown on the axes, the third argument is the text, and optional arguments specify the position of the text relative to the coördinates, the colour, text size, and font:

```
text(1, 2.4, "Three species of Iris", pos=4, col="navyblue")
```

A special kind of text is the *legend*, added with the legend method;

The abline method can also add lines computed from a model, for example the least-squares regression (using the lm method) and a robust regression (using the lqs method of the MASS package):

```
abline(lm(Petal.Width ~ Petal.Length), lty="longdash", col="red")
abline(lqs(Petal.Width ~ Petal.Length), lty=2, col="blue")
```

This customized plot is shown in Figure 4.

Returning results from graphics methods Many high-level graphics methods return results, which may be assigned to an S object or used directly

Anderson Iris data

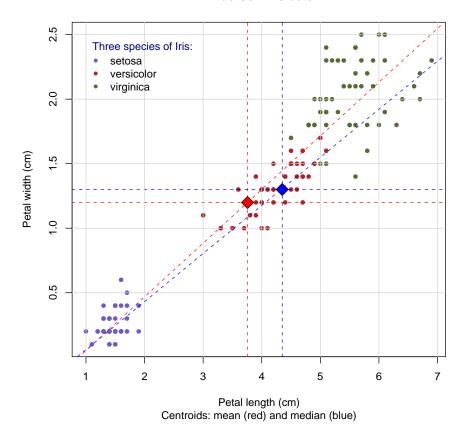


Figure 4: Custom scatterplot

in an expression. For example, the hist method returns the break and mid points, counts and densities:

```
> data(trees)
> h <- hist(trees$Volume)</pre>
> str(h)
List of 7
              : num [1:8] 10 20 30 40 50 60 70 80
 $ breaks
              : int [1:7] 10 9 5 1 5 0 1
 $ counts
 $ intensities: num [1:7] 0.03226 0.02903 0.01613 0.00323 0.01613 ...
              : num [1:7] 0.03226 0.02903 0.01613 0.00323 0.01613 ...
 $ density
              : num [1:7] 15 25 35 45 55 65 75
 $ mids
              : chr "trees$Volume"
 $ xname
             : logi TRUE
 $ equidist
  attr(*, "class")= chr "histogram"
> (hist(trees$Volume))$mids
[1] 15 25 35 45 55 65 75
```

5.1.1 Types of base graphics plots

Table 2 lists the principal plot types; see the help for each one for more details.

assocplot	Association Plots
barplot	Bar Plots
boxplot	Box Plots
contour	Contour Plots
coplot	Conditioning Plots
dotchart	Cleveland Dot Plots
filled.contour	Level (Contour) Plots
fourfoldplot	Fourfold Plots
hist	Histograms
image	Display a Colour Image
matplot	Plot Columns of Matrices
mosaicplot	Mosaic Plots
pairs	Scatterplot Matrices
persp	Perspective (3D) Plots
plot	Generic X-Y Plotting
stars	Star (Spider/Radar) Plots
stem	Stem-and-Leaf Plots
stripchart	1-D Scatter Plots
sunflowerplot	Sunflower Scatter Plots

Table 2: Base graphics plot types

Figure 5 shows examples of a boxplot, a conditioning plot, a pairwise scatterplot, and a star plot, all applied to the Anderson iris dataset.

```
boxplot(Petal.Length ~ Species, horizontal=T,
   col="lightblue", boxwex=.5,
   xlab="Petal length (cm)", ylab="Species",
   main="Grouped box plot")
coplot(Petal.Width ~ Petal.Length | Species,
   col=as.numeric(Species), pch=as.numeric(Species))
pairs(iris[,1:4], col=as.numeric(Species),
   main="Pairwise scatterplot")
stars(iris[,1:4], key.loc=c(2,35), mar=c(2, 2, 10, 2),
   main="Star plot of individuals", frame=T)
```

Some packages have implemented their own variations of these and other plots, for example scatterplot and scatterplot.matrix in the car package and truehist in the MASS package.

5.1.2 Interacting with base graphics plots

If the output graphics device is a screen, e.g. as initialised with the windows method, it is possible to *query* the graph with the identify method for scatterplots. This reads the position of the graphics pointer when the *left* mouse button is pressed, and searches the coördinates given as its for the closest point in the plot. If this point is close enough to the pointer, its index is added to a list to be returned, once the *right* mouse button is pressed.

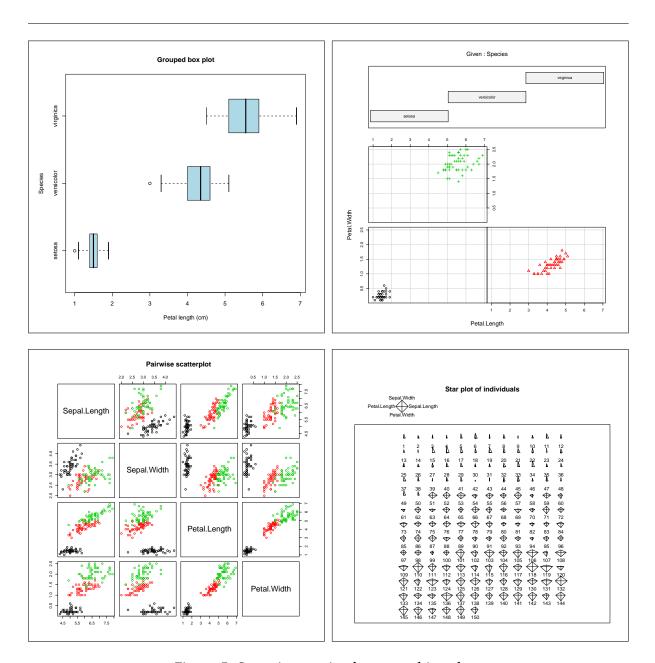


Figure 5: Some interesting base graphics plots

The coördinate pairs for identify is normally the same as the scatterplot:

```
> plot(Petal.Length, Petal.Width)
> (p <- identify(Petal.Length, Petal.Width))
[1] 44 65 99
> iris[p,]
   Sepal.Length Sepal.Width Petal.Length Petal.Width
                                                             Species
44
             5.0
                          3.5
                                        1.6
                                                              setosa
65
             5.6
                          2.9
                                        3.6
                                                      1.3 versicolor
99
             5.1
                          2.5
                                        3.0
                                                      1.1 versicolor
```

This is quite useful for identifying unusual points in the plot.

5.2 Trellis graphics

The Trellis graphics system is framework for data visualization developed at Bell Labs (where S originated) based on the ideas in Cleveland [3]. It was implemented in S-PLUS and then in R with the lattice package; its design and basic use are well-explained by its author Sarkar [29] in the R Newsletter. It is harder to learn than R base graphics, but can produce higher-quality graphics, especially for *multivariate visualisation* when the relationship between variables changes with some grouping factor; this is called *conditioning* the graph on the factor. It uses *formulae* similar to the statistical formulae introduced in §4.17 to specify the variables to be plotted and their relation in the plot. Customization of Trellis graphics parameters (for example, default background and symbol colours) is explained in §5.2.2.

Univariate plots As a simple example, consider the iris dataset. To produce a kernel density plot (a sophisticated histogram) on the whole dataset, use the densityplot method:

```
densityplot(~ Petal.Length, data=iris)
```

The ~ operator here has no left-hand side, since there is no dependent variable in the plot; it is univariate. The petal length is the independent variable, and we get one plot; this is shown shown on the left side of Figure 6.

To add *conditioning*, we use the | operator, which can be read as "conditioned on" the variable(s) named on its right side:

```
densityplot(~ Petal.Length | Species, data=iris)
```

Here there is one *panel* per species; this is shown shown on the right side of Figure 6. We can clearly see that the multi-modal distribution of the entire data set is due to the different distributions for each species.

Bivariate plots The workhorse here is the xyplot method, now with a dependent (y-axis) and independent (x-axis) variable; this can also be conditioned on one or more grouping factors:

```
xyplot(Petal.Width ~ Petal.Length, data=iris,
    groups=Species, auto.key=T)
xyplot(Petal.Width ~ Petal.Length | Species, data=iris,
    groups=Species)
```

These are shown in Figure 7. Note the use of the groups argument to specify a different graphic treatment (in this case colour) for each species,

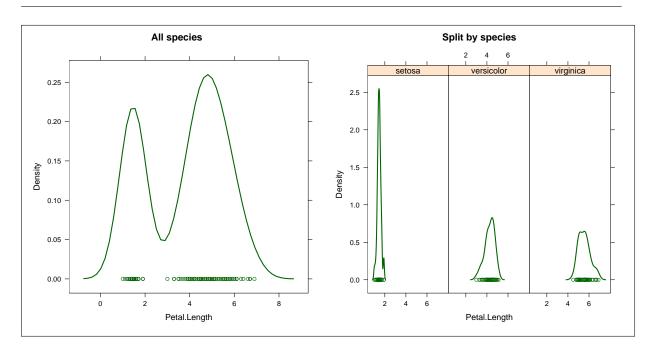


Figure 6: Trellis density plots, without and with a conditioning factor

and the auto.key argument to get a simple key to the colours used for each species.

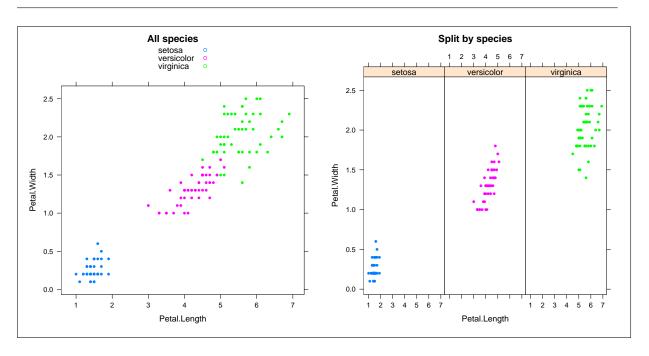


Figure 7: Trellis scatter plots, without and with a conditioning factor

Triivariate plots The most useful plots here are the levelplot and contourplot methods for 2D plotting of one response variable on two continuous dependent variables (for example, elevation vs. two coördinates), the wireframe method for a 3D version of this, and the cloud method for a 3D scatterplot of three variables. All can be conditioned on a factor. Figure 8 shows some examples, produced by the following code:

```
pl1 <- cloud(Sepal.Length ~ Petal.Length * Petal.Width,
 groups=Species,
 data=iris, pch=20, main="Anderson Iris data, all species",
 screen=list(z=30, x=-60))
data(volcano)
pl2 <- wireframe(volcano,
 shade = TRUE, aspect = c(61/87, 0.4),
 light.source = c(10, 0, 10), zoom=1.1, box=F,
 scales=list(draw=F), xlab="", ylab="", zlab=""
 main="Wireframe plot, Maunga Whau Volcano, Auckland")
pl3 <- levelplot(volcano,
      col.regions=gray(0:16/16),
     main="Levelplot, Maunga Whau Volcano, Auckland")
pl4 <- contourplot(volcano, at=seq(floor(min(volcano)/10)*10,
         ceiling(max(volcano)/10)*10, by=10),
         main="Contourplot, Maunga Whau Volcano, Auckland",
         sub="contour interval 10 m",
         region=T,
         col.regions=terrain.colors(100))
print(pl1, split=c(1,1,2,2), more=T)
print(pl2, split=c(2,1,2,2), more=T)
print(pl3, split=c(1,2,2,2), more=T)
print(pl4, split=c(2,2,2,2), more=F)
rm(pl1, pl2, pl3, pl4)
```

Note that the volcano data set is just a matrix of elevations:

```
> str(volcano)
num [1:87, 1:61] 100 101 102 103 104 105 105 106 107 108 ...
```

The levelplot method converts this into one response variable (the z values) and two predictors, i.e. the row and column of the matrix. (the x and y values).

This example shows that high-level lattice methods do not themselves draw a graph; they return an object of class trellis which can be printed with the print method. R's default behaviour when working interactively (at the console) is to print the results of any expression except an assignment, so the casual user doesn't see this behaviour. It is however quite useful to place multiple graphs on the same page as illustrated here and explained in more detail in §5.4.

Panel functions A Trellis plot must be constructed in one go, unlike in the base graphics package, where elements can be added later. Each additional element beyond the default is specified by a so-called *panel function*. For example, suppose we want to add a least-squares regression line

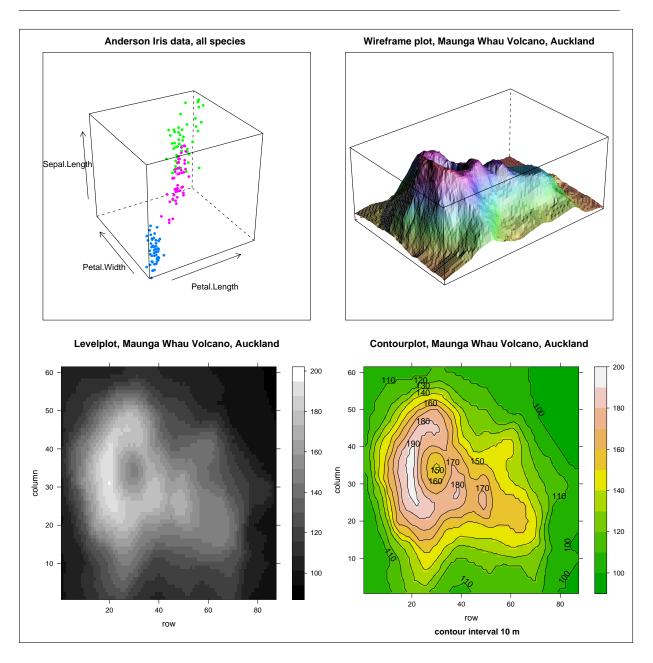


Figure 8: Trellis trivariate plots

as well as regression lines for each species to the scatterplot of petal width and length:

```
panel.xyplot(x, y, ...);
panel.abline(lm(y ~ x), col="black");
for (lvl in 1:length(levels(Species))) {
   panel.abline(lm(y ~ x,
        subset=(Species==levels(Species)[lvl])),
        col=c("darkgreen", "navyblue", "firebrick")[lvl],
        lty=2)
   }
})
```

This plot is shown in Figure 9.

2.5 - 2.0 -

Figure 9: Trellis scatter plot with some added elements

The panel argument is used whenever we want to control the appearance of the panel beyond the default plot. Here it is a function, which takes as arguments the *dummy variables* x and y, which represent the two variables of the x-y plot. The ... argument to the panel passes through all the extra arguments specified previously, e.g. data=iris. Within the un-named panel function, several pre-defined panel functions are called to add graphic elements. These all have names beginning with panel.. First we use panel.fill to change the main plot background, then panel.xyplot to draw the points; note that this must be called explicitly if there is a panel function. Then we add the regression lines with

panel.abline. Note the use of the for loop to add one line for each species.

See ?panel.functions and the explanation of the panel parameter in ?xyplot for details.

5.2.1 Types of Trellis graphics plots

Table 3 lists the principal plot types; see the help for each one for more details.

Univariate				
assocplot	Association Plots			
barchart	bar plots			
bwplot	box and whisker plots			
densityplot	kernel density plots			
dotplot	dot plots			
histogram	histograms			
qqmath	quantile plots against mathematical dis-			
	tributions			
stripplot	1-dimensional scatterplot			
Bivariate				
qq	q-q plot for comparing two distribu-			
	tions			
xyplot	scatter plots			
Trivariate				
levelplot	level plots			
contourplot	contour plots			
cloud	3-D scatter plots			
wireframe	3-D surfaces			
Hypervariate				
splom	scatterplot matrix			
parallel	parallel coördinate plots			
Miscellaneous				
rfs	residual and fitted value plot			
tmd	Tukey Mean-Difference plot			

Table 3: Trellis graphics plot types

5.2.2 Adjusting Trellis graphics parameters

The Trellis graphics environment as implemented in the lattice package sets reasonable defaults for its graphics parameters, based on the output device (screen, PDF file ...). Changing these requires three steps: (1) retrieve the parameters into a data structure in memory; (2) modify them; (3) write the modified parameters back as permanent options.

Parameters are retrieved with the trellis.par.get method and set with

the trellis.par.set method. In the following example we change the 'superposition' symbol which is used in the xyplot method to show groups of points, as in the example just above.

The current settings are shown graphically by the show.settings method.

```
> show.settings()
> options <- trellis.par.get()</pre>
> names(options)
 [1] "fontsize"
                         "background"
                                             "clip"
 [4] "add.line"
                         "add.text"
                                             "bar.fill"
 [7] "box.dot"
                         "box.rectangle"
                                             "box.umbrella"
[10] "dot.line"
                         "dot.symbol"
                                             "plot.line"
[13] "plot.symbol"
                         "reference.line"
                                             "strip.background"
[16] "strip.shingle"
                         "superpose.line"
                                             "regions"
[19] "shade.colors"
                         "superpose.symbol" "axis.line"
[22] "axis.text"
                         "box.3d"
                                             "par.xlab.text"
[25] "par.ylab.text"
                                             "par.main.text"
                         "par.zlab.text"
[28] "par.sub.text"
> options$superpose.symbol
$cex
[1] 0.8
$col
[1] "#00ffff" "#ff00ff" "#00ff00" "#ff7f00" "#007eff"
[6] "#ffff00" "#ff0000"
$font
[1] 1 1 1 1 1 1 1
$pch
[1] 1
> options$superpose.symbol$pch
> options$superpose.symbol$pch <- 20</pre>
> options$superpose.symbol$col <- c("blue", "green", "red", "magenta",</pre>
+ "cyan", "black", "grey")
> options$superpose.symbol$cex <- 1.4</pre>
> trellis.par.set("superpose.symbol", options$superpose.symbol)
> xyplot(Sepal.Width ~ Sepal.Length, group=Species, iris)
```

There are a large number of options, each with sub-options. For example, the superposition symbol has a character code (pch), a vector of colours (col), a vector of fonts (font), and a character expansion fraction (cex). These can all be set and then written back as shown. Subsequent graphs use the changed parameters.

5.3 Multiple graphics windows

To open several graphics windows at the same time, use the windows method. R opens the first graphics window automatically in response to the first graphics method such as plot or hist; in the following example we assume no such commands have yet been given.

```
> dev.list()
NULL
> windows()
> dev.list()
```

```
windows
2
> dev.cur()
windows
2
```

At this point, there is only one window and it is, of course, the current graphics device, i.e. number 2 (for some reason, 1 is not used). The results of any plotting commands will be displayed in this window.

Now we open another window; it becomes the current window:

```
> windows()
> dev.list()
windows windows
2  3
> dev.cur()
windows
3
```

At this point, any plot commands will go to the most recently-opened window, i.e. number 3.

Switching between windows The dev.set method specifies which graphics device to use for the next graphics output. For example, to compare scatterplots of tree volume vs. two possible predictors (height and girth) in adjacent windows:

```
> dev.set(2)
> plot(Height, Volume)
> dev.set(3)
> plot(Girth, Volume)
```

5.4 Multiple graphs in the same window

This depends on the graphics system: *base* or *trellis* (§5.2), as implemented in the lattice R package. You can determine which system is used by a given graphics command at the top of its help page. For example:

?boxplot

shows the page title as boxplot (graphics) indicating that it's in the base graphics package, whereas

?xyplot

shows the page title as xyplot (lattice) indicating that it's a trellis plot.

Base graphics The *parameters* of the active graphics device are set with the par method. One of these parameters is the number of rows and

columns of indivual plots in the device. By default this is (1, 1), i.e. one plot per device. You can set up a matrix of any size with the par(mfrow=...) or par(mfcol=...) commands. The difference is the order in which figures will be drawn, either row- or column-wise.

For example, to set up a two-by-two matrix of four histograms, and fill them from left-to-right, top-to-bottom:

```
# the `par' method refers to the active device
par(mfrow=c(2, 2))
hist(rnorm(100)); hist(rbinom(100, 20, .5)
hist(rpois(100, 1)); hist(runif(100)
par(mfrow=c(1,1))
# next plot will fill the window
```

Trellis graphics A trellis (§5.2) graphics window can also be split, but in this case the print method of the lattice package must be used on an object of class trellis (which might be built in the same command), using the split = optional argument to specify the position (x and y) within a matrix of plots. For all but the last plot the more=T argument must be specified.

Repeating the previous example:

```
 \begin{array}{lll} & \text{print(histogram(rnorm(100)), split=c(1,1,2,2), more=T);} \\ & \text{print(histogram(rbinom(100, 20, .5)), split=c(2,1,2,2), more=T);} \\ & \text{print(histogram(rpois(100, 1)), split=c(1,2,2,2), more=T);} \\ & \text{print(histogram(runif(100)), split=c(2,2,2,2), more=F)} \end{array}
```

A more elegant way to do this is to create plots with any lattice method, including levelplot, xyplot, and histogram, but instead of displaying them directly, *saving* them (using the assignment operator <-) as *trellis objects* (this is the object type created by lattice graphics methods), and then print them with lattice's print method. The advantage is that the same plot can be printed in a group of several plots, alone, or on different devices, without having to be recomputed.

For example:

```
h1 <- histogram(rnorm(100), col="lightblue");
h2 <- histogram(rbinom(100, 20, .5), col="snow3");
h3 <- histogram(rpois(100, 1), col="springgreen1");
h4 <- histogram(runif(100), col="red4");
print(h1, split=c(1,1,2,2), more=T);
print(h2, split=c(2,1,2,2), more=T);
print(h3, split=c(1,2,2,2), more=T);
print(h4, split=c(2,2,2,2), more=F);
rm(h1, h2, h3, h4)</pre>
```

5.5 Colours

Both base ($\S5.1$) and Trellis ($\S5.2$) graphics have many places where colours can be specified, often with the col (foreground colour) or bg (background colour) optional arguments to graphics methods such as plot.

Colours may be specified either by name, by code (colour specification), or by their numeric position in the active *colour palette*. There are a large number of named colours, but only eight of these in the default palette.

To get a list of possible colour names use the colours method; to see the numeric colours in the active palette use the palette method:

```
> colours()
  [1] "white"
                       "aliceblue"
                                         "antiquewhite"
  [4] "antiquewhite1" "antiquewhite2"
                                         "antiquewhite3"
[655] "yellow3"
                       "vellow4"
                                         "yellowgreen"
> colours()[655]
[1] "yellow3"
> palette()
[1] "black"
              "red"
                        "green3" "blue"
                                             "cyan"
                                                       "magenta"
[7] "yellow" "gray"
> palette()[4]
[1] "blue"
```

The named colours can be visualised as a bar graph:

Then an individual colour number can be identified interactively by leftclicking on the vertical colour bar at the midpoint; right-click anywhere in the graph when done:

```
> abline(h=0.5, lwd=3) # to aim at
> selected <- identify(tmp, rep(0.5, length(tmp)))
> selected # colour number
> colors()[selected] # colour name
```

The Red, Green, Blue of any colour can be examined with the col2rgb method:

```
> col2rgb("yellow3")
        [,1]
red     205
green    205
blue     0
```

Single colours can be created with the rgb method, specifying Red, Green and Blue contributions each in the range 0...1 (completely absent ... saturated):

```
> rgb(0.25 0.5, 0)
[1] "#408000"
```

There are several built-in *colour ramps* (sequences of colours that give a pleasing visual impression); these are returned by the heat.colors, terrain.colors, topo.colors, and cm.colors methods; another palette is provided by the bpy.colors method of th gstat package.³⁰ These all return a vector of colours from defined endpoints, according to the number of levels requested:

```
> terrain.colors(5)
[1] "#00A600" "#E6E600" "#EAB64E" "#EEB99F" "#F2F2F2"
> terrain.colors(10)
[1] "#00A600" "#2DB600" "#63C600" "#A0D600" "#E6E600" "#E8C32E"
[7] "#EBB25E" "#EDB48E" "#F0C9C0" "#F2F2F2"
> terrain.colors(10)[1]
[1] "#00A600"
```

The hexidecimal codes here represent Red, Green, and Blue; from 00 (no colour) to FF (full colour); thus there are $256^3 = 16\,777\,216$ possible colours.

Grey scales use the slightly different gray method; its argument is a vector of values between 0...1 giving the gray level:

Custom colour ramps can be produced with the hsv and rainbow methods; see their help for details.

All of these ramps can be indexed to get individual colours. They are most useful, however, when these colours are linked to data values. For example, to plot soil sample points in the meuse soil pollution data set, with the points coloured in order of their rank (from least to most polluted by cadmium):

```
> library(sp)
> data(meuse)
> attach(meuse)
> xyplot(y ~ x , data=meuse, asp="iso", pch=20,cex=2,
```

³⁰ Note the American spelling of 'colour'.

This plot is shown in Figure 10. Note the use of the asp argument to xyplot to specify the *aspect* (ratio of axes), in this case proportional to the two scales ("isometric").

Soil samples, Meuse; colour ramp by Cd value

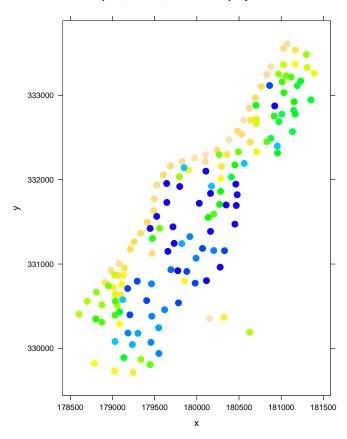


Figure 10: Example of a colour ramp

The key methods here are topo.colors to return a range of colours from dark blue through light pink, length to find the number of points and from this set the length of the colour ramp, and rank to return the rank of each sample, based on its cadmium content: the lowest pollution is rank 1, and so on to the most polluted with rank equal to the number of samples. Then the correct colour for each sample is extracted from the vector with the [] (subscript) operator.

6 Preparing your own data for R

R comes with many interesting example datasets (§3.12), but of course you are most interested in your own data. There are many ways to prepare this for R; a comprehensive guide is given in the **R Data Import/Export** manual provided as a PDF file.³¹

6.1 Preparing data directly

A small dataset may be entered directly in R in several ways. Here we illustrate this with the winning times from the 100 m footrace in the modern Olympic games [31], which we will assemble into a data frame, with the cases being each year and the fields being the year number, the men's winning time, and the women's winning time.

One method is to assign a vector directly to a variable. In the case of regular data, this can be easily accomplished with the seq or rep methods. For irregular data, the c method must be used to create a list.

```
> yr <- seq(1900,2004,4) # produces 1900, 1904, 1908, ... 2004
> men <- c(11, 11, 10.8, 10.8, NA, 10.8, 10.6, 10.8, 10.3,
+ 10.3, NA, NA,
+ 10.3, 10.4, 10.5, 10.2, 10, 9.95, 10.14, 10.06,
+ 10.25, 9.99, 9.92, 9.96, 9.84, 9.87, 9.85)</pre>
```

Note the + *continuation prompt* from R; as long as the list was not completed (not enough) to match the open (), R could determine that the expression was not complete, and prompted for more input.

Also note the use of the special NA value to indicate a *missing value*; no Olympic games were held in 1916, 1940 or 1944, so there is no time for those years.

Vectors can also be entered with the scan method. This waits for you to type at the console, until a blank line is entered. It shows the number of the next data item as a continuation prompt:

```
> women <- scan()
1: NA NA NA NA NA NA NA
8: 12.2 11.9 11.5 NA NA
13: 11.9 11.5 11.5 11 11.4 11.08 11.07 11.08 11.06 10.97
23: 10.54 10.82 10.94 10.75 10.93
28:</pre>
```

When the 28 was displayed, the user pressed the "Enter" key, and R realised the list was complete.

The three vectors are then gathered a data frame, and the local copies are discarded. By default the fields in the frame are named from the local

³¹ In RGui, select menu command <u>H</u>elp | <u>M</u>anuals | R <u>D</u>ata Import/Export

variables, but new names can be given with the fieldname = variable syntax. For example:

```
> oly.100 <- data.frame(year=yr, men, women)
> str(oly.100)
`data.frame': 27 obs. of 3 variables:
$ year : num 1900 1904 1908 1912 1916 ...
$ men : num 11 11 10.8 10.8 NA 10.8 10.6 10.8 10.3 10.3 ...
$ women: num NA NA NA NA NA NA NA 12.2 11.9 11.5 ...
> rm(yr, men, women)
```

To enter a **matrix**, first enter the data with the scan method or as a list with the c method, and then place it in matrix form with the matrix ("create a matrix") method. We illustrate this with the sample confusion matrix of Congalton *et al.* [4], also used as an example by Skidmore [30] and Rossiter [24].³² This example also illustrates the rownames and colnames methods to assign (or read) the row and column names of a matrix.

```
> cm <- scan()
1 : 35 14 11 1 4 11 3 0 12 9 38 4 2 5 12 2
> cm <- matrix(cm, 4, 4, byrow=T)</pre>
> cm
     [,1] [,2] [,3] [,4]
[1,] 35 14 11
[2,]
       4
           11
                3
                       0
          9
      12
                38
[3,]
                      4
           5 12
      2
[4,]
> colnames(cm) <- c ("A", "B", "C", "D")</pre>
> rownames(cm) <- LETTERS[1:4]</pre>
> cm
   A B C D
A 35 14 11 1
B 4 11 3 0
C 12 9 38 4
D 2 5 12 2
> cm[1, ]
 A B C D
35 14 11 1
> cm["A", "C"]
[1] 11
```

Note the use of the byrow optional argument to the matrix method, to indicate that we entered the data by row, also the use of the rownames and colnames methods to label the matrix with upper-case letters supplied conveniently by the LETTERS built-in constant.

6.2 Importing data from a CSV file

The *Comma-Separated Values* or "CSV" file is a common interchange format which can be prepared in many ways. For example, a CSV file can be created directly as a text file, using Notepad or some other plain-text edi-

This matrix is also used as an example in §4.6

tor. However, it is common to have data already in a spreadsheet such as Excel. In this case the procedure is as follows:

- 1. Prepare the data as an Excel spreadsheet with named columns;
- 2. Export from Excel to a (CSV) file, using Excel's File | Save As ... menu item;
- 3. Import into R with the read.csv method;
- 4. Adjust data types in R if necessary.

We illustrate this with a simplified version of the meuse dataset from the gstat and sp packages, which has been prepared to illustrate some issues with import.

Here is a small CSV file written by Excel and viewed in a plain text editor such as Notepad:

```
x,y,cadmium,elev,dist,om,ffreq,soil,lime,landuse 181072,333611,11.7,7.909,0.00135803,13.6,1,1,1,Ah 181025,333558,8.6,6.983,0.0122243,14,1,1,1,Ah 181165,333537,6.5,7.8,0.103029,13,1,1,1,Ah 181298,333484,2.6,7.655,0.190094,8,1,2,0,Ga 181307,333330,2.8,7.48,0.27709,8.7,1,2,0,Ah 181390,333260,3,7.791,0.364067,7.8,1,2,0,Ga
```

Note that:

- · There is one line per observation (*record*);
- Each record consists of the same number of *fields*, which are separated by commas;
- The first line has the same number of fields as the others but consists of the field *names*.

Suppose this file is named example.csv. To read into R, we first change to the directory where the file is stored and then read into an R object with the read.csv method³³.

³³ read.csv is a specialised *wrapper* to the very general read.table method which can deal with tables in many other formats

```
$ soil : int 1 1 1 2 2 2
$ lime : int 1 1 1 0 0 0
$ landuse: Factor w/ 2 levels "Ah", "Ga": 1 1 1 2 1 2
```

Notice that R could determine that landuse is a *factor* (categorical variable), because it was non-numeric. It could also determine the variable names from the first row. The other factors were not recognized, and in fact they have different R data types, which we now assign, using the as.* methods to change data types:

Using the correct data type is important for many modelling methods; here we inform R that lime was either applied (logical TRUE, associated by R with the number 1) or not (logical FALSE, associated by R with the number 0); that there are three soil types arbitrarily named "1", "2" and "3"³⁴ (not in any order); and that there are three flood frequency classes named "1", "2" and "3", and these are in this order.

Missing values Missing values are expressed in CSV files by the two letters NA (without quotes). For example:

```
x,y,cadmium,elev,dist,om,ffreq,soil,lime,landuse
181072,333611,NA,7.909,0.00135803,NA,1,1,1,Ah
181025,333558,8.6,6.983,0.0122243,14,1,1,1,Ah
```

In the first record neither the cadmium concentration nor organic matter proportion are known; these will be imported as missing values, symbolized in R by NA.

7 Exporting from R

Data frames are easily exported from R. For all the possibilities, see the R Data Import/Export manual. Here we explain the most common operation: exporting a data frame to a CSV file. This format can be read into Excel, ILWIS, and many other programs.

 $^{^{34}}$ These are *not* the *numbers* 1, 2, and 3.

A common reason for exporting is that you have computed some result in R which you want to use in another program. For example, suppose you've computed a kriging interpolation with the krige method of the gstat package:

```
> # load sp library to support spatial classes
> # load gstat for variograms and kriging
> library(sp); library(gstat)
> # load sample data and interpolation grid
> data(meuse); data(meuse.grid)
> # convert these to spatial objects
> coordinates(meuse) <- ~ x + y; coordinates(meuse.grid) <- ~ x + y</pre>
> # krige using a known variogram model
> kxy <- krige(log(lead)~x+y, locations=meuse,</pre>
        newdata=meuse.grid, maxdist=800,
        model=vgm(0.34, "Sph", 1140, 0.08))
[using universal kriging]
> str(as.data.frame(kxy))
`data.frame': 3103 obs. of 4 variables:
 $ x
           : num 181180 181140 181180 181220 181100 ...
           : num 333740 333700 333700 333660 ...
 $ var1.pred: num 5.72 5.68 5.61 5.54 5.67 ...
 $ var1.var : num   0.293  0.225  0.239  0.257  0.173  ...
```

Note the use of the coordinates method to promote the meuse and meuse.grid data frames to objects of class SpatialPointsDataFrame as required by the krige method, and the as.data.frame method to extract the data frame from the kriged object as required by the write.table method.

To export this data frame use the write.table method:

```
> write.table(round(as.data.frame(kxy), 4), file="KrigeResult.csv",
+     sep=",", quote=T, row.names=F,
+     col.names=c("E", "N", "LPb", "LPb.var"))
```

In this example the precision of the output was limited with the round method, and named the fields with the row.names= optional argument to write.table.

Here are the first few lines of the file KrigeResult.csv viewed in a plaintext editor such as Notepad:

```
"E","N","LPb","LPb.var"
181180,333740,5.7214,0.2932
181140,333700, 5.6772,0.2254
181180,333700, 5.6064,0.2391
```

8 Miscellaneous R tricks

In this section I've collected tips for some tasks which have puzzled ITC users.

8.1 Setting up a regular grid

This is done with the expand.grid method. First a step-by-step approach, also using the seq and names methods.

```
> # specify the limits of the grid
> utm.n.min <- 210000; utm.n.max <- 216000
> utm.e.min <- 620000; utm.e.max <- 628000
> # specify the spacing between points; they can be different
> x.spacing <- 500
> y.spacing <- 250
> # sequences of coordinates
> xseq <- seq(utm.e.min, utm.e.max, by=x.spacing)
> yseq <- seq(utm.n.min, utm.n.max, by=y.spacing)
> # all combinations, making a rectangular grid
> sample.pts <- expand.grid(xseq, yseq)
> # name the fields in the data frame
> names(sample.pts) <- c("x", "y")</pre>
```

The same result can be achieved with one command:

```
> sample.pts <- expand.grid(x=seq(210000, 216000, by=500),
+ y=seq(620000, 628000, by=250))
> plot(sample.pts$x, sample.pts$y)
```

The above grid is suitable for a regular interpolation grid, e.g. for kriging. If the grid is intended for field sampling, it may be wise to add a small random "jitter" to each coördinate to avoid undetected periodic effects in the field, using the rnorm method:

```
> jitter.sd <- 10
> sample.pts$x <- sample.pts$x + rnorm(length(sample.pts$x),
+ 0, jitter.sd)
> sample.pts$y <- sample.pts$y + rnorm(length(sample.pts$y),
+ 0, jitter.sd)
> plot(sample.pts$x, sample.pts$y)
```

This scheme is illustrated on the left side of Figure 11.

(See also the spsample method in the sp package.)

8.2 Setting up a random sampling scheme

A common problem is to draw a completely random sample in some geographic space, where the two coordinates are independent and both on a uniform distribution. This is easily done with the runif (random uniform)

method to draw samples for each coördinate and the data.frame method to put the two coördinates together.

```
> n.pt <- ((utm.e.max-utm.e.min)*(utm.n.max-utm.n.min))/spacing^2
> x <- runif(n.pt, utm.e.min, utm.e.max)
> y <- runif(n.pt, utm.n.min, utm.n.max)
> sample.pts <- data.frame(id = 1:n.pt, x, y)
> str(sample.pts)
`data.frame': 192 obs. of 3 variables:
$ id: int 1 2 3 4 5 6 7 8 9 10 ...
$ x : num 625215 627837 623322 620016 620142 ...
$ y : num 214168 212769 211254 212812 214317 ..
> attach(sample.pts); plot(x,y, type="n"); text(x, y, id)
```

This scheme is illustrated on the right side of Figure 11.

(See also the spsample method in the sp package.)

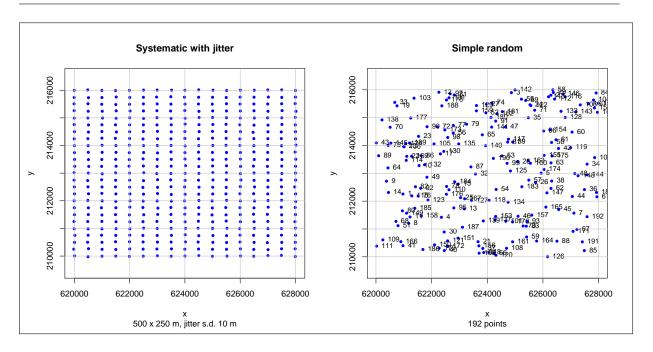


Figure 11: Two sampling schemes

9 Learning R

The present manual explains the basics of using R ($\S 3$), the S language ($\S 4$), and R graphics ($\S 5$). The on-line help system is explained in $\S 3.6$.

Task Views

Some applications are covered in so-called **Task Views**, on-line at http://cran.r-project.org/src/contrib/Views/. These are a summary by a task maintainer of the facilities in R to accomplish certain tasks. For example, Roger Bivand maintains an excellent task view "Analysis of Spatial Data" (http://cran.r-project.org/src/contrib/Views/Spatial.html) which discusses how to represent spatial data in R, how to read and write it, how to analyze point patterns, and geostatistical analysis. Another useful task view is "Multivariate Statistics" (http://cran.r-project.org/src/contrib/Views/Multivariate.html) maintained by Paul Hewson.

9.1 R tutorials and introductions

A good introduction to R concepts is the 100-page "R for Beginners" by Emmanuel Paradis of the University of Montpellier (F) [14]. This is also availble in his native French [16] and in a Spanish translation [15]; Correa & González [5]. is a Spanish-language introduction to R graphics. Dalgaard [6] is a clearly-written introduction to statistics, using R in all examples. Another useful introduction is "simpleR" by John Verzani of the City University of New York [34], also available as a set of web pages (§9.4). This shows how to use R for the usual univariate and bivariate statistics and tests, linear regression, and ANOVA.

Within R itself, you can access the introductory course "An Introduction to R" as follows.

- 1. **Select menu command** Help | Html help; a web page will appear in your browser.
- 2. In this web page, **select the link** "An Introduction to R"; another web page will appear.

You will probably want to start with the section "A sample session" (scroll down on the web page to find this in the table of contents). This will give you some familiarity with the style of R sessions and more importantly some instant feedback on what actually happens. Don't worry if you don't understand everything; this is just to give you a feel for how R works and what it can do. For individual commands, it is always best to look at its help topic.

9.2 Textbooks using R

Dalgaard [6] was mentioned above. Venables & Ripley [33] present a wide variety of up-to-date statistical methods (including spatial statistics) with

algorithms coded in S-PLUS. Most of these will run unchanged in R. There are a variety of other texts using S or S-PLUS, which are mostly applicable to R. Fox [11] explains how to use R for regression analysis, including advanced techniques; this is a companion to his text [10]. A more mathematically-sophisticated approach, but with a heavy emphasis on R techniques, is the text by Faraway [9], which is freely-available for download as a PDF.

9.3 Technical notes using R

I have written several technical notes on statistical topics, using R to compute and graph; these are all available as PDF files on-line, from which code can be cut and then pasted into R. If you work through these and use them as starting points for your own analysis, you will have a good basis in R.

One note [25] is designed to show as many R techniques as possible: exploratory data analysis, univariate statistics, bivariate correlation and regression, multivariate analysis including PCA, and some geostatistics.

Others are more specialised: land cover change with logistic regression [28], assessing map accuracy [24], co-kriging [26], fitting rational functions to time series [27], and optimal partitioning of soil transects [23].

These technical notes, their sample data sets and R code are stored at http://www.itc.nl/personal/rossiter/pubs/list.html#pubs_m_R.

9.4 Web Pages to learn R

http://www.math.csi.cuny.edu/Statistics/R/simpleR/index.html

"simpleR: Using R for Introductory Statistics". This is an excellent and well-paced tutorial from simple to complex techniques; also available as a single document (§9.1).

http://wwwmaths.anu.edu.au/~johnm/r/

"Data Analysis and Graphics Using R: An Introduction" by John Maindonald (Australian National University)

http://www.stat.lsa.umich.edu/~faraway/book/

"Practical Regression and Anova in R" by Julian Faraway (University of Michigan)

9.5 Keeping up with developments in R

R is a dynamic environment, with a large number of dedicated scientists working to make it both a rich statistical computing environment and a modern computing platform. Almost every day there are new and modified packages added to CRAN, and new versions of the R base appear regularly. But that means you need to invest some time to keep up with developments:

- Read the **R Newsletter**: follow the "Newsletter" link on the R Project home page (http://www.r-project.org/. This is issued from two to four times a year, and is announced on R home page. It is an attractive PDF document with news, announcements, tutorials, programmer's tips, bibliographies and much more.
- Subscribe to one or more **mailing lists**: follow the "Mailing Lists" link on the R Project home page (http://www.r-project.org/. The most relevant for most ITC users are:
 - *R-announce*: major announcements, e.g. new versions
 - *R-packages*: announcements of new or updated packages
 - R-help: discussion about problems using R, and their solutions.
 The R gurus monitor this list and reply as necessary. A search through the archives is a good way to see if your problem was already discussed.
- Attend the useR! user's conference every two years; follow the link on the R home page. The papers from the 2004 meeting are available at http://www.ci.tuwien.ac.at/Conferences/useR-2004/.

10 Frequently-asked questions

10.1 Help! I got an error, what did I do wrong?

1. **Read the error message carefully**. Often it says exactly what is wrong. For example:

```
> x <- rnorm(100)
> summary(X)
Error in summary(X) : Object "X" not found
```

This means exactly what it says: there is no object named X in the workspace nor in attached data frames, so R could not find it when it tried to execute the summary method. In this case the solution is clear: the variable is a lower-case x, not an upper-case X:

```
> summary(x)
    Min. 1st Qu. Median Mean 3rd Qu. Max.
-2.750 -0.561 -0.070 -0.014 0.745 2.350
```

2. If the command involves an **external file**, make sure your R session is in the right directory, or else use the full path name. For example, the read.csv method requires a file name:

```
> dlv <- read.csv("dlv.csv")
Error in file(file, "r") : unable to open connection
In addition: Warning message:
cannot open file 'dlv.csv'</pre>
```

The "unable to open connection" message means that the file could not be found.

Check the current working directory with the getwd method, and see if the file is there with the list.files method (or, you could look for the file in Windows Explorer):

```
> getwd()
[1] "/Users/rossiter/ds/DavisGeostats"
> list.files(pattern="dlv.csv")
character(0)
```

In fact this file is in another directory. One way is to give the full path name; note the use of the front slash / as in Unix; R interprets this correctly for MS-Windows:

```
> dlv <- read.csv("/Users/rossiter/ds/DLV/dlv.csv")
> dim(dlv)
[1] 88 33
```

Another way is to change the working directory with the setwd method:

```
> setwd("/Users/rossiter/ds/DLV")
```

```
> getwd()
[1] "/Users/rossiter/ds/DLV"
> dlv <- read.csv("dlv.csv")
> dim(dlv)
[1] 88 33
```

3. A common problem is the **attempt to use a method that is in an unloaded package**:

Suppose we try to run a resistant regression with the lqs method:

```
> lqs(lead ~ om, data=meuse)
Error: couldn't find function "lqs"
```

This error has two possible causes: either there is no such method anywhere (for example, if it had been misspelled lqr), or the method is available in an unloaded package.

To find out if the method is available in any package, search for the topic with the help.search method:

```
> help.search("lqs")
```

In this case, the list of matches to the search term "lqs" shows two, both associated with package MASS.

Once the required package is loaded, the method is available:

- 4. If the command which produced the error is **compound**, break it down into small pieces, beginning with the innermost command and then working outwards.
- 5. **Review the documentation for the command**; it may explain situations in which an error will be produced. For example, if we try to compute the non-parametric correlation between lead and organic matter in the Meuse data set, we get an error:

```
> library(gstat); data(meuse)
> cor(meuse$lead, meuse$om, method="spearman")
Error in cor(lead, om) : missing observations in cov/cor
> ?cor
```

The help for cor says: "If use is "all.obs", then the presence of missing observations will produce an error"; in the usage section it shows that use = "all.obs" is the default; so we must have some missing

values. We can check for these with the is.na method:

```
> sum(is.na(lead)); sum(is.na(om))
[1] 0
[1] 2
```

There are two missing values of organic matter (but none of lead). Then we must decide how to deal with them; one way is to compute the correlation without the missing cases:

```
> cor(lead, om, method="spearman", use="complete")
[1] 0.59759
```

10.2 Why didn't my command(s) do what I expected?

Because R does what you said, not what you meant! Some ideas to make the two match:

- 1. Review the on-line documentation for the command to see what the command actually does.
- 2. Look for the command in a tutorial or text and follow the examples.
- 3. Break down the command into smaller parts; make sure each part does what you think.
- 4. Experiment with test data or "toy" examples to understand how the command really works.
- 5. Look at the data structures with the str and class: sometimes it has a different structure than you thought.
- 6. A common problem occurs when a *variable defined in the workspace*, also called a *local* variable, has the same name as a *field in a data frame*. The local variable is found by R when it looks for the name, and *masks* the field name.

This is not the expected value; it is very low, and we know that a tree's volume should be fairly well correlated with its girth. What is

wrong? Listing the workspace gives a clue:

```
> ls()
[1] "Volume" "trees"
```

The name Volume occurs *twice*: once as a local variable, visible with ls(), and once as a field name, visible with str(trees). Even though the trees frame is attached, the Volume field is masked by the Volume local variable, which in this case is just a random permutation of the integers from 1 to 31, so the cor method gives an incorrect result.

One way around this problem is to name the field explicitly within its frame using \$, e.g. trees\$Volume:

```
> cor(trees$Volume, Girth)
[1] 0.96712
```

Another way is to delete the workspace variable with rm(); this makes the field name in the attached frame visible:

```
> rm(Volume)
> cor(Volume, Girth)
[1] 0.96712
```

Another way is to use names for local variables that do not conflict with field names in the attached data frames.

10.3 How do I find the method to do what I want?

R has a very rich set of methods, and there are often several ways to accomplish the same thing, especially with contributed packages.

- 1. Look at the **help pages for methods you do know**; they often list related methods. For example, the help page for the linear models method (?1m) gives related methods for prediction, summary, regression diagnostics, analysis of variance, and generalised linear models, with hyperlinks (in the HTML help) to directly access their help.
- 2. **Search for keywords**. For example help.search("sequence") lists methods to generate sequences, vectors of sequences, and sequences of dates for time-series analysis.
- 3. Look at the **Task Views**, on-line at http://cran.r-project.org/src/contrib/Views/. These are a summary of the facilities in R to accomplish certain tasks, including the names of the applicable methods.
- 4. Review the **tutorials**; they cover many common methods.
- 5. Some **textbooks** use R to illustrate their discussions (e.g. [6, 11, 33,

9]); you can adapt their examples to your needs.

6. If you don't find what you're looking for, perhaps the method is in a contributed package which has not yet been installed on your system. You can search for it on CRAN (the R archive), http://cran.r-project.org/.

For example, the von Mises distribution is the circular analogue of the normal distribution [7, p. 322]. On R with the default installation, a search for this term with the help.search method will give no results:

```
> help.search("von Mises")
No help files found with alias or concept or title
    matching 'von Mises'
```

However, you can search the R archive for the term "Von Mises" with the RSiteSearch method:

```
> RSiteSearch("von Mises")
> RSiteSearch("von Mises", restrict="functions")
```

The second form restricts the search to just functions; by default documentation and the R-help mailing list archives are also searched. This opens the search page http://search.r-project.org/ in a browser.

In this case, several matches are shown, including two packages. A review of their contents shows that the circular package for circular statistics is the more complete, so it should be installed on your system (§B.1).

Once the new package is installed, its contents are available to be searched, and this time the term "von Mises" is found. Several methods in the circular package are relevant:

```
> help.search("von Mises")
dmixedvonmises(circular)
    Mixture of von Mises Distributions
mle.vonmises(circular)
    von Mises Maximum Likelihood Estimates
mle.vonmises.bootstrap.ci(circular)
    Bootstrap Confidence Intervals
pp.plot(circular)
    von Mises Probability-Probability Plot
dvonmises(circular)
    von Mises Density Function
```

You can get help on any of these by loading the package and viewing the help:

```
> library(circular)
```

> ?dvonmises

10.4 What statistical procedure should I use?

This of course depends on your application field, your research questions, and your dataset. You should always refer to textbooks and research papers; R is only a computer program, not a statistical wizard.

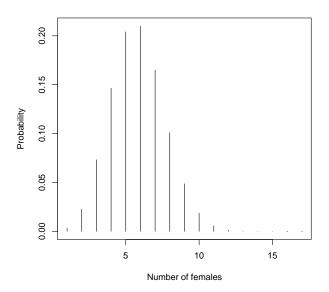
Within R, each help page gives references to textbooks or articles which you should consult if you are unsure about the theory behind the method or its options. You can also look up technical terms in your favourite statistics textbook.

A A sample R session

This appendix takes you through some of R's vast repertoire of analysis and visualisation with minimal to no explanation. It is intended to give the beginner a feel for how R is used and what it can accomplish. The commands are shown in this typeface; you can type them at the R command prompt (>) or cut-and-paste from this document.

First, you have to start R; see §3.

We begin with some probability calculations (§4.11). Suppose sixteen students are chosen at random from a population that is 30% female. What is the probability that none, one, two ...sixteen of the chosen students are female?



Suppose that only two of the sixteen chosen are female. What is the probability that two or fewer females could be chosen by chance?

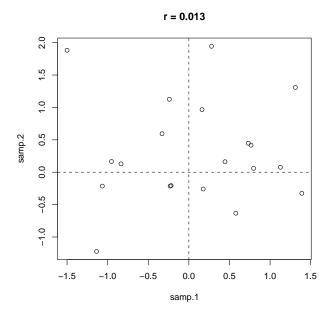
```
> pbinom(2, 16, 0.3, lower.tail = T)
[1] 0.09936
```

(Is this observed event evidence that females did not have a fair chance of

being selected for the sample?)

Two independent normally-distributed random samples should be uncorrelated; let's simulate this several times to estimate the correlation coefficient at which the probability of a Type I error (rejecting a true null hypothesis of no correlation) is 10%. First, one drawing:

```
> size <- 20
> samp.1 <- rnorm(size)</pre>
> samp.2 <- rnorm(size)</pre>
> cor.test(samp.1, samp.2)
        Pearson's product-moment correlation
data: samp.1 and samp.2
t = -0.3806, df = 18, p-value = 0.708
alternative hypothesis: true correlation is not equal to 0
95 percent confidence interval:
 -0.51164 0.36771
sample estimates:
      cor
-0.089344
> plot(samp.1, samp.2)
> abline(h = 0, lty = 2)
> abline(v = 0, lty = 2)
> title(paste("r =", round(cor(samp.1, samp.2), 3)))
```

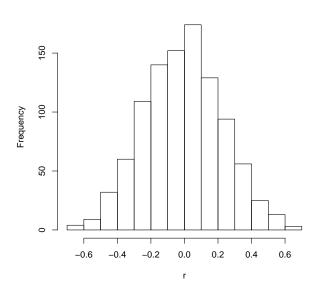


Your results will be different, since the sample is random. This can be repeated if you wish.

Then, a large number of drawings, collecting their statistics; this makes use of a user-defined function:

```
> cor.2 <- function(size) {</pre>
      samp.1 <- rnorm(size)</pre>
      samp.2 <- rnorm(size)</pre>
+
+
      cor(samp.1, samp.2)
+ }
> results <- NULL
 length <- 1000
 for (i in 1:length) {
      results[i] <- cor.2(20)
+
> hist(results, xlab = "r", main = "Correlation coefficients")
> (paste("5% have r more negative than", round(sort(results)[length/20],
      3)))
[1] "5% have r more negative than -0.411"
> (paste("5% have r more positive than", round(sort(results)[length -
      length/20], 3)))
[1] "5% have r more positive than 0.355"
```

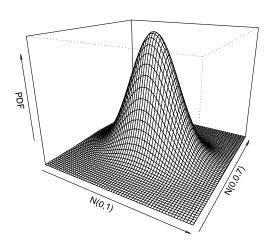
Correlation coefficients



It looks like an interval of about -0.38...+0.38 covers 90% of the sample correlation coefficients r for sample size 20. Again, your results will be slightly different.

A perspective plot of a bivariate normal distribution:

Bivariate normal distribution



Clean up the workspace:

Sepal.Width

Min. :2.00

1st Qu.:2.80

Sepal.Length Min. :4.30

1st Qu.:5.10

Now we move to a typical data visualization and analysis example. Load one of the built-in example datasets (§3.12) and view its metadata, data structure, and a summary of the data items:

Petal.Width

Min. :0.1

1st Qu.:0.3

Petal.Length

Min. :1.00

1st Qu.:1.60

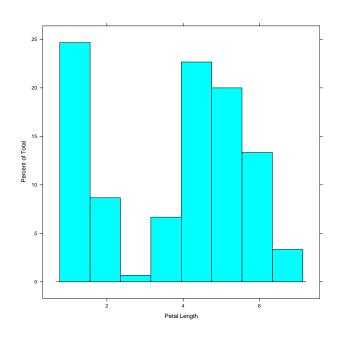
```
Median :5.80
                            Median :4.35
              Median :3.00
                                          Median :1.3
Mean :5.84
              Mean :3.06
                            Mean :3.76
                                          Mean :1.2
3rd Qu.:6.40
              3rd Qu.:3.30
                            3rd Qu.:5.10
                                          3rd Qu.:1.8
Max.
      :7.90
              Max. :4.40
                            Max.
                                  :6.90
                                          Max.
                                               :2.5
     Species
setosa
         :50
versicolor:50
virginica:50
```

We'll use the trellis graphics environment (§5.2) for much of the visualisation; this is included in the lattice add-on package which must be loaded:

> library(lattice)

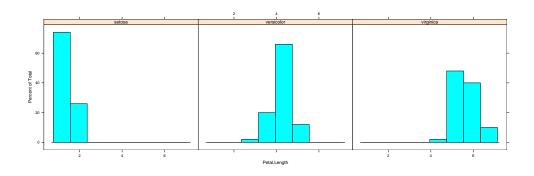
Plot the histogram of petal lengths:

> histogram(~Petal.Length, data = iris)



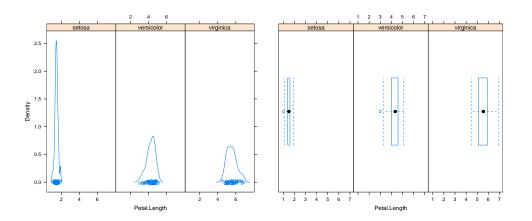
This is multi-modal; does it depend on the plant species?

> histogram(~Petal.Length | Species, data = iris)



Yes; we can see this several other ways:

- > densityplot(~Petal.Length | Species, data = iris)
- > bwplot(~Petal.Length | Species, data = iris)



This suggests the mean petal length is different between species; can we prove it? We try linear modelling ($\S4.17$):

```
> model <- lm(Petal.Length ~ Species, data = iris)
> summary(model)

Call:
lm(formula = Petal.Length ~ Species, data = iris)
Residuals:
```

Min 1Q Median 3Q Max -1.260 -0.258 0.038 0.240 1.348

Coefficients:

	Estimate	Sta. Error	t valu	e Pr(> t)
(Intercept)	1.4620	0.0609	24.	0 <2e-16
Speciesversicolor	2.7980	0.0861	32.	5 <2e-16
Speciesvirginica	4.0900	0.0861	47.	5 <2e-16

Residual standard error: 0.43 on 147 degrees of freedom Multiple R-Squared: 0.941, Adjusted R-squared: 0.941 F-statistic: 1.18e+03 on 2 and 147 DF, p-value: <2e-16

> anova(mode1)

Analysis of Variance Table

```
Response: Petal.Length

Df Sum Sq Mean Sq F value Pr(>F)
Species 2 437 219 1180 <2e-16
Residuals 147 27 0.19
```

The three species can definitely be separated; we can compute the differences, confidence intervals of these, and probability of overlap:

> TukeyHSD(aov(mode1))

```
Tukey multiple comparisons of means 95% family-wise confidence level
```

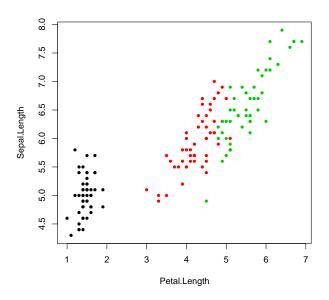
Fit: aov(formula = model)

\$Species

```
diff lwr upr p adj
versicolor-setosa 2.798 2.5942 3.0018 0
virginica-setosa 4.090 3.8862 4.2938 0
virginica-versicolor 1.292 1.0882 1.4958 0
```

Is there a consistent relation between petal and sepal length, irrespective of species?

```
> plot(Sepal.Length ~ Petal.Length, data = iris, col = as.numeric(Species),
+ pch = 20)
```

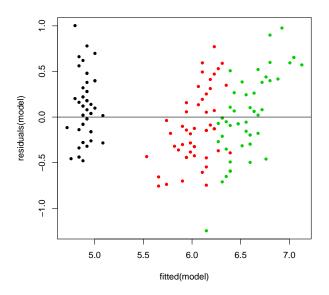


Try to model this, first without considering species:

```
> model <- lm(Sepal.Length ~ Petal.Length, data = iris)
> summary(model)
```

Call: lm(formula = Sepal.Length ~ Petal.Length, data = iris) Residuals: Min 1Q Median 3Q Max -1.2468 -0.2966 -0.0152 0.2768 1.0027 Coefficients: Estimate Std. Error t value Pr(>|t|) 0.0784 54.9 <2e-16 (Intercept) 4.3066 <2e-16 Petal.Length 0.4089 0.0189 21.6 Residual standard error: 0.407 on 148 degrees of freedom Multiple R-Squared: 0.76, Adjusted R-squared: 0.758 F-statistic: 469 on 1 and 148 DF, p-value: <2e-16

Petal length explains 76% of the variability of sepal length; but there are problems with this fit, which we can see with model diagnostics (§4.18.1):



The first species has many more high than low residuals, and there is a clear pattern to the residuals for the other two species, suggesting a poor adjustment to the line. It seems the species have different relations between the two lengths; confirm with a mixed model:

```
> model <- lm(Sepal.Length ~ Petal.Length * Species, data = iris)
> summary(model)

Call:
lm(formula = Sepal.Length ~ Petal.Length * Species, data = iris)
```

Residuals:

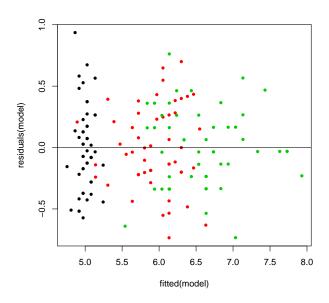
```
Min 1Q Median 3Q Max
-0.7348 -0.2279 -0.0313 0.2437 0.9361
```

Coefficients:

	estimate sta.	EL.LOL.	t varue	Pr(> L)
(Intercept)	4.213	0.407	10.34	< 2e-16
Petal.Length	0.542	0.277	1.96	0.052
Speciesversicolor	-1.806	0.598	-3.02	0.003
Speciesvirginica	-3.154	0.634	-4.97	1.8e-06
Petal.Length:Speciesversicolor	0.286	0.295	0.97	0.334
Petal.Length:Speciesvirginica	0.453	0.290	1.56	0.120

Residual standard error: 0.336 on 144 degrees of freedom Multiple R-Squared: 0.84, Adjusted R-squared: 0.835

F-statistic: 152 on 5 and 144 DF, p-value: <2e-16



Much better; but are the interaction terms needed? We compare with a nested (parallel regression) model:

```
> mode1.2 <- lm(Sepa1.Length ~ Peta1.Length/Species, data = iris)
> anova(mode1, mode1.2)
```

Analysis of Variance Table

```
Model 1: Sepal.Length ~ Petal.Length * Species
Model 2: Sepal.Length ~ Petal.Length/Species
Res.Df RSS Df Sum of Sq F Pr(>F)
1 144 16.3
2 146 19.2 -2 -2.9 12.8 7.6e-06
```

Yes.

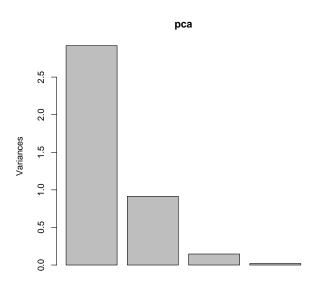
How much redundancy is there in the four variables?

```
> pca <- prcomp(iris[, 1:4], scale = T)
> summary(pca)
```

Importance of components:

PC1 PC2 PC3 PC4
Standard deviation 1.71 0.96 0.383 0.1439
Proportion of Variance 0.73 0.23 0.037 0.0052
Cumulative Proportion 0.73 0.96 0.995 1.0000

> screeplot(pca)



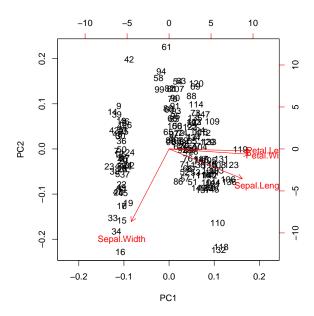
Quite a bit; the first two standardized principal components include 96% of the total variance.

How are these two components associated with variables and observations?

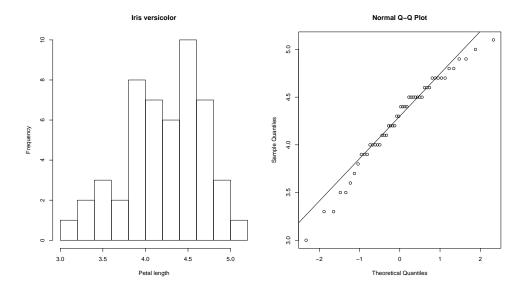
> pca\$rotation

```
PC1 PC2 PC3 PC4
Sepal.Length 0.52107 -0.377418 0.71957 0.26129
Sepal.Width -0.26935 -0.923296 -0.24438 -0.12351
Petal.Length 0.58041 -0.024492 -0.14213 -0.80145
Petal.Width 0.56486 -0.066942 -0.63427 0.52360
```

> biplot(pca)



Now we try to model the distribution of the petal lengths for one of the species; a first guess is that this should be normally-distributed:



The graphs seem to show deviations from normality but the Shapiro test can not reject the *a priori* null hypothesis of normality; so we estimate the parameters:

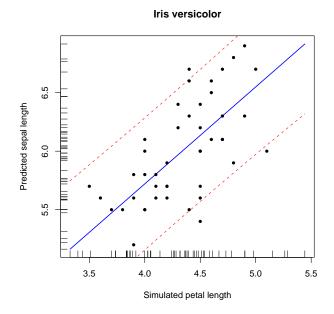
```
> mu <- mean(petal.v)
> sigma <- sd(petal.v)</pre>
```

Simulate another sample of flowers from the same population:

```
> petal.v.2 <- sort(rnorm(length(petal.v), mu, sigma))
> summary(petal.v.2)

Min. 1st Qu. Median Mean 3rd Qu. Max.
3.33 3.90 4.32 4.29 4.54 5.44
```

What would the sepal lengths of these be? We can show a 90% prediction inteval along with the original sample (§4.18.2); we expect about 5 of the 50 observations to be near or beyond this limit:



Clean up the workspace:

Stop the program:

> q()

You will be asked if you want to save the workspace; answer No.

B Obtaining your own copy of R

You may want your own copy of R for your portable computer, your home computer, or your organisation's computer or network. **This is free and legal!** Everything R is found via the R Project Home Page: http://www.r-project.org/

This has links to:

- Download from CRAN (The Comprehensive R Archive Network) at http://cran.r-project.org/; you will be asked to select a *mirror*, i.e. a server near you.
- · Installation instructions
- · Manuals
- The R Newsletter, including innovative statistical applications, clever uses of R, and R programming
- Frequently Asked Questions (FAQ)

Installing R for Windows To install R on Windows, download the setup program from CRAN (follow the links for "Windows", then the "base" package, then select the setup program, which has a name like R-2.2.0-win32.exe, the exact name depending on the version). Download the file (about 25 Mb) and run it.

The following stable link will redirect to the current Windows binary release:

http://mirrors.dotsrc.org/cran/bin/windows/base/release.htm.

Note for Windows system managers: the "R Windows FAQ" in the same directory as the setup program has extensive information on administering R for Windows.

The setup installs the base R system and some of the most common libraries (Table 4).

It also installs **six manuals** in both PDF and HTML format: (1) An Introduction to R; (2) R Installation and Administration; (3) R Language Definition; (4) Reference Index; (5) R Data Import/Export; (6) Writing R Extensions.

base	The R Base Package	
chron	Chronological objects which can handle dates and times	
class	Functions for classification	
cluster	Functions for clustering	
datasets	The R Datasets Package	
foreign	Read data stored by Minitab, S, SAS, SPSS, Stata,	
graphics	The R Graphics Package	
grDevices	The R graphics devices;s upport for colours and fonts	
grid	The Grid Graphics Package	
KernSmooth	Functions for kernel smoothing	
lattice	Lattice Graphics	
MASS	Main Library of Venables and Ripley's MASS	
methods	Formal Methods and Classes	
mle	Maximum likelihood estimation	
multcomp	Multiple Tests and Simultaneous Confidence Intervals	
mvtnorm	Multivariate Normal and T Distribution	
nlme	Linear and nonlinear mixed effects models	
nnet	Feed-forward neural networks	
rgl	3D visualization device system (OpenGL)	
rpart	Recursive partitioning	
SparseM	Sparse Linear Algebra	
spatial	Functions for Kriging and point pattern analysis	
splines	Regression Spline Functions and Classes	
stats	The R Stats Package (includes classical tests, exploratory	
	data anlysis, smoothing and local methods for regres-	
	sion, multivariate analysis, non-linear least squares, time	
	series analysis)	
stepfun	Step Functions, including Empirical Distributions	
survival	Survival analysis, including penalised likelihood.	
utils	R Utilities	

Table 4: Most important packages in the base R 2.1 distribution for Windows; libraries loaded when R starts are shown in **boldface**.

abind	Combine multi-dimensional arrays
akima	Interpolation of irregularly spaced data
car	Companion to Applied Regression
effects	Effect displays for linear and generalized linear models
gstat	Geostatistical modelling, prediction and simulation
lmtest	Testing linear regression models
Rcmdr	R Commander GUI

Table 5: Extra packages installed at ITC; these are not loaded by default

Other operating systems For Mac OS X or a Unix-based system, follow the appropriate links from the CRAN home page and read the installation instructions.

Cross-platform The JGR project at the University of Augsburg (D) 35 has developed a Java-based GUI which runs on any platform with industry-standard Java Runtime Engine, including Mac OS X and most Windows systems. This includes the iplots interactive graphics package.

B.1 Installing new packages

The ITC installation includes the most popular optional packages. If you need to install packages on your own copy of R, use the Packages | Install Package(s) from CRAN ... menu item while connected to the Internet. A brief description and full documentation of the available packages is available from the CRAN home page; click on the link for "Packages". Table 5 lists the extra packages installed on the ITC network. New packages on the network must be installed by the ITC computer department; you can install packages on your own system if you were able to install the base program.

B.2 Customizing your installation

(This section is not necessary to get started with R.)

Many aspects of R's interactive behaviour can be changed to suit your preferences. For example, you can set up your own copy of R to load libraries at startup, and you can also change many default options. You do this by creating a file named .Rprofile either in your *home directory*, or in a *working directory* from which you will start R, or both. The second of these is used if it exists, otherwise the master copy in the home directory.

To see the current options setings, use the options method without any

³⁵ http://www.rosuda.org/

arguments; it's easier to review these by viewing its structure. Individual settings can then be viewed by their field name.

Here is an example .Rprofile which sets some options and loads some libraries that will always be used in a project:

C An example script

This is an example of a moderately complicated script, which gives both a numerical and a visual impression of the variability of small random samples. The output is shown in Figure 12 on the following page. If you want to experiment with the script, cut-and-paste it into a text editor, modify it as you like (for example, change the sample size n or the number of replications), save it as a command file, and run it with the source method as explained in §3.9.

You prepare this with a plain-text editor like Notepad in a text file, for example plot4.R and then "source" it into R, which executes the commands immediately.

```
> source("plot4.R")
```

If you want to change the plotting parameters, you have to change the script and re-source it. The next section offers a better solution.

A note on R style It is good practice to make all parameters into variables at the beginning of the script, so they can be easily adjusted. If you find yourself repeating the same number in many expressions, it probably should be converted to a variable. Examples here are the sample size and parameters of the normal distribution. You could write:

```
v <- rnorm(30, 180, 20)
hist(v, breaks = seq(800, 280, by=(20/3)))
points(x, dnorm(x, 180, 20)*(30*(20/3)))

but it is more elegant to write:

n <- 30; mu <- 180; sd <- 20; bin.width <- sd/3
v <- rnorm(n, mu, sd)
hist(v, breaks = seq(mu-5*sd, mu+5*sd, by=bin.width))
points(x, dnorm(x, mu, sd)*(n*bin.width))</pre>
```

```
### visualise the variability of small random samples
                               # sample size
n <- 30
                               # number of plot rows, columns
rows <- 2; cols <- 2; reps <- rows*cols
                               # parameters of the normal distribution
mu <- 180; sd <- 20
                               # set up graphic display
par(mfrow=c(rows, cols))
                               # number of s.d.'s for histogram display
sdd <- 3.5
                               # compute bin width from s.d and
                                 the number of bars for each
bin.width=sd/3
                               # scale x-axis
x.min <- mu-(sdd*sd); x.max <- mu+(sdd*sd)</pre>
                               # scale y-axis
y.max <- n*0.5*bin.width/sd
                               # compute and display each graph
for (i in 1:reps) {
  v <- rnorm(n, mu, sd)</pre>
  hist(v, xlim=c(x.min,x.max), ylim=c(0, y.max),
       breaks = seq(mu-5*sd, mu+5*sd, by=bin.width),
       main="", xlab=paste("Sample",i));
  x \leftarrow seq(x.min, x.max, length=120)
                              # true normal distribution
  points(x,dnorm(x, mu, sd)*(n*bin.width),
         type="l", col="blue", lty=1, lwd=1.8)
                               # distribution estimated from sample
  points(x,dnorm(x, mean(v), sd(v))*(n*bin.width),
         type="1", col="red", lty=2, lwd=1.8)
                               # print sample params.
                               # and Pr(Type I error)
  text(x.min, 0.9*y.max, paste("mean:", round(mean(v),2)),pos=4)
  text(x.min, 0.8*y.max, paste("sdev:", round(sd(v),2)),pos=4)
  text(x.min, 0.7*y.max,
       paste("Pr(t):", round((t.test(v, mu=mu))$p.value,2)),pos=4)
}
                               # clean up
par(mfrow=c(1,1))
rm(n, rows, cols, reps, mu, sd, v, i, sdd, bin.width, x.min, x.max, y.max, x)
```

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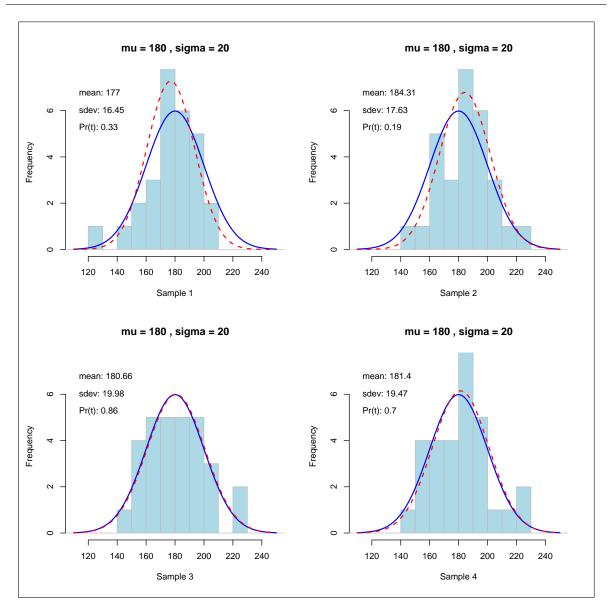


Figure 12: A visualisation of the variability of small random samples. Each sample of 30 has been divided into ten histogram bins on [130...230]. The blue (solid) normal curves all have $\mu=180$ and $\sigma=20$; the red (dashed) normal curves are estimated from each sample. Note the bias (left or right of the blue curves) and variances (narrower or wider than the blue curves).

D An example function

A more powerful approach than writing and sourcing a script is to write a *function* which is loaded into the workspace with the source method and then run as if it were a built-in R method. The main advantage is that you can make the function adaptable with a set of *arguments* (parameters that can be sent to the function), so you don't have to edit the script.

Here we have converted the script of Appendix C into a function, with only one required *argument* (the sample size) and six optional arguments which control aspects of the display, for example the number of samples to compare on one plot.

You prepare this with a plain-text editor like Notepad in a text file, for example plot_normals.R and then read it into R. Once it is in the workspace (which you can verify with the ls method), you run it just like a built-in R method.

```
> source("plot_normals.R")
> ls()
plot.normals
> plot.normals(60)
> plot.normals(60, mu=100, sd=15)
> plot.normals(60, rows=3, cols=3, mu=100, sd=15)
```

```
### function to visualise the variability of small random samples
##
    required arguments:
##
       n : sample size
    arguments with reasonable defaults:
       rows, cols: dimensions of display
##
       mu, sd: mean, s.d. of normal distribution to sample
##
       bsd: histogram bins to represent each s.d.
##
       sdd : +/- number of s.d. to display
plot.normals <- function(n, rows=2, cols=2, mu=0, sd=1,
                        bsd = 2, sdd=3.5) {
                               # set up graphic display
par(mfrow=c(rows, cols))
                                # number of random samples
reps <- rows*cols
                                # histogram bin width
bin.width=sd/bsd
                                # scale x-axis
x.min <- mu-(sdd*sd); x.max <- mu+(sdd*sd)</pre>
                                # scale y-axis; max. dnorm(1,0)=0.3989
                                # adjust to sample and bin sizes
                                # and normalize by s.d.
                                # and leave room for higher bars
y.max <- n*0.5*bin.width/sd
                                # compute and display each graph
for (i in 1:reps) {
  v <- rnorm(n, mu, sd)</pre>
  hist(v, xlim=c(x.min,x.max), ylim=c(0,y.max),
       breaks = seq(mu-5*sd, mu+5*sd, by=bin.width),
       main=paste("mu =", mu, ", sigma =", sd),
       xlab=paste("Sample",i), col="lightblue", border="gray",
       freq=TRUE)
  x <- seq(x.min,x.max,length=120)</pre>
                                # true normal distribution
  points(x,dnorm(x, mu, sd)*(n*bin.width),
         type="1", col="blue", lty=1, lwd=1.8)
                                # normal dist. estimated from sample
  points(x,dnorm(x,\ mean(v),\ sd(v))*(n*bin.width),
         type="1", col="red", lty=2, lwd=1.8)
                                # print sample params.
                                # and Pr(Type I error)
  text(x.min, 0.9*y.max, paste("mean:", round(mean(v),2)),pos=4) text(x.min, 0.8*y.max, paste("sdev:", round(sd(v),2)),pos=4)
  text(x.min, 0.7*y.max,
       paste("Pr(t):", round((t.test(v, mu=mu))$p.value,2)),pos=4)
}
                                # clean up
par(mfrow=c(1,1))
```

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