# A Handbook of Statistical Analyses Using ${\bf R}$

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# Preface

This book is intended as a guide to data analysis with the R system for statistical computing. R is an environment incorporating an implementation of the S programming language, which is powerful, flexible and has excellent graphical facilities (R Development Core Team, 2005). In the Handbook we aim to give relatively brief and straightforward descriptions of how to conduct a range of statistical analyses using R. Each chapter deals with the analysis appropriate for one or several data sets. A brief account of the relevant statistical background is included in each chapter along with appropriate references, but our prime focus is on how to use R and how to interpret results. We hope the book will provide students and researchers in many disciplines with a self-contained means of using R to analyse their data. R is an open-source project developed by dozens of volunteers for more than ten years now and is available from the Internet under the General Public Licence. R has become the lingua franca of statistical computing. Increasingly, implementations of new statistical methodology first appear as R add-on packages. In some communities, such as in bioinformatics, R already is the primary workhorse for statistical analyses. Because the sources of the R system are open and available to everyone without restrictions and because of its powerful language and graphical capabilities, R has started to become the main computing engine for reproducible statistical research (Leisch, 2002a,b, 2003, Leisch and Rossini, 2003, Gentleman, 2005). For a reproducible piece of research, the original observations, all data preprocessing steps, the statistical analysis as well as the scientific report form a unity and all need to be available for inspection, reproduction and modification by the readers. Reproducibility is a natural requirement for textbooks such as the 'Handbook of Statistical Analyses Using R' and therefore this book is fully reproducible using an R version greater or equal to 2.4.0. All analyses and results, including figures and tables, can be reproduced by the reader without having to retype a single line of R code. The data sets presented in this book are collected in a dedicated add-on package called HSAUR accompanying this book. The package can be installed from the Comprehensive R Archive Network (CRAN) via

R> install.packages("HSAUR")

and its functionality is attached by

#### R> library("HSAUR")

The relevant parts of each chapter are available as a *vignette*, basically a document including both the R sources and the rendered output of every

analysis contained in the book. For example, the first chapter can be inspected by

R> vignette("Ch\_introduction\_to\_R", package = "HSAUR")

and the R sources are available for reproducing our analyses by

R> edit(vignette("Ch\_introduction\_to\_R", package = "HSAUR"))

An overview on all chapter vignettes included in the package can be obtained from

R> vignette(package = "HSAUR")

We welcome comments on the R package HSAUR, and where we think these add to or improve our analysis of a data set we will incorporate them into the package and, hopefully at a later stage, into a revised or second edition of the book. Plots and tables of results obtained from R are all labelled as 'Figures' in the text. For the graphical material, the corresponding figure also contains the 'essence' of the R code used to produce the figure, although this code may differ a little from that given in the HSAUR package, since the latter may include some features, for example thicker line widths, designed to make a basic plot more suitable for publication. We would like to thank the R Development Core Team for the R system, and authors of contributed add-on packages, particularly Uwe Ligges and Vince Carey for helpful advice on scatterplot3d and gee. Kurt Hornik, Ludwig A. Hothorn, Fritz Leisch and Rafael Weißbach provided good advice with some statistical and technical problems. We are also very grateful to Achim Zeileis for reading the entire manuscript, pointing out inconsistencies or even bugs and for making many suggestions which have led to improvements. Lastly we would like to thank the CRC Press staff, in particular Rob Calver, for their support during the preparation of the book. Any errors in the book are, of course, the joint responsibility of the two authors.

> Brian S. Everitt and Torsten Hothorn London and Erlangen, December 2005

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# CHAPTER 1

# An Introduction to R

# 1.1 What Is R?

The R system for statistical computing is an environment for data analysis and graphics. The root of R is the S language, developed by John Chambers and colleagues (Becker et al., 1988, Chambers and Hastie, 1992, Chambers, 1998) at Bell Laboratories (formerly AT&T, now owned by Lucent Technologies) starting in the 1960s. The S language was designed and developed as a programming language for data analysis tasks but in fact it is a full-featured programming language in its current implementations. The development of the R system for statistical computing is heavily influenced by the open source idea: The base distribution of R and a large number of user contributed extensions are available under the terms of the Free Software Foundation's GNU General Public License in source code form. This licence has two major implications for the data analyst working with R. The complete source code is available and thus the practitioner can investigate the details of the implementation of a special method, can make changes and can distribute modifications to colleagues. As a side-effect, the R system for statistical computing is available to everyone. All scientists, especially including those working in developing countries, have access to state-of-the-art tools for statistical data analysis without additional costs. With the help of the R system for statistical computing, research really becomes reproducible when both the data and the results of all data analysis steps reported in a paper are available to the readers through an R transcript file. R is most widely used for teaching undergraduate and graduate statistics classes at universities all over the world because students can freely use the statistical computing tools. The base distribution of R is maintained by a small group of statisticians, the R Development Core Team. A huge amount of additional functionality is implemented in add-on packages authored and maintained by a large group of volunteers. The main source of information about the R system is the world wide web with the official home page of the R project being

# http://www.R-project.org

All resources are available from this page: the R system itself, a collection of add-on packages, manuals, documentation and more. The intention of this chapter is to give a rather informal introduction to basic concepts and data manipulation techniques for the R novice. Instead of a rigid treatment of the technical background, the most common tasks are illustrated by practical

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examples and it is our hope that this will enable readers to get started without too many problems.

# 1.2 Installing R

The R system for statistical computing consists of two major parts: the base system and a collection of user contributed add-on packages. The R language is implemented in the base system. Implementations of statistical and graphical procedures are separated from the base system and are organised in the form of packages. A package is a collection of functions, examples and documentation. The functionality of a package is often focused on a special statistical methodology. Both the base system and packages are distributed via the Comprehensive R Archive Network (CRAN) accessible under

http://CRAN.R-project.org

#### 1.2.1 The Base System and the First Steps

The base system is available in source form and in precompiled form for various Unix systems, Windows platforms and Mac OS X. For the data analyst, it is sufficient to download the precompiled binary distribution and install it locally. Windows users follow the link

# http://CRAN.R-project.org/bin/windows/base/release.htm

download the corresponding file (currently named rw2040.exe), execute it locally and follow the instructions given by the installer.



>

Depending on the operating system, R can be started either by typing 'R' on the shell (Unix systems) or by clicking on the R symbol (as shown left) created by the installer (Windows). R comes without any frills and on start up shows simply a short introductory message including the version number and a prompt '>':

R : Copyright 2006 The R Foundation for Statistical Computing Version 2.4.0 (2006-10-03), ISBN 3-900051-07-0

R is free software and comes with ABSOLUTELY NO WARRANTY. You are welcome to redistribute it under certain conditions. Type 'license()' or 'licence()' for distribution details.

R is a collaborative project with many contributors. Type 'contributors()' for more information and 'citation()' on how to cite R or R packages in publications.

Type 'demo()' for some demos, 'help()' for on-line help, or 'help.start()' for an HTML browser interface to help. Type 'q()' to quit R.

#### INSTALLING R

One can change the appearance of the prompt by

> options(prompt = "R> ")

and we will use the prompt R> for the display of the code examples throughout this book. Essentially, the R system evaluates commands typed on the R prompt and returns the results of the computations. The end of a command is indicated by the return key. Virtually all introductory texts on R start with an example using R as pocket calculator, and so do we:

R> x <- sqrt(25) + 2

This simple statement asks the R interpreter to calculate  $\sqrt{25}$  and then to add 2. The result of the operation is assigned to an R object with variable name x. The assignment operator <- binds the value of its right hand side to a variable name on the left hand side. The value of the object x can be inspected simply by typing

R> x

[1] 7

which, implicitly, calls the print method:

R> print(x)

[1] 7

# 1.2.2 Packages

The base distribution already comes with some high-priority add-on packages, namely

| KernSmooth | MASS    | boot     | class     |
|------------|---------|----------|-----------|
| cluster    | foreign | lattice  | mgcv      |
| nlme       | nnet    | rpart    | spatial   |
| survival   | base    | datasets | grDevices |
| graphics   | grid    | methods  | splines   |
| stats      | stats4  | tcltk    | tools     |
| utils      |         |          |           |

The packages listed here implement standard statistical functionality, for example linear models, classical tests, a huge collection of high-level plotting functions or tools for survival analysis; many of these will be described and used in later chapters. Packages not included in the base distribution can be installed directly from the R prompt. At the time of writing this chapter, 858 user contributed packages covering almost all fields of statistical methodology were available. Given that an Internet connection is available, a package is installed by supplying the name of the package to the function install.packages. If, for example, add-on functionality for robust estimation of covariance matrices via sandwich estimators is required (for example in Chapter 11), the sandwich package (Zeileis, 2004) can be downloaded and installed via

R> install.packages("sandwich")

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The package functionality is available after *attaching* the package by

R> library("sandwich")

A comprehensive list of available packages can be obtained from

http://CRAN.R-project.org/src/contrib/PACKAGES.html

Note that on Windows operating systems, precompiled versions of packages are downloaded and installed. In contrast, packages are compiled locally before they are installed on Unix systems.

## 1.3 Help and Documentation

Roughly, three different forms of documentation for the R system for statistical computing may be distinguished: online help that comes with the base distribution or packages, electronic manuals and publications work in the form of books etc. The help system is a collection of manual pages describing each user-visible function and data set that comes with R. A manual page is shown in a pager or web browser when the name of the function we would like to get help for is supplied to the help function

R> help("mean")

or, for short,

R> ?mean

Each manual page consists of a general description, the argument list of the documented function with a description of each single argument, information about the return value of the function and, optionally, references, cross-links and, in most cases, executable examples. The function help.search is helpful for searching within manual pages. An overview on documented topics in an add-on package is given, for example for the *sandwich* package, by

# R> help(package = "sandwich")

Often a package comes along with an additional document describing the package functionality and giving examples. Such a document is called a *vignette* (Leisch, 2003, Gentleman, 2005). The *sandwich* package vignette is opened using

# R> vignette("sandwich")

More extensive documentation is available electronically from the collection of manuals at

# http://CRAN.R-project.org/manuals.html

For the beginner, at least the first and the second document of the following four manuals (R Development Core Team, 2005a,b,c,d) are mandatory:

- An Introduction to R: A more formal introduction to data analysis with R than this chapter.
- **R Data Import/Export:** A very useful description of how to read and write various external data formats.

#### DATA OBJECTS IN R

- **R Installation and Administration:** Hints for installing R on special platforms.
- Writing R Extensions: The authoritative source on how to write R programs and packages.

Both printed and online publications are available, the most important ones are 'Modern Applied Statistics with S' (Venables and Ripley, 2002), 'Introductory Statistics with R' (Dalgaard, 2002), 'R Graphics' (Murrell, 2005) and the R Newsletter, freely available from

# http://CRAN.R-project.org/doc/Rnews/

In case the electronically available documentation and the answers to frequently asked questions (FAQ), available from

http://CRAN.R-project.org/faqs.html

have been consulted but a problem or question remains unsolved, the **r-help** email list is the right place to get answers to well-thought-out questions. It is helpful to read the posting guide

```
http://www.R-project.org/posting-guide.html
```

before starting to ask.

# 1.4 Data Objects in R

The data handling and manipulation techniques explained in this chapter will be illustrated by means of a data set of 2000 world leading companies, the Forbes 2000 list for the year 2004 collected by 'Forbes Magazine'. This list is originally available from

```
http://www.forbes.com
```

and, as an R data object, it is part of the *HSAUR* package (*Source*: From Forbes.com, New York, New York, 2004. With permission.). In a first step, we make the data available for computations within R. The data function searches for data objects of the specified name ("Forbes2000") in the package specified via the package argument and, if the search was successful, attaches the data object to the global environment:

```
R> data("Forbes2000", package = "HSAUR")
R> ls()
```

[1] "Forbes2000" "a" "x"

The output of the 1s function lists the names of all objects currently stored in the global environment, and, as the result of the previous command, a variable named Forbes2000 is available for further manipulation. The variable x arises from the pocket calculator example in Subsection 1.2.1. As one can imagine, printing a list of 2000 companies via

R> print(Forbes2000)

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category sales rank name country Citigroup United States Banking 94.71 1 1 2 2 General Electric United States Conglomerates 134.19 3 3 American Intl Group United States Insurance 76.66 profits assets marketvalue 17.85 1264.03 1 255.30 2 15.59 626.93 328.54 3 6.46 647.66 194.87

. . .

will not be particularly helpful in gathering some initial information about the data; it is more useful to look at a description of their structure found by using the following command

# R> str(Forbes2000)

```
'data.frame':
                    2000 obs. of 8 variables:
             : int 12345...
$ rank
                   "Citigroup" "General Electric" ...
$ name
             : chr
$ country
            : Factor w/ 61 levels "Africa", "Australia",...: 60 60 60 60 56 ...
            : Factor w/ 27 levels "Aerospace & defense",..: 2 6 16 19 19 ...
$ category
                    94.7 134.2 ...
$ sales
            : num
$ profits
             : num 17.9 15.6 ...
$ assets
            : num 1264 627 ...
$ marketvalue: num 255 329 ...
```

The output of the str function tells us that Forbes2000 is an object of class *data.frame*, the most important data structure for handling tabular statistical data in R. As expected, information about 2000 observations, i.e., companies, are stored in this object. For each observation, the following eight variables are available:

rank: the ranking of the company,

name: the name of the company,

country: the country the company is situated in,

category: a category describing the products the company produces,

sales: the amount of sales of the company in billion US dollars,

profits: the profit of the company in billion US dollars,

assets: the assets of the company in billion US dollars,

marketvalue: the market value of the company in billion US dollars.

A similar but more detailed description is available from the help page for the Forbes2000 object:

R> help("Forbes2000")

or

R> ?Forbes2000

#### DATA OBJECTS IN R

All information provided by str can be obtained by specialised functions as well and we will now have a closer look at the most important of these. The R language is an object-oriented programming language, so every object is an instance of a class. The name of the class of an object can be determined by

#### R> class(Forbes2000)

[1] "data.frame"

Objects of class *data.frame* represent data the traditional table oriented way. Each row is associated with one single observation and each column corresponds to one variable. The dimensions of such a table can be extracted using the dim function

R> dim(Forbes2000)

[1] 2000 8

Alternatively, the numbers of rows and columns can be found using

R> nrow(Forbes2000)

[1] 2000

R> ncol(Forbes2000)

[1] 8

The results of both statements show that Forbes2000 has 2000 rows, i.e., observations, the companies in our case, with eight variables describing the observations. The variable names are accessible from

#### R> names(Forbes2000)

| [1] | "rank"  | "name"    | "country" | "category"    |
|-----|---------|-----------|-----------|---------------|
| [5] | "sales" | "profits" | "assets"  | "marketvalue" |

The values of single variables can be extracted from the Forbes2000 object by their names, for example the ranking of the companies

R> class(Forbes2000[, "rank"])

[1] "integer"

is stored as an integer variable. Brackets [] always indicate a subset of a larger object, in our case a single variable extracted from the whole table. Because *data.frames* have two dimensions, observations and variables, the comma is required in order to specify that we want a subset of the second dimension, i.e., the variables. The rankings for all 2000 companies are represented in a *vector* structure the length of which is given by

R> length(Forbes2000[, "rank"])

[1] 2000

A *vector* is the elementary structure for data handling in R and is a set of simple elements, all being objects of the same class. For example, a simple vector of the numbers one to three can be constructed by one of the following commands

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```
R> 1:3
[1] 1 2 3
R> c(1, 2, 3)
[1] 1 2 3
R> seq(from = 1, to = 3, by = 1)
[1] 1 2 3
```

The unique names of all 2000 companies are stored in a character vector R> class(Forbes2000[, "name"])

[1] "character"

R> length(Forbes2000[, "name"])

[1] 2000

and the first element of this vector is

```
R> Forbes2000[, "name"][1]
```

```
[1] "Citigroup"
```

Because the companies are ranked, Citigroup is the world's largest company according to the Forbes 2000 list. Further details on vectors and subsetting are given in Section 1.6. Nominal measurements are represented by *factor* variables in R, such as the category of the company's business segment

```
R> class(Forbes2000[, "category"])
```

[1] "factor"

Objects of class *factor* and *character* basically differ in the way their values are stored internally. Each element of a vector of class *character* is stored as a *character* variable whereas an integer variable indicating the level of a *factor* is saved for *factor* objects. In our case, there are

R> nlevels(Forbes2000[, "category"])

[1] 27

different levels, i.e., business categories, which can be extracted by
R> levels(Forbes2000[, "category"])

```
[1] "Aerospace & defense"
[2] "Banking"
[3] "Business services & supplies"
...
```

As a simple summary statistic, the frequencies of the levels of such a factor variable can be found from

```
R> table(Forbes2000[, "category"])
```

| Aerospace & defense          | Banking |
|------------------------------|---------|
| 19                           | 313     |
| Business services & supplies |         |
| 70                           |         |

#### DATA IMPORT AND EXPORT

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The sales, assets, profits and market value variables are of type numeric, the natural data type for continuous or discrete measurements, for example

R> class(Forbes2000[, "sales"])

[1] "numeric"

and simple summary statistics such as the mean, median and range can be found from

R> median(Forbes2000[, "sales"])

[1] 4.365

R> mean(Forbes2000[, "sales"])

[1] 9.69701

R> range(Forbes2000[, "sales"])

[1] 0.01 256.33

The summary method can be applied to a numeric vector to give a set of useful summary statistics namely the minimum, maximum, mean, median and the 25% and 75% quartiles; for example

```
R> summary(Forbes2000[, "sales"])
```

Min. 1st Qu. Median Mean 3rd Qu. Max. 0.010 2.018 4.365 9.697 9.548 256.300

#### 1.5 Data Import and Export

In the previous section, the data from the Forbes 2000 list of the world's largest companies were loaded into R from the *HSAUR* package but we will now explore practically more relevant ways to import data into the R system. The most frequent data formats the data analyst is confronted with are comma separated files, Excel spreadsheets, files in SPSS format and a variety of SQL data base engines. Querying data bases is a non-trivial task and requires additional knowledge about querying languages and we therefore refer to the 'R Data Import/Export' manual – see Section 1.3. We assume that a comma separated file containing the Forbes 2000 list is available as Forbes2000.csv (such a file is part of the *HSAUR* source package in directory HSAUR/inst/rawdata). When the fields are separated by commas and each row begins with a name (a text format typically created by Excel), we can read in the data as follows using the read.table function

```
R> csvForbes2000 <- read.table("Forbes2000.csv", header = TRUE,
+ sep = ",", row.names = 1)
```

The argument header = TRUE indicates that the entries in the first line of the text file "Forbes2000.csv" should be interpreted as variable names. Columns are separated by a comma (sep = ","), users of continental versions of Excel should take care of the character symbol coding for decimal points (by default

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dec = "."). Finally, the first column should be interpreted as row names but
not as a variable (row.names = 1). Alternatively, the function read.csv can
be used to read comma separated files. The function read.table by default
guesses the class of each variable from the specified file. In our case, character
variables are stored as factors

R> class(csvForbes2000[, "name"])

[1] "factor"

which is only suboptimal since the names of the companies are unique. However, we can supply the types for each variable to the colClasses argument

```
R> csvForbes2000 <- read.table("Forbes2000.csv", header = TRUE,
+ sep = ",", row.names = 1, colClasses = c("character",
+ "integer", "character", "factor", "factor",
+ "numeric", "numeric", "numeric", "numeric"))
R> class(csvForbes2000[, "name"])
```

[1] "character"

and check if this object is identical with our previous Forbes 2000 list object R> all.equal(csvForbes2000, Forbes2000)

[1] TRUE

The argument colClasses expects a character vector of length equal to the number of columns in the file. Such a vector can be supplied by the c function that combines the objects given in the parameter list into a *vector* 

```
R> classes <- c("character", "integer", "character",
+ "factor", "factor", "numeric", "numeric", "numeric",
+ "numeric")
R> length(classes)
[1] 9
```

R> class(classes)

[1] "character"

An R interface to the open data base connectivity standard (ODBC) is available in package *RODBC* and its functionality can be used to assess Excel and Access files directly:

```
R> library("RODBC")
```

```
R> cnct <- odbcConnectExcel("Forbes2000.xls")</pre>
```

```
R> sqlQuery(cnct, "select * from \"Forbes2000$\"")
```

The function odbcConnectExcel opens a connection to the specified Excel or Access file which can be used to send SQL queries to the data base engine and retrieve the results of the query. Files in SPSS format are read in a way similar to reading comma separated files, using the function read.spss from package *foreign* (which comes with the base distribution). Exporting data from R is now rather straightforward. A comma separated file readable by Excel can be constructed from a *data.frame* object via

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```
R> write.table(Forbes2000, file = "Forbes2000.csv",
+ sep = ",", col.names = NA)
```

The function write.csv is one alternative and the functionality implemented in the *RODBC* package can be used to write data directly into Excel spreadsheets as well. Alternatively, when data should be saved for later processing in R only, R objects of arbitrary kind can be stored into an external binary file via

R> save(Forbes2000, file = "Forbes2000.rda")

where the extension .rda is standard. We can get the file names of all files with extension .rda from the working directory

R> list.files(pattern = ".rda")

[1] "Forbes2000.rda"

and we can load the contents of the file into R by

R> load("Forbes2000.rda")

# 1.6 Basic Data Manipulation

The examples shown in the previous section have illustrated the importance of data.frames for storing and handling tabular data in R. Internally, a data.frame is a *list* of vectors of a common length n, the number of rows of the table. Each of those vectors represents the measurements of one variable and we have seen that we can access such a variable by its name, for example the names of the companies

```
R> companies <- Forbes2000[, "name"]</pre>
```

Of course, the companies vector is of class *character* and of length 2000. A subset of the elements of the vector companies can be extracted using the [] subset operator. For example, the largest of the 2000 companies listed in the Forbes 2000 list is

R> companies[1]

[1] "Citigroup"

and the top three companies can be extracted utilising an integer vector of the numbers one to three:

R> 1:3

[1] 1 2 3

R> companies[1:3]

[1] "Citigroup" "General Electric"
[3] "American Intl Group"

In contrast to indexing with positive integers, negative indexing returns all elements which are *not* part of the index vector given in brackets. For example, all companies except those with numbers four to two-thousand, i.e., the top three companies, are again

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```
R> companies[-(4:2000)]
```

[1] "Citigroup" "General Electric"
[3] "American Intl Group"

The complete information about the top three companies can be printed in a similar way. Because *data.frames* have a concept of rows and columns, we need to separate the subsets corresponding to rows and columns by a comma. The statement

R> Forbes2000[1:3, c("name", "sales", "profits", "assets")]

name sales profits assets 1 Citigroup 94.71 17.85 1264.03 2 General Electric 134.19 15.59 626.93 3 American Intl Group 76.66 6.46 647.66

extracts the variables name, sales, profits and assets for the three largest companies. Alternatively, a single variable can be extracted from a *data.frame* by

R> companies <- Forbes2000\$name

which is equivalent to the previously shown statement

R> companies <- Forbes2000[, "name"]

We might be interested in extracting the largest companies with respect to an alternative ordering. The three top selling companies can be computed along the following lines. First, we need to compute the ordering of the companies' sales

```
R> order_sales <- order(Forbes2000$sales)
```

which returns the indices of the ordered elements of the numeric vector sales. Consequently the three companies with the lowest sales are

R> companies[order\_sales[1:3]]

```
[1] "Custodia Holding" "Central European Media"
[3] "Minara Resources"
```

The indices of the three top sellers are the elements 1998, 1999 and 2000 of the integer vector order\_sales

Another way of selecting vector elements is the use of a logical vector being TRUE when the corresponding element is to be selected and FALSE otherwise. The companies with assets of more than 1000 billion US dollars are

```
R> Forbes2000[Forbes2000$assets > 1000, c("name", "sales",
+ "profits", "assets")]
```

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```
name sales profits assets
1 Citigroup 94.71 17.85 1264.03
9 Fannie Mae 53.13 6.48 1019.17
403 Mizuho Financial 24.40 -20.11 1115.90
```

where the expression Forbes2000sassets > 1000 indicates a logical vector of length 2000 with

R> table(Forbes2000\$assets > 1000)

FALSE TRUE 1997 3

elements being either FALSE or TRUE. In fact, for some of the companies the measurement of the profits variable are missing. In R, missing values are treated by a special symbol, NA, indicating that this measurement is not available. The observations with profit information missing can be obtained via

```
R> na_profits <- is.na(Forbes2000$profits)
R> table(na_profits)
na_profits
      TRUE
FALSE
 1995
          5
R> Forbes2000[na_profits, c("name", "sales", "profits",
      "assets")]
                       name sales profits assets
772
                        AMP
                             5.40
                                        NA
                                            42.94
1085
                                            51.65
                        HHG
                             5.68
                                        NA
1091
                                            10.59
                        NTL
                             3.50
                                        NA
1425
                                             8.58
          US Airways Group
                             5.50
                                        NA
1909 Laidlaw International
                                             3.98
                             4.48
                                        NA
```

where the function is.na returns a logical vector being TRUE when the corresponding element of the supplied vector is NA. A more comfortable approach is available when we want to remove all observations with at least one missing value from a *data.frame* object. The function complete.cases takes a *data.frame* and returns a logical vector being TRUE when the corresponding observation does not contain any missing value:

R> table(complete.cases(Forbes2000))

FALSE TRUE 5 1995

Subsetting *data.frames* driven by logical expressions may induce a lot of typing which can be avoided. The **subset** function takes a *data.frame* as first argument and a logical expression as second argument. For example, we can select a subset of the Forbes 2000 list consisting of all companies situated in the United Kingdom by

R> UKcomp <- subset(Forbes2000, country == "United Kingdom")
R> dim(UKcomp)

[1] 137 8

i.e., 137 of the 2000 companies are from the UK. Note that it is not necessary to extract the variable country from the *data.frame* Forbes2000 when formulating the logical expression.

# 1.7 Simple Summary Statistics

Two functions are helpful for getting an overview about R objects: str and summary, where str is more detailed about data types and summary gives a collection of sensible summary statistics. For example, applying the summary method to the Forbes2000 data set,

# R> summary(Forbes2000)

results in the following output

| rank              | name      |           |             | country           |
|-------------------|-----------|-----------|-------------|-------------------|
| Min. : 1.0        | Length:20 | 00        | United Sta  | tes :751          |
| 1st Qu.: 500.8    | Class :ch | aracter d | Japan       | :316              |
| Median :1000.5    | Mode :ch  | aracter   | United King | gdom <b>:</b> 137 |
| Mean :1000.5      |           | (         | Germany     | : 65              |
| 3rd Qu.:1500.2    |           |           | France      |                   |
| Max. :2000.0      |           | (         | Canada      | : 56              |
|                   |           |           | (Other)     | :612              |
|                   | category  | sa.       | les         |                   |
| Banking           | : 31      | 3 Min.    | : 0.010     |                   |
| Diversified final |           |           | .: 2.018    |                   |
| Insurance         | : 11.     | 2 Median  | : 4.365     |                   |
| Utilities         | : 11      | 0 Mean    | : 9.697     |                   |
| Materials         | : 9       | 7 3rd Ou  | .: 9.547    |                   |
| Oil & gas operat. | ions : 9  | 0 Max.    | :256.330    |                   |
|                   | :112      |           |             |                   |
| profits           |           |           | marketva    | alue              |
| Min. :-25.8300    |           | : 0.270   |             |                   |
| 1st Qu.: 0.0800   | 1st Qu.   | : 4.025   | 1st Qu.:    | 2.72              |
| Median : 0.2000   |           | : 9.345   |             |                   |
| Mean : 0.3811     | Mean      | : 34.042  | Mean :      | 11.88             |
| 3rd Qu.: 0.4400   | 3rd Ou.   | : 22.793  | 3rd Qu.:    | 10.60             |
| Max. : 20.9600    |           | :1264.030 | Max. :      |                   |
| NA's : 5.0000     |           |           |             |                   |

From this output we can immediately see that most of the companies are situated in the US and that most of the companies are working in the banking sector as well as that negative profits, or losses, up to 26 billion US dollars occur. Internally, summary is a so-called *generic function* with methods for a multitude of classes, i.e., summary can be applied to objects of different classes and will report sensible results. Here, we supply a *data.frame* object to summary where it is natural to apply summary to each of the variables in this *data.frame*. Because a *data.frame* is a *list* with each variable being an element of that *list*, the same effect can be achieved by

#### SIMPLE SUMMARY STATISTICS

# R> lapply(Forbes2000, summary)

The members of the apply family help to solve recurring tasks for each element of a *data.frame*, *matrix*, *list* or for each level of a factor. It might be interesting to compare the profits in each of the 27 categories. To do so, we first compute the median profit for each category from

# R> mprofits <- tapply(Forbes2000\$profits, Forbes2000\$category, + median, na.rm = TRUE)

a command that should be read as follows. For each level of the factor category, determine the corresponding elements of the numeric vector profits and supply them to the median function with additional argument na.rm = TRUE. The latter one is necessary because profits contains missing values which would lead to a non-sensible result of the median function

# R> median(Forbes2000\$profits)

[1] NA

The three categories with highest median profit are computed from the vector of sorted median profits

#### R> rev(sort(mprofits))[1:3]

| Oil & gas operations          | Drugs & biotechnology |
|-------------------------------|-----------------------|
| 0.35                          | 0.35                  |
| Household & personal products |                       |
| 0.31                          |                       |

where **rev** rearranges the vector of median profits **sort**ed from smallest to largest. Of course, we can replace the **median** function with **mean** or whatever is appropriate in the call to **tapply**. In our situation, **mean** is not a good choice, because the distributions of profits or sales are naturally skewed. Simple graphical tools for the inspection of distributions are introduced in the next section.

#### 1.7.1 Simple Graphics

The degree of skewness of a distribution can be investigated by constructing histograms using the hist function. (More sophisticated alternatives such as smooth density estimates will be considered in Chapter 7.) For example, the code for producing Figure 1.1 first divides the plot region into two equally spaced rows (the layout function) and then plots the histograms of the raw market values in the upper part using the hist function. The lower part of the figure depicts the histogram for the log transformed market values which appear to be more symmetric. Bivariate relationships of two continuous variables are usually depicted as scatterplots. In R, regression relationships are specified by so-called *model formulae* which, in a simple bivariate case, may look like

R> fm <- marketvalue ~ sales
R> class(fm)

```
R> layout(matrix(1:2, nrow = 2))
R> hist(Forbes2000$marketvalue)
R> hist(log(Forbes2000$marketvalue))
```

# Histogram of Forbes2000\$marketvalue



Histogram of log(Forbes2000\$marketvalue)



Figure 1.1 Histograms of the market value and the logarithm of the market value for the companies contained in the Forbes 2000 list.

#### [1] "formula"

with the dependent variable on the left hand side and the independent variable on the right hand side. The tilde separates left and right hand side. Such a model formula can be passed to a model function (for example to the linear model function as explained in Chapter 5). The plot generic function implements a *formula* method as well. Because the distributions of both market value and sales are skewed we choose to depict their logarithms. A raw scatterplot of 2000 data points (Figure 1.2) is rather uninformative due to areas with very high density. This problem can be avoided by choosing a transparent color for the dots (currently only possible with the PDF graphics device) as

#### ORGANISING AN ANALYSIS

```
R> plot(log(marketvalue) ~ log(sales), data = Forbes2000,
+ pch = ".")
```



Figure 1.2 Raw scatterplot of the logarithms of market value and sales.

shown in Figure 1.3. If the independent variable is a factor, a boxplot representation is a natural choice. For four selected countries, the distributions of the logarithms of the market value may be visually compared in Figure 1.4. Here, the width of the boxes are proportional to the square root of the number of companies for each country and extremely large or small market values are depicted by single points.

# 1.8 Organising an Analysis

Although it is possible to perform an analysis typing all commands directly on the R prompt it is much more comfortable to maintain a separate text file collecting all steps necessary to perform a certain data analysis task. Such



Figure 1.3 Scatterplot with transparent shading of points of the logarithms of market value and sales.

an R transcript file, for example <code>analysis.R</code> created with your favourite text editor, can be sourced into R using the <code>source</code> command

R> source("analysis.R", echo = TRUE)

When all steps of a data analysis, i.e., data preprocessing, transformations, simple summary statistics and plots, model building and inference as well as reporting, are collected in such an R transcript file, the analysis can be reproduced at any time, maybe with modified data as it frequently happens in our consulting practice.

# 1.9 Summary

Reading data into R is possible in many different ways, including direct connections to data base engines. Tabular data are handled by *data.frames* in R, and the usual data manipulation techniques such as sorting, ordering or sub-

## SUMMARY

R> boxplot(log(marketvalue) ~ country, data = subset(Forbes2000, + country %in% c("United Kingdom", "Germany", + "India", "Turkey")), ylab = "log(marketvalue)",

+ varwidth = TRUE)



Figure 1.4 Boxplots of the logarithms of the market value for four selected countries, the width of the boxes is proportional to the square-roots of the number of companies.

setting can be performed by simple R statements. An overview on data stored in a *data.frame* is given mainly by two functions: summary and str. Simple graphics such as histograms and scatterplots can be constructed by applying the appropriate R functions (hist and plot) and we shall give many more examples of these functions and those that produce more interesting graphics in later chapters.

#### AN INTRODUCTION TO R

# Exercises

Ex. 1.1 Calculate the median profit for the companies in the United States and the median profit for the companies in the UK, France and Germany.

Ex. 1.2 Find all German companies with negative profit.

- Ex. 1.3 Which business category are most of the companies situated at the Bermuda island working in?
- Ex. 1.4 For the 50 companies in the Forbes data set with the highest profits, plot sales against assets (or some suitable transformation of each variable), labelling each point with the appropriate country name which may need to be abbreviated (using abbreviate) to avoid making the plot look too 'messy'.
- Ex. 1.5 Find the average value of sales for the companies in each country in the Forbes data set, and find the number of companies in each country with profits above 5 billion US dollars.

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# CHAPTER 2

# Simple Inference: Guessing Lengths, Wave Energy, Water Hardness, Piston Rings, and Rearrests of Juveniles

# 2.1 Introduction

2.2 Statistical Tests

# 2.3 Analysis Using R

2.3.1 Estimating the Width of a Room

The data shown in Table ?? are available as roomwidth *data.frame* from the *HSAUR* package and can be attached by using

R> data("roomwidth", package = "HSAUR")

If we convert the estimates of the room width in metres into feet by multiplying each by 3.28 then we would like to test the hypothesis that the mean of the population of 'metre' estimates is equal to the mean of the population of 'feet' estimates. We shall do this first by using an independent samples *t*-test, but first it is good practice to, informally at least, check the normality and equal variance assumptions. Here we can use a combination of numerical and graphical approaches. The first step should be to convert the metre estimates into feet, i.e., by a factor

R> convert <- ifelse(roomwidth\$unit == "feet", 1, 3.28)

which equals one for all feet measurements and 3.28 for the measurements in metres. Now, we get the usual summary statistics and standard deviations of each set of estimates using

```
R> tapply(roomwidth$width * convert, roomwidth$unit,
      summary)
+
$feet
   Min. 1st Qu.
                 Median
                            Mean 3rd Ou.
                                             Max.
   24.0
           36.0
                    42.0
                             43.7
                                     48.0
                                              94.0
$metres
                 Median
   Min. 1st Qu.
                            Mean 3rd Qu.
                                             Max.
          36.08
                   49.20
                           52.55
                                    55.76
                                           131.20
  26.24
R> tapply(roomwidth$width * convert, roomwidth$unit,
      sd)
+
```

#### SIMPLE INFERENCE

# feet metres 12.49742 23.43444

where tapply applies summary, or sd, to the converted widths for both groups of measurements given by roomwidth\$unit. A boxplot of each set of estimates might be useful and is depicted in Figure 2.1. The layout function (line 1 in Figure 2.1) divides the plotting area in three parts. The boxplot function produces a boxplot in the upper part and the two qqnorm statements in lines 8 and 11 set up the normal probability plots that can be used to assess the normality assumption of the *t*-test. The boxplots indicate that both sets of estimates contain a number of outliers and also that the estimates made in metres are skewed and more variable than those made in feet, a point underlined by the numerical summary statistics above. Both normal probability plots depart from linearity, suggesting that the distributions of both sets of estimates are not normal. The presence of outliers, the apparently different variances and the evidence of non-normality all suggest caution in applying the *t*-test, but for the moment we shall apply the usual version of the test using the t.test function in R. The two-sample test problem is specified by a *formula*, here by

# I(width \* convert) ~ unit

where the response, width, on the left hand side needs to be converted first and, because the star has a special meaning in formulae as will be explained in Chapter 4, the conversion needs to be embedded by I. The factor unit on the right hand side specifies the two groups to be compared.

# 2.3.2 Wave Energy Device Mooring

# The data from Table ?? are available as *data.frame* waves

#### R> data("waves", package = "HSAUR")

and requires the use of a matched pairs *t*-test to answer the question of interest. This test assumes that the differences between the matched observations have a normal distribution so we can begin by checking this assumption by constructing a boxplot and a normal probability plot – see Figure 2.5.

# 2.3.3 Mortality and Water Hardness

There is a wide range of analyses we could apply to the data in Table ?? available from

## R> data("water", package = "HSAUR")

But to begin we will construct a scatterplot of the data enhanced somewhat by the addition of information about the marginal distributions of water hardness (calcium concentration) and mortality, and by adding the estimated linear regression fit (see Chapter 5) for mortality on hardness. The plot and the

## ANALYSIS USING R

```
R> layout(matrix(c(1, 2, 1, 3), nrow = 2, ncol = 2,
```

- + byrow = FALSE))
- R> boxplot(I(width \* convert) ~ unit, data = roomwidth,
- 4 + ylab = "Estimated width (feet)", varwidth = TRUE,
- 5 + names = c("Estimates in feet", "Estimates in metres (converted to feet)"))

- 6 R> feet <- roomwidth\$unit == "feet"
- 7 R> qqnorm(roomwidth\$width[feet], ylab = "Estimated width (feet)")
- 8 R> qqline(roomwidth\$width[feet])
- 9 R> qqnorm(roomwidth\$width[!feet], ylab = "Estimated width (metres)")
- R> qqline(roomwidth\$width[!feet])





Figure 2.1 Boxplots of estimates of width of room in feet and metres (after conversion to feet) and normal probability plots of estimates of room width made in feet and in metres.

Figure 2.2 R output of the independent samples *t*-test for the roomwidth data.

```
R> t.test(I(width * convert) ~ unit, data = roomwidth,
+ var.equal = FALSE)
Welch Two Sample t-test
data: I(width * convert) by unit
t = -2.3071, df = 58.788, p-value = 0.02459
alternative hypothesis: true difference in means is not equal to 0
95 percent confidence interval:
-16.54308 -1.17471
sample estimates:
mean in group feet mean in group metres
43.69565 52.55455
```

Figure 2.3 R output of the independent samples Welch test for the roomwidth data.

required R code is given along with Figure 2.8. In line 1 of Figure 2.8, we divide the plotting region into four areas of different size. The scatterplot (line 3) uses a plotting symbol depending on the location of the city (by the pch argument), a legend for the location is added in line 6. We add a least squares fit (see Chapter 5) to the scatterplot and, finally, depict the marginal distributions by means of a boxplot and a histogram. The scatterplot shows that as hardness increases mortality decreases, and the histogram for the water hardness shows it has a rather skewed distribution.

## 2.3.4 Piston-ring Failures

Rather than looking at the simple differences of observed and expected values for each cell which would be unsatisfactory since a difference of fixed size is clearly more important for smaller samples, it is preferable to consider a

ANALYSIS USING R

Figure 2.4 R output of the Wilcoxon rank sum test for the roomwidth data.

standardised residual given by dividing the observed minus expected difference by the square root of the appropriate expected value. The  $X^2$  statistic for assessing independence is simply the sum, over all the cells in the table, of the squares of these terms. We can find these values extracting the **residuals** element of the object returned by the **chisq.test** function

# R> chisq.test(pistonrings)\$residuals

| -          | Leg        |            |            |
|------------|------------|------------|------------|
| compressor | North      | Centre     | South      |
| C1         | 0.6036154  | 1.6728267  | -1.7802243 |
| C2         | 0.1429031  | 0.2975200  | -0.3471197 |
| С3         | -0.3251427 | -0.4522620 | 0.6202463  |
| C4         | -0.4157886 | -1.4666936 | 1.4635235  |

A graphical representation of these residuals is called *association plot* and is available via the **assoc** function from package vcd (Meyer et al., 2006) applied to the contingency table of the two categorical variables. Figure 2.11 depicts the residuals for the piston ring data. The deviations from independence are largest for C1 and C4 compressors in the centre and south leg.

#### 2.3.5 Rearrests of Juveniles

The data in Table ?? are available as *table* object via R> data("rearrests", package = "HSAUR") R> rearrests Juvenile court

| Adult | court    | Rearrest | NO | rearrest |
|-------|----------|----------|----|----------|
| Rea   | rrest    | 158      |    | 515      |
| No    | rearrest | 290      |    | 1134     |

and in **rearrests** the counts in the four cells refer to the matched pairs of subjects; for example, in 158 pairs both members of the pair were rearrested.

```
8 SIMPLE INFERENCE
R> mooringdiff <- waves$method1 - waves$method2
R> layout(matrix(1:2, ncol = 2))
R> boxplot(mooringdiff, ylab = "Differences (Newton metres)",
+ main = "Boxplot")
R> abline(h = 0, lty = 2)
R> qqnorm(mooringdiff, ylab = "Differences (Newton metres)")
R> qqline(mooringdiff)
```



Figure 2.5 Boxplot and normal probability plot for differences between the two mooring methods.

Here we need to use McNemar's test to assess whether rearrest is associated with type of court where the juvenile was tried. We can use the R function mcnemar.test. The test statistic shown in Figure 2.12 is 62.888 with a single degree of freedom – the associated *p*-value is extremely small and there is strong evidence that type of court and the probability of rearrest are related. It appears that trial at a juvenile court is less likely to result in rearrest (see Exercise 2.4). An exact version of McNemar's test can be obtained by testing whether *b* and *c* are equal using a binomial test (see Figure 2.13).

# ANALYSIS USING R

# R> t.test(mooringdiff)

One Sample t-test

```
data: mooringdiff
t = 0.9019, df = 17, p-value = 0.3797
alternative hypothesis: true mean is not equal to 0
95 percent confidence interval:
-0.08258476 0.20591810
sample estimates:
mean of x
0.06166667
```



Figure 2.7 R output of the Wilcoxon signed rank test for the waves data.



9 R> boxplot(water\$mortality)

Histogram of water\$hardness







**Figure 2.8** Enhanced scatterplot of water hardness and mortality, showing both the joint and the marginal distributions and, in addition, the location of the city by different plotting symbols.

ANALYSIS USING R

```
R> cor.test(~mortality + hardness, data = water)
```

Pearson's product-moment correlation

Figure 2.9 R output of Pearsons' correlation coefficient for the water data.

Figure 2.10 R output of the chi-squared test for the pistonrings data.

# SIMPLE INFERENCE



Figure 2.11 Association plot of the residuals for the pistonrings data.

 $\label{eq:Figure 2.12} Figure \ 2.12 \quad {\sf R} \ {\rm output} \ {\rm of} \ {\rm McNemar's} \ {\rm test} \ {\rm for} \ {\rm the} \ {\rm rearrests} \ {\rm data}.$ 

# ANALYSIS USING R

```
Figure 2.13 R output of an exact version of McNemar's test for the rearrests data computed via a binomal test.
```
\_\_\_\_| |\_\_\_\_

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## CHAPTER 3

## Conditional Inference: Guessing Lengths, Suicides, Gastrointestinal Damage, and Newborn Infants

## 3.1 Introduction

### 3.2 Conditional Test Procedures

## 3.3 Analysis Using R

#### 3.3.1 Estimating the Width of a Room Revised

The unconditional analysis of the room width estimated by two groups of students in Chapter ?? lead to the conclusion that the estimates in metres are slightly larger than the estimates in feet. Here, we reanalyse these data in a conditional framework. First, we convert metres into feet and store the vector of observations in a variable y:

```
R> data("roomwidth", package = "HSAUR")
R> convert <- ifelse(roomwidth$unit == "feet", 1, 3.28)
R> feet <- roomwidth$unit == "feet"
R> metre <- !feet
R> y <- roomwidth$width * convert</pre>
```

The test statistic is simply the difference in means

R> T <- mean(y[feet]) - mean(y[metre]) R> T

[1] -8.858893

In order to approximate the conditional distribution of the test statistic T we compute 9999 test statistics for shuffled y values. A permutation of the y vector can be obtained from the sample function.

```
R> meandiffs <- double(9999)
R> for (i in 1:length(meandiffs)) {
+    sy <- sample(y)
+    meandiffs[i] <- mean(sy[feet]) - mean(sy[metre])
+ }</pre>
```

The distribution of the test statistic T under the null hypothesis of independence of room width estimates and groups is depicted in Figure 3.1. Now, the value of the test statistic T for the original unshuffled data can be compared

```
R> hist(meandiffs)
R> abline(v = T, lty = 2)
R> abline(v = -T, lty = 2)
```

## Histogram of meandiffs 2000 1500 Frequency 1000 500 0 Τ Т 0 5 -10 -5 10 -15 meandiffs

Figure 3.1 Approximated conditional distribution of the difference of mean roomwidth estimates in the feet and metres group under the null hypothesis. The vertical lines show the negative and positive absolute value of the test statistic T obtained from the original data.

with the distribution of T under the null hypothesis (the vertical lines in Figure 3.1). The *p*-value, i.e., the proportion of test statistics T larger than 8.859 or smaller than -8.859 is

```
R> greater <- abs(meandiffs) > abs(T)
R> mean(greater)
```

[1] 0.0080008

with a confidence interval of

R> binom.test(sum(greater), length(greater))\$conf.int

```
[1] 0.006349087 0.009947933
attr(,"conf.level")
[1] 0.95
```

Note that the approximated conditional *p*-value is roughly the same as the *p*-value reported by the *t*-test in Chapter 2.

Figure 3.2 R output of the exact permutation test applied to the roomwidth data.

Figure 3.3 R output of the exact conditional Wilcoxon rank sum test applied to the roomwidth data.

3.3.2 Crowds and Threatened Suicide

#### 3.3.3 Gastrointestinal Damages

Here we are interested in the comparison of two groups of patients, where one group received a placebo and the other one Misoprostol. In the trials shown here, the response variable is measured on an ordered scale – see Table ??. Data from four clinical studies are available and thus the observations are naturally grouped together. From the *data.frame* Lanza we can construct a three-way table as follows:

```
R> data("Lanza", package = "HSAUR")
R> xtabs(~treatment + classification + study, data = Lanza)
, , study = I
```

Figure 3.4 R output of Fisher's exact test for the suicides data.

```
classification
treatment
           1 2 3 4 5
 Misoprostol 21 2 4 2 0
          2 2 4 9 13
 Placebo
, , study = II
          classification
treatment 1 2 3 4 5
 Misoprostol 20 4 6 0 0
 Placebo
           8 4 9 4 5
, , study = III
          classification
treatment
          1 2 3 4 5
 Misoprostol 20 4 3 1 2
 Placebo
            0 2 5 5 17
, , study = IV
          classification
           1 2 3 4 5
treatment
 Misoprostol 1 4 5 0 0
            0 0 0 4 6
 Placebo
```

For the first study, the null hypothesis of independence of treatment and gastrointestinal damage, i.e., of no treatment effect of Misoprostol, is tested by

```
R> library("coin")
R> cmh_test(classification ~ treatment, data = Lanza,
```

```
6
```

```
+ scores = list(classification = c(0, 1, 6, 17,
+ 30)), subset = Lanza$study == "I")
```

Asymptotic Linear-by-Linear Association Test

data: classification (ordered) by groups Misoprostol, Placebo chi-squared = 28.8478, df = 1, p-value = 7.83e-08

and, by default, the conditional distribution is approximated by the corresponding limiting distribution. The p-value indicates a strong treatment effect. For the second study, the asymptotic p-value is a little bit larger

```
R> cmh_test(classification ~ treatment, data = Lanza,
+ scores = list(classification = c(0, 1, 6, 17,
+ 30)), subset = Lanza$study == "II")
```

Asymptotic Linear-by-Linear Association Test

data: classification (ordered) by groups Misoprostol, Placebo chi-squared = 12.0641, df = 1, p-value = 0.000514

and we make sure that the implied decision is correct by calculating a confidence interval for the exact p-value

```
R> p <- cmh_test(classification ~ treatment, data = Lanza,
+ scores = list(classification = c(0, 1, 6, 17,
+ 30)), subset = Lanza$study == "II", distribution = approximate(B = 19999))
R> pvalue(p)
[1] 5.00025e-05
99 percent confidence interval:
```

```
2.506396e-07 3.714653e-04
```

The third and fourth study indicate a strong treatment effect as well

```
R> cmh_test(classification ~ treatment, data = Lanza,
+ scores = list(classification = c(0, 1, 6, 17,
+ 30)), subset = Lanza$study == "III")
```

Asymptotic Linear-by-Linear Association Test

data: classification (ordered) by groups Misoprostol, Placebo chi-squared = 28.1587, df = 1, p-value = 1.118e-07

```
R> cmh_test(classification ~ treatment, data = Lanza,
+ scores = list(classification = c(0, 1, 6, 17,
+ 30)), subset = Lanza$study == "IV")
```

Asymptotic Linear-by-Linear Association Test

```
data: classification (ordered) by groups Misoprostol, Placebo
chi-squared = 15.7414, df = 1, p-value = 7.262e-05
```

At the end, a separate analysis for each study is unsatisfactory. Because the design of the four studies is the same, we can use **study** as a block variable

#### CONDITIONAL INFERENCE

and perform a global linear-association test investigating the treatment effect of Misoprostol in all four studies. The block variable can be incorporated into the *formula* by the | symbol.

Based on this result, a strong treatment effect can be established.

#### 3.3.4 Teratogenesis

In this example, the medical doctor (MD) and the research assistant (RA) assessed the number of anomalies (0, 1, 2 or 3) for each of 395 babies:

```
R> anomalies <- as.table(matrix(c(235, 23, 3, 0, 41,</pre>
+
      35, 8, 0, 20, 11, 11, 1, 2, 1, 3, 1), ncol = 4,
      dimnames = list(MD = 0:3, RA = 0:3)))
+
R> anomalies
   RA
MD
       0
           1
                2
                    3
  0 235
          41
               20
                    2
  1
     23
          35
               11
                    1
                    3
  2
       3
           8
              11
  3
       0
           0
                    1
                1
```

We are interested in testing whether the number of anomalies assessed by the medical doctor differs structurally from the number reported by the research assistant. Because we compare *paired* observations, i.e., one pair of measurements for each newborn, a test of marginal homogeneity (a generalisation of McNemar's test, see Chapter 2) needs to be applied:

R> mh\_test(anomalies)

Asymptotic Marginal-Homogeneity Test

```
data: response by
    groups MD, RA
    stratified by block
chi-squared = 21.2266, df = 3, p-value = 9.446e-05
```

The *p*-value indicates a deviation from the null hypothesis. However, the levels of the response are not treated as ordered. Similar to the analysis of the gastrointestinal damage data above, we can take this information into account by the definition of an appropriate score. Here, the number of anomalies is a natural choice:

```
R> mh_test(anomalies, scores = list(c(0, 1, 2, 3)))
```

Asymptotic Marginal-Homogeneity Test for Ordered Data

```
data: response (ordered) by
    groups MD, RA
    stratified by block
chi-squared = 21.0199, df = 1, p-value = 4.545e-06
```

In our case, both versions coincide and one can conclude that the assessment of the number of anomalies differs between the medical doctor and the research assistant.

## CHAPTER 4

## Analysis of Variance: Weight Gain, Foster Feeding in Rats, Water Hardness and Male Egyptian Skulls

## 4.1 Introduction

4.2 Analysis of Variance

### 4.3 Analysis Using R

#### 4.3.1 Weight Gain in Rats

Before applying analysis of variance to the data in Table ?? we should try to summarise the main features of the data by calculating means and standard deviations and by producing some hopefully informative graphs. The data is available in the *data.frame* weightgain. The following R code produces the required summary statistics

```
R> data("weightgain", package = "HSAUR")
R> tapply(weightgain$weightgain, list(weightgain$source,
+
      weightgain$type), mean)
        High Low
Beef
       100.0 79.2
Cereal
        85.9 83.9
R> tapply(weightgain$weightgain, list(weightgain$source,
      weightgain$type), sd)
+
           High
                      LOW
       15.13642 13.88684
Beef
Cereal 15.02184 15.70881
```

To apply analysis of variance to the data we can use the **aov** function in R and then the **summary** method to give us the usual analysis of variance table. The model *formula* specifies a two-way layout with interaction terms, where the first factor is **source**, and the second factor is **type**.

R> wg\_aov <- aov(weightgain ~ source \* type, data = weightgain) The estimates of the intercept and the main and interaction effects can be extracted from the model fit by

R> coef(wg\_aov)

| (Intercept) | sourceCereal | typeLow |
|-------------|--------------|---------|
| 100.0       | -14.1        | -20.8   |

#### ANALYSIS OF VARIANCE

R> plot.design(weightgain)



Factors

Figure 4.1 Plot of mean weight gain for each level of the two factors.

sourceCereal:typeLow
 18.8

Note that the model was fitted with the restrictions  $\gamma_1 = 0$  (corresponding to **Beef**) and  $\beta_1 = 0$  (corresponding to **High**) because treatment contrasts were used as default as can be seen from

## R> options("contrasts")

| \$contrasts       |              |  |  |  |
|-------------------|--------------|--|--|--|
| unordered         | ordered      |  |  |  |
| "contr.treatment" | "contr.poly" |  |  |  |

Thus, the coefficient for source of -14.1 can be interpreted as an estimate of the difference  $\gamma_2 - \gamma_1$ . Alternatively, we can use the restriction  $\sum_i \gamma_i = 0$  by R> coef(aov(weightgain ~ source + type + source:type,

+ data = weightgain, contrasts = list(source = contr.sum)))



| (Intercept)              | source1 | typeLow |
|--------------------------|---------|---------|
| 92.95                    | 7.05    | -11.40  |
| source1:typeLow<br>-9.40 |         |         |

#### 4.3.2 Foster Feeding of Rats of Different Genotype

As in the previous subsection we will begin the analysis of the foster feeding data in Table ?? with a plot of the mean litter weight for the different geno-types of mother and litter (see Figure 4.4). The data are in the *data.frame* foster

```
R> data("foster", package = "HSAUR")
```

We can derive the two analyses of variance tables for the foster feeding example by applying the R code

```
R> summary(aov(weight ~ litgen * motgen, data = foster))
to give
                 Sum Sq Mean Sq F value
              Df
                                           Pr(>F)
                          20.05 0.3697 0.775221
litgen
               3
                   60.16
               3 775.08
                         258.36 4.7632 0.005736 **
motgen
litgen:motgen 9 824.07
                           91.56
                                  1.6881 0.120053
              45 2440.82
Residuals
                           54.24
Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
and then the code
R> summary(aov(weight ~ motgen * litgen, data = foster))
to give
                 Sum Sq Mean Sq F value
              Df
                                           Pr(>F)
                  771.61 257.20 4.7419 0.005869 **
motgen
               3
                           21.21 0.3911 0.760004
litgen
               3
                   63.63
motgen:litgen 9 824.07
                           91.56
                                 1.6881 0.120053
Residuals
              45 2440.82
                           54.24
___
Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

#### ANALYSIS OF VARIANCE



**Figure 4.3** Interaction plot of type  $\times$  source.

There are (small) differences in the sum of squares for the two main effects and, consequently, in the associated F-tests and p-values. This would not be true if in the previous example in Subsection 4.3.1 we had used the code

## R> summary(aov(weightgain ~ type \* source, data = weightgain))

instead of the code which produced Figure 4.2 (readers should confirm that this is the case). We can investigate the effect of genotype B on litter weight in more detail by the use of *multiple comparison procedures* (see Everitt, 1996). Such procedures allow a comparison of all pairs of levels of a factor whilst maintaining the nominal significance level at its selected value and producing adjusted confidence intervals for mean differences. One such procedure is called *Tukey honest significant differences* suggested by Tukey (1953), see Hochberg and Tamhane (1987) also. Here, we are interested in simultaneous confidence

## ANALYSIS USING R R> plot.design(foster)



Factors

Figure 4.4 Plot of mean litter weight for each level of the two factors for the foster data.

intervals for the weight differences between all four genotypes of the mother. First, an ANOVA model is fitted

```
R> foster_aov <- aov(weight ~ litgen * motgen, data = foster)
which serves as the basis of the multiple comparisons, here with allpair differences by</pre>
```

```
R> foster_hsd <- TukeyHSD(foster_aov, "motgen")
R> foster_hsd
Tukey multiple comparisons of means
```

```
95% family-wise confidence level
Fit: aov(formula = weight ~ litgen * motgen, data = foster)
```

R> plot(foster\_hsd)



## 95% family-wise confidence level

Figure 4.5 Graphical presentation of multiple comparison results for the foster feeding data.

\$motgen diff lwr upr p adj B-A 3.330369 -3.859729 10.5204672 0.6078581 I-A -1.895574 -8.841869 5.0507207 0.8853702 J-A -6.566168 -13.627285 0.4949498 0.0767540 I-B -5.225943 -12.416041 1.9641552 0.2266493 J-B -9.896537 -17.197624 -2.5954489 0.0040509 J-I -4.670593 -11.731711 2.3905240 0.3035490

A convenient plot method exists for this object and we can get a graphical representation of the multiple confidence intervals as shown in Figure 4.5. It appears that there is only evidence for a difference in the B and J genotypes.

### 4.3.3 Water Hardness and Mortality

The water hardness and mortality data for 61 large towns in England and Wales (see Table 2.3) was analysed in Chapter 2 and here we will extend the analysis by an assessment of the differences of both hardness and mortality in the North or South. The hypothesis that the two-dimensional mean-vector of water hardness and mortality is the same for cities in the North and the South can be tested by *Hotelling-Lawley* test in a multivariate analysis of variance framework. The R function manova can be used to fit such a model and the corresponding summary method performs the test specified by the test argument

```
R> data("water", package = "HSAUR")
R> summary(manova(cbind(hardness, mortality) ~ location,
+ data = water), test = "Hotelling-Lawley")
```

Df Hotelling-Lawley approx F num Df den Df Pr(>F) location 1 0.9002 26.1062 2 58 8.217e-09 Residuals 59

```
location ***
Residuals
---
Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

The cbind statement in the left hand side of the formula indicates that a *multivariate* response variable is to be modelled. The *p*-value associated with the *Hotelling-Lawley* statistic is very small and there is strong evidence that the mean vectors of the two variables are not the same in the two regions. Looking at the sample means

## R> tapply(water\$hardness, water\$location, mean)

```
North South
30.40000 69.76923
```

#### R> tapply(water\$mortality, water\$location, mean)

North South 1633.600 1376.808

we see large differences in the two regions both in water hardness and mortality, where low mortality is associated with hard water in the South and high mortality with soft water in the North (see Figure ?? also).

#### 4.3.4 Male Egyptian Skulls

We can begin by looking at a table of mean values for the four measurements within each of the five epochs. The measurements are available in the *data.frame* skulls and we can compute the means over all epochs by

```
R> data("skulls", package = "HSAUR")
R> means <- aggregate(skulls[, c("mb", "bh", "bl",</pre>
```

```
ANALYSIS OF VARIANCE
```

```
R> pairs(means[, -1], panel = function(x, y) {
+ text(x, y, abbreviate(levels(skulls$epoch)))
+ })
```

10



Figure 4.6 Scatterplot matrix of epoch means for Egyptian skulls data.

```
+ "nh")], list(epoch = skulls$epoch), mean)
R> means
```

epochmbbhblnh1c4000BC131.3667133.600099.1666750.533332c3300BC132.3667132.700099.0666750.233333c1850BC134.4667133.800096.0333350.566674c200BC135.5000132.300094.5333351.966675cAD150136.1667130.333393.5000051.36667

It may also be useful to look at these means graphically and this could be done in a variety of ways. Here we construct a scatterplot matrix of the means using the code attached to Figure 4.6. There appear to be quite large differences

between the epoch means, at least on some of the four measurements. We can now test for a difference more formally by using MANOVA with the following R code to apply each of the four possible test criteria mentioned earlier;

```
R> skulls_manova <- manova(cbind(mb, bh, bl, nh) ~
      epoch, data = skulls)
+
R> summary(skulls_manova, test = "Pillai")
           Df Pillai approx F num Df den Df
                                                Pr(>F)
            4 0.3533 3.5120
epoch
                                   16
                                          580 4.675e-06 ***
Residuals 145
Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
R> summary(skulls_manova, test = "Wilks")
              Df Wilks approx F num Df den Df
                                                  Pr(>F)
            4.00 0.6636
                           3.9009 16.00 434.45 7.01e-07 ***
epoch
Residuals 145.00
Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
R> summary(skulls_manova, test = "Hotelling-Lawley")
           Df Hotelling-Lawley approx F num Df den Df
epoch
            4
                        0.4818
                                 4.2310
                                            16
                                                    562
Residuals 145
             Pr(>F)
epoch
          8.278e-08 ***
Residuals
Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
R> summary(skulls_manova, test = "Roy")
           Df
                  Roy approx F num Df den Df
                                                  Pr(>F)
               0.4251 15.4097
                                 4 145 1.588e-10 ***
epoch
            4
Residuals 145
___
Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
The p-value associated with each four test criteria is very small and there is
strong evidence that the skull measurements differ between the five epochs. We
might now move on to investigate which epochs differ and on which variables.
We can look at the univariate F-tests for each of the four variables by using
the code
R> summary.aov(manova(cbind(mb, bh, bl, nh) ~ epoch,
```

```
12
                                      ANALYSIS OF VARIANCE
Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
Response bh :
            Df Sum Sq Mean Sq F value Pr(>F)
                         57.5 2.4474 0.04897 *
epoch
             4 229.9
           145 3405.3
Residuals
                         23.5
Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
Response bl :
            Df Sum Sq Mean Sq F value
                                         Pr(>F)
            4 803.3
                       200.8 8.3057 4.636e-06 ***
epoch
Residuals
           145 3506.0
                         24.2
Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
Response nh :
            Df Sum Sq Mean Sq F value Pr(>F)
epoch
             4
                 61.20
                        15.30
                                 1.507 0.2032
           145 1472.13
                         10.15
Residuals
```

We see that the results for the maximum breadths (mb) and basialiveolar length (bl) are highly significant, with those for the other two variables, in particular for nasal heights (nh), suggesting little evidence of a difference. To look at the pairwise multivariate tests (any of the four test criteria are equivalent in the case of a one-way layout with two levels only) we can use the summary method and manova function as follows:

```
R> summary(manova(cbind(mb, bh, bl, nh) ~ epoch, data = skulls,
     subset = epoch %in% c("c4000BC", "c3300BC")))
+
          Df Pillai approx F num Df den Df Pr(>F)
          1 0.02767 0.39135
epoch
                                 4
                                       55 0.814
Residuals 58
R> summary(manova(cbind(mb, bh, bl, nh) ~ epoch, data = skulls,
     subset = epoch %in% c("c4000BC", "c1850BC")))
+
          Df Pillai approx F num Df den Df Pr(>F)
epoch
          1 0.1876
                      3.1744
                                 4
                                       55 0.02035 *
Residuals 58
___
Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
R> summary(manova(cbind(mb, bh, bl, nh) ~ epoch, data = skulls,
     subset = epoch %in% c("c4000BC", "c200BC")))
+
          Df Pillai approx F num Df den Df
                                              Pr(>F)
                     5.9766
epoch
          1 0.3030
                                4
                                       55 0.0004564 ***
Residuals 58
Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

```
R> summary(manova(cbind(mb, bh, bl, nh) ~ epoch, data = skulls,
+ subset = epoch %in% c("c4000BC", "cAD150")))
Df Pillai approx F num Df den Df Pr(>F)
epoch 1 0.3618 7.7956 4 55 4.736e-05 ***
Residuals 58
---
```

```
Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

To keep the overall significance level for the set of all pairwise multivariate tests under some control (and still maintain a reasonable power), Stevens (2001) recommends setting the nominal level  $\alpha = 0.15$  and carrying out each test at the  $\alpha/m$  level where m s the number of tests performed. The results of the four pairwise tests suggest that as the epochs become further separated in time the four skull measurements become increasingly distinct.

\_\_\_\_| |\_\_\_\_

## Bibliography

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- Hochberg, Y. and Tamhane, A. C. (1987), *Multiple Comparison Procedures*, New York, USA: John Wiley & Sons.
- Stevens, J. (2001), Applied Multivariate Statistics for the Social Sciences, Mahwah, New Jersey, USA: Lawrence Erlbaum, 4th edition.
- Tukey, J. W. (1953), "The problem of multiple comparisons (unpublished manuscript)," in *The Collected Works of John W. Tukey VIII. Multiple Comparisons: 1948-1983*, New York, USA: Chapman & Hall.

## CHAPTER 5

## Multiple Linear Regression: Cloud Seeding

#### 5.1 Introduction

#### 5.2 Multiple Linear Regression

### 5.3 Analysis Using R

Both the boxplots (Figure 5.1) and the scatterplots (Figure 5.2) show some evidence of outliers. The row names of the extreme observations in the clouds data.frame can be identified via

R> rownames(clouds)[clouds\$rainfall %in% c(bxpseeding\$out,

```
bxpecho$out)]
```

[1] "1" "15"

where bxpseeding and bxpecho are variables created by boxplot in Figure 5.1. For the time being we shall not remove these observations but bear in mind during the modelling process that they may cause problems.

#### 5.3.1 Fitting a Linear Model

In this example it is sensible to assume that the effect that some of the other explanatory variables is modified by seeding and therefore consider a model that allows interaction terms for **seeding** with each of the covariates except **time**. This model can be described by the *formula* 

and the design matrix  $\mathbf{X}^{\star}$  can be computed via

R> Xstar <- model.matrix(clouds\_formula, data = clouds)

By default, treatment contrasts have been applied to the dummy codings of the factors seeding and echomotion as can be seen from the inspection of the contrasts attribute of the model matrix

R> attr(Xstar, "contrasts")

```
$seeding
[1] "contr.treatment"
```

\$echomotion
[1] "contr.treatment"

MULTIPLE LINEAR REGRESSION

```
R> data("clouds", package = "HSAUR")
R> layout(matrix(1:2, nrow = 2))
R> bxpseeding <- boxplot(rainfall ~ seeding, data = clouds,
+ ylab = "Rainfall", xlab = "Seeding")
R> bxpecho <- boxplot(rainfall ~ echomotion, data = clouds,
+ ylab = "Rainfall", xlab = "Echo Motion")</pre>
```



Seeding



Echo Motion

Figure 5.1 Boxplots of rainfall.

```
ANALYSIS USING R
R> layout(matrix(1:4, nrow = 2))
R> plot(rainfall ~ time, data = clouds)
R> plot(rainfall ~ sne, data = clouds, xlab = "S-NE criterion")
R> plot(rainfall ~ cloudcover, data = clouds)
R> plot(rainfall ~ prewetness, data = clouds)
```



Figure 5.2 Scatterplots of rainfall against the continuous covariables.

The default contrasts can be changed via the contrasts.arg argument to model.matrix or the contrasts argument to the fitting function, for example lm or aov as shown in Chapter 4. However, such internals are hidden and performed by high-level model fitting functions such as lm which will be used to fit the linear model defined by the *formula* clouds\_formula:

```
R> clouds_lm <- lm(clouds_formula, data = clouds)
R> class(clouds_lm)
```

[1] "lm"

## MULTIPLE LINEAR REGRESSION

The results of the model fitting is an object of class lm for which a summary method showing the conventional regression analysis output is available. The output in Figure 5.3 shows the estimates  $\hat{\beta}^*$  with corresponding standard errors and t-statistics as well as the F-statistic with associated p-value.

| R> summary(clouds_lm)   |          |                    |  |  |
|---|----------|--------------------|--|--|
| Call:   |          |                    |  |  |
| lm(formula = clouds_formula, data = clouds)                   |          |                    |  |  |
| Residuals:  |          |                    |  |  |
| Min 1Q Median 3Q  | Max      |                    |  |  |
| -2.5259 -1.1486 -0.2704 1.0401                                | 4.3913   |                    |  |  |
| Coefficients:   |          |                    |  |  |
|   | Estimate | Std. Error t value |  |  |
| (Intercept)   | -0.34624 | 2.78773 -0.124     |  |  |
| seedingyes  | 15.68293 |                    |  |  |
| sne   | 0.38786  |                    |  |  |
| cloudcover  | 0.41981  | 0.84453 0.497      |  |  |
| prewetness  | 4.10834  | 3.60101 1.141      |  |  |
| echomotionstationary  | 3.15281  | 1.93253 1.631      |  |  |
| time  | -0.04497 | 0.02505 -1.795     |  |  |
| seedingyes:sne  | -0.48625 | 0.24106 -2.017     |  |  |
| seedingyes:cloudcover   | -3.19719 | 1.26707 -2.523     |  |  |
| seedingyes:prewetness   | -2.55707 | 4.48090 -0.571     |  |  |
| seedingyes:echomotionstationary                               | -0.56222 | 2.64430 -0.213     |  |  |
|   | Pr(> t ) |                    |  |  |
| (Intercept)   | 0.90306  |                    |  |  |
| seedingyes  | 0.00372  | * *                |  |  |
| sne   | 0.09839  |                    |  |  |
| cloudcover  | 0.62742  |                    |  |  |
| prewetness  | 0.27450  |                    |  |  |
| echomotionstationary  | 0.12677  |                    |  |  |
| time  | 0.09590  |                    |  |  |
| seedingyes:sne  | 0.06482  |                    |  |  |
| seedingyes:cloudcover   | 0.02545  | *                  |  |  |
| seedingyes:prewetness   | 0.57796  |                    |  |  |
| seedingyes:echomotionstationary 0.83492                       |          |                    |  |  |
|   |          |                    |  |  |
| Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1 |          |                    |  |  |
| Residual standard error: 2.205 on 13 degrees of freedom       |          |                    |  |  |
| Multiple R-Squared: 0.7158, Adjusted R-squared: 0.4972        |          |                    |  |  |
| F-statistic: 3.274 on 10 and 13 DF, p-value: 0.02431          |          |                    |  |  |

### Figure 5.3 R output of the linear model fit for the clouds data.

Many methods are available for extracting components of the fitted model. The estimates  $\hat{\beta}^{\star}$  can be assessed via

```
R> betastar <- coef(clouds_lm)
R> betastar
```

```
(Intercept)
                     -0.34624093
                     seedingyes
                     15.68293481
                             sne
                      0.38786207
                     cloudcover
                     0.41981393
                     prewetness
                      4.10834188
           echomotionstationary
                     3.15281358
                            time
                     -0.04497427
                 seedingyes:sne
                    -0.48625492
          seedingyes:cloudcover
                     -3.19719006
          seedingyes: prewetness
                     -2.55706696
seedingyes:echomotionstationary
                     -0.56221845
```

and the corresponding covariance matrix  $\mathsf{Cov}(\hat{\beta}^\star)$  is available from the  $\mathtt{vcov}$  method

R> Vbetastar <- vcov(clouds\_lm)

where the square roots of the diagonal elements are the standard errors as shown in Figure 5.3

R> sqrt(diag(Vbetastar))

```
(Intercept)
2.78773403
seedingyes
4.44626606
sne
0.21785501
cloudcover
0.84452994
prewetness
3.60100694
echomotionstationary
1.93252592
time
0.02505286
```

#### MULTIPLE LINEAR REGRESSION

seedingyes:sne 0.24106012 seedingyes:cloudcover 1.26707204 seedingyes:prewetness 4.48089584 seedingyes:echomotionstationary 2.64429975

### 5.3.2 Regression Diagnostics

In order to investigate the quality of the model fit, we need access to the residuals and the fitted values. The residuals can be found by the residuals method and the fitted values of the response from the fitted (or predict) method

R> clouds\_resid <- residuals(clouds\_lm)
R> clouds\_fitted <- fitted(clouds\_lm)</pre>

Now the residuals and the fitted values can be used to construct diagnostic plots; for example the residual plot in Figure 5.5 where each observation is labelled by its number. Observations 1 and 15 give rather large residual values and the data should perhaps be reanalysed after these two observations are removed. The normal probability plot of the residuals shown in Figure 5.6 shows a reasonable agreement between theoretical and sample quantiles, however, observations 1 and 15 are extreme again. An index plot of the Cook's distances for each observation (and many other plots including those constructed above from using the basic functions) can be found from applying the **plot** method to the object that results from the application of the 1m function. Figure 5.7 suggests that observations 2 and 18 have undue influence on the estimated regression coefficients, but the two outliers identified previously do not. Again it may be useful to look at the results after these two observations have been removed (see Exercise 5.2).

```
R> psymb <- as.numeric(clouds$seeding)
R> plot(rainfall ~ cloudcover, data = clouds, pch = psymb)
R> abline(lm(rainfall ~ cloudcover, data = clouds,
+ subset = seeding == "no"))
R> abline(lm(rainfall ~ cloudcover, data = clouds,
+ subset = seeding == "yes"), lty = 2)
R> legend("topright", legend = c("No seeding", "Seeding"),
+ pch = 1:2, lty = 1:2, bty = "n")
```



Figure 5.4 Regression relationship between cloud coverage and rainfall with and without seeding.

```
10
                                MULTIPLE LINEAR REGRESSION
R> plot(clouds_fitted, clouds_resid, xlab = "Fitted values",
+
      ylab = "Residuals", ylim = max(abs(clouds_resid)) *
         c(-1, 1), type = "n")
+
R> abline(h = 0, lty = 2)
R> text(clouds_fitted, clouds_resid, labels = rownames(clouds))
```



Figure 5.5 Plot of residuals against fitted values for clouds seeding data.

```
ANALYSIS USING R
R> qqnorm(clouds_resid, ylab = "Residuals")
R> qqline(clouds_resid)
```



Normal Q–Q Plot

Figure 5.6 Normal probability plot of residuals from cloud seeding model clouds\_lm.

## MULTIPLE LINEAR REGRESSION

R> plot(clouds\_lm)



 ${\bf Figure \ 5.7} \quad {\rm Index \ plot \ of \ Cook's \ distances \ for \ cloud \ seeding \ data}.$ 

## CHAPTER 6

## Logistic Regression and Generalised Linear Models: Blood Screening, Women's Role in Society, and Colonic Polyps

## 6.1 Introduction

#### 6.2 Logistic Regression and Generalised Linear Models

#### 6.3 Analysis Using R

#### 6.3.1 ESR and Plasma Proteins

We can now fit a logistic regression model to the data using the glm function. We start with a model that includes only a single explanatory variable, fibrinogen. The code to fit the model is

### R> plasma\_glm\_1 <- glm(ESR ~ fibrinogen, data = plasma, + family = binomial())

The formula implicitly defines a parameter for the global mean (the intercept term) as discussed in Chapters ?? and ??. The distribution of the response is defined by the family argument, a binomial distribution in our case. (The default link function when the binomial family is requested is the logistic function.) From the results in Figure 6.2 we see that the regression coefficient for fibrinogen is significant at the 5% level. An increase of one unit in this variable increases the log-odds in favour of an ESR value greater than 20 by an estimated 1.83 with 95% confidence interval

#### R> confint(plasma\_glm\_1, parm = "fibrinogen")

2.5 % 97.5 % 0.3389465 3.9988602

These values are more helpful if converted to the corresponding values for the odds themselves by exponentiating the estimate

R> exp(coef(plasma\_glm\_1)["fibrinogen"])

fibrinogen 6.215715

and the confidence interval

```
R> exp(confint(plasma_glm_1, parm = "fibrinogen"))
```

#### 4 LOGISTIC REGRESSION AND GENERALISED LINEAR MODELS

```
R> data("plasma", package = "HSAUR")
R> layout(matrix(1:2, ncol = 2))
R> cdplot(ESR ~ fibrinogen, data = plasma)
R> cdplot(ESR ~ globulin, data = plasma)
```



**Figure 6.1** Conditional density plots of the erythrocyte sedimentation rate (ESR) given fibrinogen and globulin.

2.5 % 97.5 % 1.403468 54.535954

The confidence interval is very wide because there are few observations overall and very few where the ESR value is greater than 20. Nevertheless it seems likely that increased values of fibrinogen lead to a greater probability of an ESR value greater than 20. We can now fit a logistic regression model that includes both explanatory variables using the code

```
R> plasma_glm_2 <- glm(ESR ~ fibrinogen + globulin,
+ data = plasma, family = binomial())
```

and the output of the summary method is shown in Figure 6.3. The coefficient for gamma globulin is not significantly different from zero. Subtracting the residual deviance of the second model from the corresponding value for the first model we get a value of 1.87. Tested using a  $\chi^2$ -distribution with a single degree of freedom this is not significant at the 5% level and so we conclude that gamma globulin is not associated with ESR level. In R, the task of comparing the two nested models can be performed using the **anova** function

```
R> anova(plasma_glm_1, plasma_glm_2, test = "Chisq")
```

```
R> summary(plasma_glm_1)
Call:
glm(formula = ESR ~ fibrinogen, family = binomial(), data = plasma)
Deviance Residuals:
        10
    Min
                  Median
                                ЗQ
                                        Max
-0.9298 -0.5399 -0.4382 -0.3356
                                     2.4794
Coefficients:
           Estimate Std. Error z value Pr(>|z|)
            -6.8451
                         2.7703
                                -2.471
                                         0.0135 *
(Intercept)
                         0.9009
fibrinogen
             1.8271
                                  2.028
                                         0.0425 *
Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
(Dispersion parameter for binomial family taken to be 1)
    Null deviance: 30.885 on 31 degrees of freedom
Residual deviance: 24.840 on 30 degrees of freedom
AIC: 28.840
Number of Fisher Scoring iterations: 5
```

Figure 6.2 R output of the summary method for the logistic regression model fitted to the plasma data.

Analysis of Deviance Table Model 1: ESR ~ fibrinogen Model 2: ESR ~ fibrinogen + globulin Resid. Df Resid. Dev Df Deviance P(>|Chi|) 1 30 24.8404 2 29 22.9711 1 1.8692 0.1716

Nevertheless we shall use the predicted values from the second model and plot them against the values of *both* explanatory variables using a *bubble plot* to illustrate the use of the symbols function. The estimated conditional probability of a ESR value larger 20 for all observations can be computed, following formula (??), by

R> prob <- predict(plasma\_glm\_1, type = "response")</pre>

and now we can assign a larger circle to observations with larger probability as shown in Figure 6.4. The plot clearly shows the increasing probability of an ESR value above 20 (larger circles) as the values of fibrinogen, and to a lesser extent, gamma globulin, increase.

#### 6 LOGISTIC REGRESSION AND GENERALISED LINEAR MODELS

```
R> summary(plasma_glm_2)
Call:
glm(formula = ESR ~ fibrinogen + globulin, family = binomial(),
    data = plasma)
Deviance Residuals:
          10
    Min
                 Median
                               30
                                       Max
-0.9683 -0.6122 -0.3458 -0.2116
                                    2.2636
Coefficients:
           Estimate Std. Error z value Pr(>|z|)
(Intercept) -12.7921
                     5.7963
                                -2.207
                                         0.0273 *
             1.9104
                        0.9710
                                1.967
                                         0.0491 *
fibrinogen
globulin
             0.1558
                        0.1195
                                 1.303
                                         0.1925
Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
(Dispersion parameter for binomial family taken to be 1)
    Null deviance: 30.885 on 31
                                 degrees of freedom
Residual deviance: 22.971 on 29 degrees of freedom
AIC: 28.971
Number of Fisher Scoring iterations: 5
```

Figure 6.3 Routput of the summary method for the logistic regression model fitted to the plasma data.

#### 6.3.2 Women's Role in Society

Originally the data in Table ?? would have been in a completely equivalent form to the data in Table ?? data, but here the individual observations have been grouped into counts of numbers of agreements and disagreements for the two explanatory variables, sex and education. To fit a logistic regression model to such grouped data using the glm function we need to specify the number of agreements and disagreements as a two-column matrix on the left hand side of the model formula. We first fit a model that includes the two explanatory variables using the code

```
R> data("womensrole", package = "HSAUR")
R> womensrole_glm_1 <- glm(cbind(agree, disagree) ~
+ sex + education, data = womensrole, family = binomial())</pre>
```

From the summary output in Figure 6.5 it appears that education has a highly significant part to play in predicting whether a respondent will agree with the statement read to them, but the respondent's sex is apparently unimportant. As years of education increase the probability of agreeing with the statement declines. We now are going to construct a plot comparing the observed pro-
```
ANALYSIS USING R
R> plot(globulin ~ fibrinogen, data = plasma, xlim = c(2,
+ 6), ylim = c(25, 50), pch = ".")
R> symbols(plasma$fibrinogen, plasma$globulin, circles = prob,
+ add = TRUE)
```

7



Figure 6.4 Bubble plot of fitted values for a logistic regression model fitted to the ESR data.

portions of agreeing with those fitted by our fitted model. Because we will reuse this plot for another fitted object later on, we define a function which plots years of education against some fitted probabilities, e.g.,

```
R> role.fitted1 <- predict(womensrole_glm_1, type = "response")
and labels each observation with the person's sex:</pre>
```

#### 8 LOGISTIC REGRESSION AND GENERALISED LINEAR MODELS

```
R> summary(womensrole_glm_1)
Call:
glm(formula = cbind(agree, disagree) ~ sex + education, family = binomial(),
   data = womensrole)
Deviance Residuals:
    Min
         10
                     Median
                                   30
                                            Max
-2.72544 -0.86302 -0.06525
                              0.84340
                                        3.13315
Coefficients:
           Estimate Std. Error z value Pr(>|z|)
                      0.18389 13.646
(Intercept) 2.50937
                                         <2e-16 ***
           -0.01145
                       0.08415 -0.136
                                         0.892
sexFemale
education
           -0.27062
                       0.01541 -17.560
                                         <2e-16 ***
___
Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
(Dispersion parameter for binomial family taken to be 1)
   Null deviance: 451.722 on 40 degrees of freedom
Residual deviance: 64.007 on 38 degrees of freedom
AIC: 208.07
Number of Fisher Scoring iterations: 4
```

Figure 6.5 R output of the summary method for the logistic regression model fitted to the womensrole data.

```
ylim = c(0, 1))
+
+
      lines(womensrole$education[!f], role.fitted[!f],
+
          lty = 1)
+
      lines(womensrole$education[f], role.fitted[f],
+
          lty = 2
+
      lgtxt <- c("Fitted (Males)", "Fitted (Females)")</pre>
+
      legend("topright", lgtxt, lty = 1:2, bty = "n")
+
      y <- womensrole$agree/(womensrole$agree + womensrole$disagree)
      text(womensrole$education, y, ifelse(f, "\\VE",
+
+
          "\\MA"), family = "HersheySerif", cex = 1.25)
+ }
```

The two curves for males and females in Figure 6.6 are almost the same reflecting the non-significant value of the regression coefficient for sex in wom-ensrole\_glm\_1. But the observed values plotted on Figure 6.6 suggest that there might be an interaction of education and sex, a possibility that can be investigated by applying a further logistic regression model using

### ANALYSIS USING R R> myplot(role.fitted1)



Figure 6.6 Fitted (from womensrole\_glm\_1) and observed probabilities of agreeing for the womensrole data.

```
R> womensrole_glm_2 <- glm(cbind(agree, disagree) ~
+ sex * education, data = womensrole, family = binomial())</pre>
```

The sex and education interaction term is seen to be highly significant, as can be seen from the summary output in Figure 6.7. We can obtain a plot of deviance residuals plotted against fitted values using the following code above Figure 6.9. The residuals fall into a horizontal band between -2 and 2. This pattern does not suggest a poor fit for any particular observation or subset of observations.

#### 10 LOGISTIC REGRESSION AND GENERALISED LINEAR MODELS

```
R> summary(womensrole_glm_2)
Call:
glm(formula = cbind(agree, disagree) ~ sex * education, family = binomial(),
    data = womensrole)
Deviance Residuals:
    Min
           10
                     Median
                                   30
                                            Max
-2.39097
         -0.88062
                   0.01532
                              0.72783
                                         2.45262
Coefficients:
                   Estimate Std. Error z value Pr(>|z|)
                                         8.910
(Intercept)
                    2.09820
                             0.23550
                                                < 2e-16 ***
sexFemale
                    0.90474
                               0.36007
                                         2.513
                                                0.01198 *
education
                   -0.23403
                               0.02019 -11.592
                                                < 2e-16 ***
sexFemale:education -0.08138
                               0.03109 -2.617
                                                0.00886 **
___
Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
(Dispersion parameter for binomial family taken to be 1)
    Null deviance: 451.722 on 40 degrees of freedom
Residual deviance: 57.103 on 37 degrees of freedom
AIC: 203.16
Number of Fisher Scoring iterations: 4
```

Figure 6.7 R output of the summary method for the logistic regression model fitted to the womensrole data.

#### 6.3.3 Colonic Polyps

The data on colonic polyps in Table ?? involves *count* data. We could try to model this using multiple regression but there are two problems. The first is that a response that is a count can only take positive values, and secondly such a variable is unlikely to have a normal distribution. Instead we will apply a GLM with a log link function, ensuring that fitted values are positive, and a Poisson error distribution, i.e.,

$$\mathsf{P}(y) = \frac{e^{-\lambda}\lambda^y}{y!}.$$

This type of GLM is often known as *Poisson regression*. We can apply the model using

R> data("polyps", package = "HSAUR")
R> polyps\_glm\_1 <- glm(number ~ treat + age, data = polyps,
+ family = poisson())</pre>

```
ANALYSIS USING R
R> role.fitted2 <- predict(womensrole_glm_2, type = "response")</pre>
R> myplot(role.fitted2)
```



Fitted (from womensrole\_glm\_2) and observed probabilities of agree-Figure 6.8 ing for the womensrole data.

(The default link function when the Poisson family is requested is the log We can deal with overdispersion by using a procedure known as function.) quasi-likelihood, which allows the estimation of model parameters without fully knowing the error distribution of the response variable. McCullagh and Nelder (1989) give full details of the quasi-likelihood approach. In many respects it simply allows for the estimation of  $\phi$  from the data rather than defining it to be unity for the binomial and Poisson distributions. We can apply quasilikelihood estimation to the colonic polyps data using the following R code

```
R> polyps_glm_2 <- glm(number ~ treat + age, data = polyps,</pre>
      family = quasipoisson())
+
R> summary(polyps_glm_2)
```

```
12 LOGISTIC REGRESSION AND GENERALISED LINEAR MODELS
R> res <- residuals(womensrole_glm_2, type = "deviance")
R> plot(predict(womensrole_glm_2), res, xlab = "Fitted values",
+ ylab = "Residuals", ylim = max(abs(res)) * c(-1,
+ 1))
R> abline(h = 0, lty = 2)
```



Figure 6.9 Plot of deviance residuals from logistic regression model fitted to the womensrole data.

```
Call:

glm(formula = number ~ treat + age, family = quasipoisson(),

data = polyps)

Deviance Residuals:

Min 1Q Median 3Q Max

-4.2212 -3.0536 -0.1802 1.4459 5.8301
```

```
Coefficients:
```

R> summary(polyps\_glm\_1) Call: glm(formula = number ~ treat + age, family = poisson(), data = polyps) Deviance Residuals: Min 1Q Median ЗQ Max -4.2212 -3.0536 -0.1802 1.4459 5.8301 Coefficients: Estimate Std. Error z value Pr(>|z|)4.529024 0.146872 30.84 < 2e-16 \*\*\* (Intercept) -1.359083 0.117643 treatdrug -11.55 < 2e-16 \*\*\* -0.038830 0.005955 -6.52 7.02e-11 \*\*\* age \_\_\_ Signif. codes: 0 '\*\*\*' 0.001 '\*\*' 0.01 '\*' 0.05 '.' 0.1 ' ' 1 (Dispersion parameter for poisson family taken to be 1) Null deviance: 378.66 on 19 degrees of freedom Residual deviance: 179.54 on 17 degrees of freedom AIC: 273.88 Number of Fisher Scoring iterations: 5

# Figure 6.10 R output of the summary method for the Poisson regression model fitted to the polyps data.

Estimate Std. Error t value Pr(>/t/) (Intercept) 4.52902 0.48106 9.415 3.72e-08 \*\*\* treatdrug -1.35908 0.38533 -3.527 0.00259 \*\* -0.03883 -1.991 0.06284 . age 0.01951 \_\_\_ Signif. codes: 0 '\*\*\*' 0.001 '\*\*' 0.01 '\*' 0.05 '.' 0.1 ' ' 1 (Dispersion parameter for quasipoisson family taken to be 10.72805) Null deviance: 378.66 on 19 degrees of freedom Residual deviance: 179.54 on 17 degrees of freedom AIC: NA

Number of Fisher Scoring iterations: 5

The regression coefficients for both explanatory variables remain significant but their estimated standard errors are now much greater than the values given in Figure 6.10. A possible reason for overdispersion in these data is that polyps do not occur independently of one another, but instead may 'cluster' together.

\_\_\_\_| |\_\_\_\_

# Bibliography

McCullagh, P. and Nelder, J. A. (1989), *Generalized Linear Models*, London, UK: Chapman & Hall/CRC.

#### CHAPTER 7

## Density Estimation: Erupting Geysers and Star Clusters

- 7.1 Introduction
- 7.2 Density Estimation
- 7.3 Analysis Using R
- 7.3.1 A Parametric Density Estimate for the Old Faithful Data

```
R> logL <- function(param, x) {</pre>
      d1 <- dnorm(x, mean = param[2], sd = param[3])</pre>
+
+
      d2 \leq dnorm(x, mean = param[4], sd = param[5])
      -sum(log(param[1] * d1 + (1 - param[1]) * d2))
+
+ }
R> startparam <- c(p = 0.5, mu1 = 50, sd1 = 3, mu2 = 80,
+
      sd2 = 3)
R> opp <- optim(startparam, logL, x = faithful$waiting,</pre>
      method = "L-BFGS-B", lower = c(0.01, rep(1,
+
+
          4)), upper = c(0.99, rep(200, 4)))
R> opp
$par
                 mu1
                            sd1
                                       mu2
                                                  sd2
        р
 0.360891 54.612122 5.872379 80.093415 5.867289
$value
[1] 1034.002
$counts
function gradient
      55
                55
$convergence
[1] 0
```

Of course, optimising the appropriate likelihood 'by hand' is not very convenient. In fact, (at least) two packages offer high-level functionality for estimating mixture models. The first one is package mclust (Fraley et al., 2006) implementing the methodology described in Fraley and Raftery (2002). Here,

```
DENSITY ESTIMATION
   4
   R> data("faithful", package = "datasets")
1
   R> x <- faithful$waiting
2
   R> layout(matrix(1:3, ncol = 3))
з
   R> hist(x, xlab = "Waiting times (in min.)", ylab = "Frequency",
4
          probability = TRUE, main = "Gaussian kernel",
   +
5
          border = "gray")
   +
6
   R> lines(density(x, width = 12), lwd = 2)
7
   R > rug(x)
8
   R> hist(x, xlab = "Waiting times (in min.)", ylab = "Frequency",
9
          probability = TRUE, main = "Rectangular kernel",
10
   +
11
   +
          border = "gray")
   R> lines(density(x, width = 12, window = "rectangular"),
12
          lwd = 2)
   +
^{13}
   R > rug(x)
14
   R> hist(x, xlab = "Waiting times (in min.)", ylab = "Frequency",
15
          probability = TRUE, main = "Triangular kernel",
   +
16
          border = "gray")
   +
^{17}
   R> lines(density(x, width = 12, window = "triangular"),
^{18}
          lwd = 2)
   +
19
   R > rug(x)
20
```



Figure 7.1 Density estimates of the geyser eruption data imposed on a histogram of the data.

```
ANALYSIS USING R 5
R> library("KernSmooth")
R> data("CYGOB1", package = "HSAUR")
R> CYGOB1d <- bkde2D(CYGOB1, bandwidth = sapply(CYGOB1,
+ dpik))
R> contour(x = CYGOB1d$x1, y = CYGOB1d$x2, z = CYGOB1d$fhat,
+ xlab = "log surface temperature", ylab = "log light intensity")
```



Figure 7.2 A contour plot of the bivariate density estimate of the CYGOB1 data, i.e., a two-dimensional graphical display for a three-dimensional problem.

```
6 DENSITY ESTIMATION
R> persp(x = CYGOB1d$x1, y = CYGOB1d$x2, z = CYGOB1d$fhat,
+ xlab = "log surface temperature", ylab = "log light intensity",
+ zlab = "estimated density", theta = -35, axes = TRUE,
+ box = TRUE)
```



 $\label{eq:Figure 7.3} {$ $ The bivariate density estimate of the CYGOB1 data, here shown in a three-dimensional fashion using the persp function. }$ 

a Bayesian information criterion (BIC) is applied to choose the form of the mixture model:

```
R> library("mclust")
R> mc <- Mclust(faithful$waiting)
R> mc
   best model: E with 2 components
and the estimated means are
R> mc$parameters$mean
```

1 2 54.61911 80.09384

with estimated standard deviation (found to be equal within both groups)
R> sqrt(mc\$parameters\$variance\$sigmasq)

[1] 5.86848

The proportion is  $\hat{p} = 0.36$ . The second package is called *flexmix* whose functionality is described by Leisch (2004). A mixture of two normals can be fitted using

```
R> library("flexmix")
R> fl <- flexmix(waiting ~ 1, data = faithful, k = 2) with \hat{p} = 0.36 and estimated parameters
```

R> parameters(fl, component = 1)

```
$coef
(Intercept)
54.6287
```

\$sigma
[1] 5.895234
R> parameters(fl, component = 2)
\$coef
(Intercept)

(Incercept) 80.09858

\$sigma [1] 5.871749

We can get standard errors for the five parameter estimates by using a bootstrap approach (see Efron and Tibshirani, 1993). The original data are slightly perturbed by drawing n out of n observations with replacement and those artificial replications of the original data are called *bootstrap samples*. Now, we can fit the mixture for each bootstrap sample and assess the variability of the estimates, for example using confidence intervals. Some suitable R code based on the Mclust function follows. First, we define a function that, for a bootstrap sample indx, fits a two-component mixture model and returns  $\hat{p}$ and the estimated means (note that we need to make sure that we always get an estimate of p, not 1 - p):

```
DENSITY ESTIMATION
R> opar <- as.list(opp$par)</pre>
R > rx <- seq(from = 40, to = 110, by = 0.1)
R> d1 <- dnorm(rx, mean = opar$mu1, sd = opar$sd1)
R> d2 <- dnorm(rx, mean = opar$mu2, sd = opar$sd2)
R > f <- opar p * d1 + (1 - opar p) * d2
R> hist(x, probability = TRUE, xlab = "Waiting times (in min.)",
     +
+
R> lines(rx, f, lwd = 2)
R> lines(rx, dnorm(rx, mean = mean(x), sd = sd(x)),
     lty = 2, lwd = 2)
+
R> legend(50, 0.06, legend = c("Fitted two-component mixture density",
     "Fitted single normal density"), lty = 1:2,
+
     bty = "n")
+
```



Figure 7.4 Fitted normal density and two-component normal mixture for geyser eruption data.

The function fit can now be fed into the boot function (Canty and Ripley, 2006) for bootstrapping (here 1000 bootstrap samples are drawn)

```
R> bootpara <- boot(faithful$waiting, fit, R = 1000)
```

We assess the variability of our estimates  $\hat{p}$  by means of adjusted bootstrap percentile (BCa) confidence intervals, which for  $\hat{p}$  can be obtained from

```
R> boot.ci(bootpara, type = "bca", index = 1)
```

```
BOOTSTRAP CONFIDENCE INTERVAL CALCULATIONS
Based on 1000 bootstrap replicates
```

```
CALL :
boot.ci(boot.out = bootpara, type = "bca", index = 1)
Intervals :
Level BCa
95% ( 0.3041, 0.4233 )
Calculations and Intervals on Original Scale
```

We see that there is a reasonable variability in the mixture model, however, the means in the two components are rather stable, as can be seen from

```
R> boot.ci(bootpara, type = "bca", index = 2)
```

```
BOOTSTRAP CONFIDENCE INTERVAL CALCULATIONS
Based on 1000 bootstrap replicates
```

```
CALL :
boot.ci(boot.out = bootpara, type = "bca", index = 2)
```

```
Intervals :
Level BCa
95% (53.42, 56.07)
Calculations and Intervals on Original Scale
```

```
for \hat{\mu}_1 and for \hat{\mu}_2 from
```

```
R> boot.ci(bootpara, type = "bca", index = 3)
```

```
BOOTSTRAP CONFIDENCE INTERVAL CALCULATIONS
Based on 1000 bootstrap replicates
```

```
CALL : boot.ci(boot.out = bootpara, type = "bca", index = 3)
```

Intervals : Level BCa 95% (79.05, 81.01 ) Calculations and Intervals on Original Scale

Finally, we show a graphical representation of both the bootstrap distribution of the mean estimates and the corresponding confidence intervals. For convenience, we define a function for plotting, namely

```
R> layout(matrix(1:2, ncol = 2))
R> bootplot(bootpara, 2, main = expression(mu[1]))
R> bootplot(bootpara, 3, main = expression(mu[2]))
```

10



Figure 7.5 Bootstrap distribution and confidence intervals for the mean estimates of a two-component mixture for the geyser data.

```
R> bootplot <- function(b, index, main = "") {</pre>
      dens <- density(b$t[, index])</pre>
+
      ci <- boot.ci(b, type = "bca", index = index)$bca[4:5]</pre>
+
      est <- b$t0[index]</pre>
+
      plot(dens, main = main)
+
      y <- max(dens$y)/10
+
      segments(ci[1], y, ci[2], y, lty = 2)
+
      points(ci[1], y, pch = "(")
+
      points(ci[2], y, pch = ")")
+
      points(est, y, pch = 19)
+
+ }
```

The element t of an object created by **boot** contains the bootstrap replications of our estimates, i.e., the values computed by **fit** for each of the 1000 bootstrap samples of the geyser data. First, we plot a simple density estimate and then construct a line representing the confidence interval. We apply this function to the bootstrap distributions of our estimates  $\hat{\mu}_1$  and  $\hat{\mu}_2$  in Figure 7.5.

### Bibliography

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#### CHAPTER 8

## Recursive Partitioning: Large Companies and Glaucoma Diagnosis

#### 8.1 Introduction

#### 8.2 Recursive Partitioning

#### 8.3 Analysis Using R

#### 8.3.1 Forbes 2000 Data

For some observations the profit is missing and we first remove those companies from the list

R> data("Forbes2000", package = "HSAUR")
R> Forbes2000 <- subset(Forbes2000, !is.na(profits))</pre>

The **rpart** function from *rpart* can be used to grow a regression tree. The response variable and the covariates are defined by a model formula in the same way as for 1m, say. By default, a large initial tree is grown.

```
R> library("rpart")
R> forbes_rpart <- rpart(profits ~ assets + marketvalue +
+ sales, data = Forbes2000)</pre>
```

A print method for *rpart* objects is available, however, a graphical representation shown in Figure 8.1 is more convenient. Observations which satisfy the condition shown for each node go to the left and observations which don't are element of the right branch in each node. The numbers plotted in the leaves are the mean profit for those observations satisfying the conditions stated above. For example, the highest profit is observed for companies with a market value greater than 89.33 billion US dollars and with more than 91.92 US dollars sales. To determine if the tree is appropriate or if some of the branches need to be subjected to pruning we can use the cptable element of the *rpart* object:

#### R> print(forbes\_rpart\$cptable)

|   | CP         | nsplit | rel error | xerror    | xstd      |
|---|------------|--------|-----------|-----------|-----------|
| 1 | 0.23748446 | 0      | 1.0000000 | 1.0010339 | 0.1946331 |
| 2 | 0.04600397 | 1      | 0.7625155 | 0.8397144 | 0.2174245 |
| 3 | 0.04258786 | 2      | 0.7165116 | 0.8066685 | 0.2166339 |
| 4 | 0.02030891 | 3      | 0.6739237 | 0.7625940 | 0.2089684 |
| 5 | 0.01854336 | 4      | 0.6536148 | 0.7842574 | 0.2093683 |
| 6 | 0.01102304 | 5      | 0.6350714 | 0.7925891 | 0.2106088 |

```
4 RECURSIVE PARTITIONING

R> plot(forbes_rpart, uniform = TRUE, margin = 0.1,

+ branch = 0.5, compress = TRUE)

R> text(forbes_rpart)
```



Figure 8.1 Large initial tree for Forbes 2000 data.

| 7 | 0.01076006 | 6 | 0.6240484 | 0.7931405 | 0.2128048 |
|---|------------|---|-----------|-----------|-----------|
| 8 | 0.01000000 | 7 | 0.6132883 | 0.7902771 | 0.2128037 |

#### R> opt <- which.min(forbes\_rpart\$cptable[, "xerror"])</pre>

The **xerror** column contains of estimates of cross-validated prediction error for different numbers of splits (**nsplit**). The best tree has three splits. Now we can prune back the large initial tree using

```
R> cp <- forbes_rpart$cptable[opt, "CP"]
R> forbes_prune <- prune(forbes_rpart, cp = cp)</pre>
```

The result is shown in Figure 8.2. This tree is much smaller. From the sample sizes and boxplots shown for each leaf we see that the majority of companies

is grouped together. However, a large market value, more that 32.72 billion US dollars, seems to be a good indicator of large profits.

#### 8.3.2 Glaucoma Diagnosis

```
R> data("GlaucomaM", package = "ipred")
R> glaucoma_rpart <- rpart(Class ~ ., data = GlaucomaM,
      control = rpart.control(xval = 100))
+
R> glaucoma_rpart$cptable
          CP nsplit rel error
                                                 xstd
                                   xerror
1 0.65306122
                  0 1.0000000 1.5306122 0.06054391
2 0.07142857
                   1 0.3469388 0.3877551 0.05647630
3 0.01360544
                   2 0.2755102 0.3775510 0.05590431
4 0.01000000
                   5 0.2346939 0.4489796 0.05960655
R> opt <- which.min(glaucoma_rpart$cptable[, "xerror"])</pre>
R> cp <- glaucoma_rpart$cptable[opt, "CP"]</pre>
R> glaucoma_prune <- prune(glaucoma_rpart, cp = cp)
```

As we discussed earlier, the choice of the appropriate sized tree is not a trivial problem. For the glaucoma data, the above choice of three leaves is very unstable across multiple runs of cross-validation. As an illustration of this problem we repeat the very same analysis as shown above and record the optimal number of splits as suggested by the cross-validation runs.

Although for 14 runs of cross-validation a simple tree with one split only is suggested, larger trees would have been favored in 11 of the cases. This short analysis shows that we should not trust the tree in Figure 8.3 too much. One way out of this dilemma is the aggregation of multiple trees via *bagging*. In R, the bagging idea can be implemented by three or four lines of code. Case count or weight vectors representing the bootstrap samples can be drawn from the multinominal distribution with parameters n and  $p_1 = 1/n, \ldots, p_n = 1/n$  via the **rmultinom** function. For each weight vector, one large tree is constructed without pruning and the *rpart* objects are stored in a list, here called **trees**:

```
R> trees <- vector(mode = "list", length = 25)
R> n <- nrow(GlaucomaM)
R> bootsamples <- rmultinom(length(trees), n, rep(1,</pre>
```



Figure 8.2 Pruned regression tree for Forbes 2000 data with the distribution of the profit in each leaf depicted by a boxplot.

### ANALYSIS USING R R> layout(matrix(1:2, nc = 1)) R> plot(glaucoma\_prune, uniform = TRUE, margin = 0.1, + branch = 0.5, compress = TRUE) R> text(glaucoma\_prune, use.n = TRUE) R> rn <- rownames(glaucoma\_prune\$frame) R> lev <- rn[sort(unique(glaucoma\_prune\$where))] R> where <- factor(rn[glaucoma\_prune\$where], levels = lev) R> mosaicplot(table(where, GlaucomaM\$Class), main = "", + xlab = "", las = 1) varg<0.209



Figure 8.3 Pruned classification tree of the glaucoma data with class distribution in the leaves depicted by a mosaicplot.

```
+ n)/n)
R> mod <- rpart(Class ~ ., data = GlaucomaM, control = rpart.control(xval = 0))
R> for (i in 1:length(trees)) trees[[i]] <- update(mod,
+ weights = bootsamples[, i])</pre>
```

The update function re-evaluates the call of mod, however, with the weights being altered, i.e., fits a tree to a bootstrap sample specified by the weights. It is interesting to have a look at the structures of the multiple trees. For example, the variable selected for splitting in the root of the tree is not unique as can be seen by

R> table(sapply(trees, function(x) as.character(x\$frame\$var[1])))

phcg varg vari vars 1 14 9 1

Although varg is selected most of the time, other variables such as vari occur as well – a further indication that the tree in Figure 8.3 is questionable and that hard decisions are not appropriate for the glaucoma data. In order to make use of the ensemble of trees in the list **trees** we estimate the conditional probability of suffering from glaucoma given the covariates for each observation in the original data set by

Thus, for each observation we get 25 estimates. However, each observation has been used for growing one of the trees with probability 0.632 and thus was not used with probability 0.368. Consequently, the estimate from a tree where an observation was not used for growing is better for judging the quality of the predictions and we label the other estimates with NA. Now, we can average the estimates and we vote for glaucoma when the average of the estimates of the conditional glaucoma probability exceeds 0.5. The comparison between the observed and the predicted classes does not suffer from overfitting since the predictions are computed from those trees for which each single observation was *not* used for growing.

```
R> avg <- rowMeans(classprob, na.rm = TRUE)
R> predictions <- factor(avg > 0.5, labels = levels(GlaucomaM$Class))
R> predtab <- table(predictions, GlaucomaM$Class)
R> predtab
```

| predictions | glaucoma | normal |
|-------------|----------|--------|
| glaucoma    | 78       | 15     |
| normal      | 20       | 83     |

Thus, an honest estimate of the probability of a glaucoma prediction when the patient is actually suffering from glaucoma is

```
R> round(predtab[1, 1]/colSums(predtab)[1] * 100)
```

glaucoma 80

per cent. For

```
R> round(predtab[2, 2]/colSums(predtab)[2] * 100)
```

normal 85

per cent of normal eyes, the ensemble does not predict a glaucomateous damage. The *bagging* procedure is a special case of a more general approach called *random forest* (Breiman, 2001). The package *randomForest* (Breiman et al., 2006) can be used to compute such ensembles via

```
R> library("randomForest")
R> rf <- randomForest(Class ~ ., data = GlaucomaM)
and we obtain out-of-bag estimates for the prediction error via</pre>
```

R> table(predict(rf), GlaucomaM\$Class)

|          | glaucoma | normal |
|----------|----------|--------|
| glaucoma | 81       | 11     |
| normal   | 17       | 87     |

For the glaucoma data, such a *conditional inference tree* can be computed using the  $\mathsf{ctree}$  function

```
R> library("party")
```

R> glaucoma\_ctree <- ctree(Class ~ ., data = GlaucomaM)</pre>

and a graphical representation is depicted in Figure 8.5 showing both the cutpoints and the *p*-values of the associated independence tests for each node. The first split is performed using a cutpoint defined with respect to the volume of the optic nerve above some reference plane, but in the inferior part of the eye only (vari).



Figure 8.4 Glaucoma data: Estimated class probabilities depending on two important variables. The 0.5 cut-off for the estimated glaucoma probability is depicted as horizontal line. Glaucomateous eyes are plotted as circles and normal eyes are triangles.

### ANALYSIS USING R R> plot(glaucoma\_ctree)



Figure 8.5 Glaucoma data: Conditional inference tree with the distribution of glaucomateous eyes shown for each terminal leaf.

\_\_\_\_| |\_\_\_\_

# Bibliography

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#### CHAPTER 9

## Survival Analysis: Glioma Treatment and Breast Cancer Survival

#### 9.1 Introduction

9.2 Survival Analysis

#### 9.3 Analysis Using R

#### 9.3.1 Glioma Radioimmunotherapy

Figure 9.1 leads to the impression that patients treated with the novel radioimmunotherapy survive longer, regardless of the tumor type. In order to assess if this informal finding is reliable, we may perform a log-rank test via

```
R> survdiff(Surv(time, event) ~ group, data = g3)
```

Call: survdiff(formula = Surv(time, event) ~ group, data = g3) N Observed Expected (O-E)^2/E (O-E)^2/V group=Control 6 4 1.49 4.23 6.06 group=RIT 11 2 4.51 1.40 6.06

Chisq= 6.1 on 1 degrees of freedom, p= 0.0138

which indicates that the survival times are indeed different in both groups. However, the number of patients is rather limited and so it might be dangerous to rely on asymptotic tests. As shown in Chapter 3, conditioning on the data and computing the distribution of the test statistics without additional assumptions is one alternative. The function surv\_test from package *coin* (Hothorn et al., 2006b,a) can be used to compute an exact conditional test answering the question whether the survival times differ for grade III patients:

```
4
                                                SURVIVAL ANALYSIS
R> data("glioma", package = "coin")
R> library("survival")
R> layout(matrix(1:2, ncol = 2))
R> g3 <- subset(glioma, histology == "Grade3")
R> plot(survfit(Surv(time, event) ~ group, data = g3),
      main = "Grade III Glioma", lty = c(2, 1), ylab = "Probability",
xlab = "Survival Time in Month", legend.bty = "n",
+
+
      legend.text = c("Control", "Treated"))
+
R> g4 <- subset(glioma, histology == "GBM")
R> plot(survfit(Surv(time, event) ~ group, data = g4),
      main = "Grade IV Glioma", ylab = "Probability",
+
      lty = c(2, 1), xlab = "Survival Time in Month",
+
      xlim = c(0, max(glioma$time) * 1.05))
+
```



Figure 9.1 Survival times comparing treated and control patients.

which, in this case, confirms the above results. The same exercise can be performed for patients with grade IV glioma

```
data: Surv(time, event) by groups Control, RIT
Z = 3.2215, p-value = 0.0001588
alternative hypothesis: two.sided
```

which shows a difference as well. However, it might be more appropriate to

answer the question whether the novel therapy is superior for both groups of tumors simultaneously. This can be implemented by *stratifying*, or *blocking*, with respect tumor grading:

```
R> surv_test(Surv(time, event) ~ group | histology,
+ data = glioma, distribution = approximate(B = 10000))
```

Approximative Logrank Test

```
data: Surv(time, event) by
    groups Control, RIT
    stratified by histology
Z = 3.6704, p-value = 1e-04
alternative hypothesis: two.sided
```

Here, we need to approximate the exact conditional distribution since the exact distribution is hard to compute. The result supports the initial impression implied by Figure 9.1

#### 9.3.2 Breast Cancer Survival

Before fitting a Cox model to the GBSG2 data, we again derive a Kaplan-Meier estimate of the survival function of the data, here stratified with respect to whether a patient received a hormonal therapy or not (see Figure 9.2). Fitting a Cox model follows roughly the same rules are shown for linear models in Chapters 4, 5 or 6 with the exception that the response variable is again coded as a *Surv* object. For the GBSG2 data, the model is fitted via

R> GBSG2\_coxph <- coxph(Surv(time, cens) ~ ., data = GBSG2)</pre>

and the results as given by the **summary** method are given in Figure 9.3. Since we are especially interested in the relative risk for patients who underwent a hormonal therapy, we can compute an estimate of the relative risk and a corresponding confidence interval via

This result implies that patients treated with a hormonal therapy had a lower risk and thus survived longer compared to women who were not treated this way. Model checking and model selection for proportional hazards models are complicated by the fact that easy to use residuals, such as those discussed in Chapter 5 for linear regression model are not available, but several possibilities do exist. A check of the proportional hazards assumption can be done by looking at the parameter estimates  $\beta_1, \ldots, \beta_q$  over time. We can safely assume proportional hazards when the estimates don't vary much over time. The null hypothesis of constant regression coefficients can be tested, both globally as well as for each covariate, by using the cox.zph function

 $\mathbf{6}$ 



Figure 9.2 Kaplan-Meier estimates for breast cancer patients who either received a hormonal therapy or not.

# R> GBSG2\_zph <- cox.zph(GBSG2\_coxph) R> GBSG2\_zph

|              | rho       | chisq    | р       |
|--------------|-----------|----------|---------|
| horThyes     | -2.54e-02 | 1.96e-01 | 0.65778 |
| age          | 9.40e-02  | 2.96e+00 | 0.08552 |
| menostatPost | -1.19e-05 | 3.75e-08 | 0.99985 |
| tsize        | -2.50e-02 | 1.88e-01 | 0.66436 |
| tgrade.L     | -1.30e-01 | 4.85e+00 | 0.02772 |

#### R> summary(GBSG2\_coxph)

#### Call:

coxph(formula = Surv(time, cens) ~ ., data = GBSG2)

n= 686

| coef) z                              | р  |  |  |  |
|--------------------------------------|--|--|--|--|
| 29075 -2.683                         | 7.3e-03  |  |  |  |
| 09301 -1.017                         | 3.1e-01  |  |  |  |
| 83476 1.409                          | 1.6e-01  |  |  |  |
| 03939 1.979                          | 4.8e-02  |  |  |  |
| 89844 2.904                          | 3.7e-03  |  |  |  |
| 21965 -1.649                         | 9.9e-02  |  |  |  |
| 07447 6.551                          | 5.7e-11  |  |  |  |
| 00574 -3.866                         | 1.1e-04  |  |  |  |
| 00450 0.438                          | 6.6e-01  |  |  |  |
|                                      |  |  |  |  |
| wer .95 upper                        | .95  |  |  |  |
| 0.549 0                              | .911   |  |  |  |
| 0.973 1                              | .009   |  |  |  |
| 0.904 1                              | .855   |  |  |  |
| 1.000 1                              | .016   |  |  |  |
| 1.196 2                              | 2.518  |  |  |  |
| 0.644 1                              | .039   |  |  |  |
| 1.035 1                              | .065   |  |  |  |
| 0.997 0                              | .999   |  |  |  |
| 0.999 1                              | .001   |  |  |  |
| Rsquare= 0.142 (max possible= 0.995) |  |  |  |  |
|                                      |  |  |  |  |
| p=0                                  |  |  |  |  |
| p=0                                  |  |  |  |  |
|                                      | $\begin{array}{cccccccccccccccccccccccccccccccccccc$ |  |  |  |

Figure 9.3 R output of the summary method for GBSG2\_coxph.

| tgrade.Q | 3.22e-03 | 3.14e-03 | 0.95530 |
|----------|----------|----------|---------|
| pnodes   | 5.84e-02 | 5.98e-01 | 0.43941 |
| progrec  | 5.65e-02 | 1.20e+00 | 0.27351 |
| estrec   | 5.46e-02 | 1.03e+00 | 0.30967 |
| GLOBAL   | NA       | 2.27e+01 | 0.00695 |

There seems to be some evidence of time-varying effects, especially for age and tumor grading. A graphical representation of the estimated regression coefficient over time is shown in Figure 9.4. We refer to Therneau and Grambsch (2000) for a detailed theoretical description of these topics. The treestructured regression models applied to continuous and binary responses in Chapter 8 are applicable to censored responses in survival analysis as well. Such a simple prognostic model with only a few terminal nodes might be R> plot(GBSG2\_zph, var = "age")



Figure 9.4 Estimated regression coefficient for age depending on time for the GBSG2 data.

helpful for relating the risk to certain subgroups of patients. Both **rpart** and the **ctree** function from package *party* can be applied to the GBSG2 data, where the conditional trees of the latter selects cutpoints based on log-rank statistics;

R> GBSG2\_ctree <- ctree(Surv(time, cens) ~ ., data = GBSG2)</pre>

and the plot method applied to this tree produces the graphical representation in Figure 9.6. The number of positive lymph nodes (pnodes) is the most important variable in the tree, this corresponds to the *p*-value associated with this variable in Cox's regression, see Figure 9.3. Women with not more than three positive lymph nodes who have undergone a hormonal therapy seem to have the best prognosis whereas a large number of positive lymph nodes and a small value of the progesterone receptor indicates a bad prognosis.

```
R> layout(matrix(1:3, ncol = 3))
R> res <- residuals(GBSG2_coxph)
R> plot(res ~ age, data = GBSG2, ylim = c(-2.5, 1.5),
+     pch = ".", ylab = "Martingale Residuals")
R> abline(h = 0, lty = 3)
R> plot(res ~ pnodes, data = GBSG2, ylim = c(-2.5,
+     1.5), pch = ".", ylab = "")
R> abline(h = 0, lty = 3)
R> plot(res ~ log(progrec), data = GBSG2, ylim = c(-2.5,
+     1.5), pch = ".", ylab = "")
R> abline(h = 0, lty = 3)
```



Figure 9.5 Martingale residuals for the GBSG2 data.
10 R> plot(GBSG2\_ctree)



Figure 9.6 GBSG2 data: Conditonal inference tree with the survival function, estimated by Kaplan-Meier, shown for every subgroup of patients identified by the tree.

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# CHAPTER 10

# Analysing Longitudinal Data I: Computerised Delivery of Cognitive Behavioural Therapy–Beat the Blues

# 10.1 Introduction

# 10.2 Analysing Longitudinal Data

# 10.3 Analysis Using R

We shall fit both random intercept and random intercept and slope models to the data including the baseline BDI values (pre.bdi), treatment group, drug and length as fixed effect covariates. Linear mixed effects models are fitted in R by using the lmer function contained in the *lme4* package (Bates and Sarkar, 2006, Pinheiro and Bates, 2000, Bates, 2005), but an essential first step is to rearrange the data from the 'wide form' in which they appear in the BtheB data frame into the 'long form' in which each separate repeated measurement and associated covariate values appear as a separate row in a *data.frame*. This rearrangement can be made using the following code:

```
R> data("BtheB", package = "HSAUR")
R> BtheB$subject <- factor(rownames(BtheB))
R> nobs <- nrow(BtheB)
R> BtheB_long <- reshape(BtheB, idvar = "subject",
+ varying = c("bdi.2m", "bdi.4m", "bdi.6m", "bdi.8m"),
+ direction = "long")
R> BtheB_long$time <- rep(c(2, 4, 6, 8), rep(nobs,
+ 4))</pre>
```

such that the data are now in the form (here shown for the first three subjects)
R> subset(BtheB\_long, subject %in% c("1", "2", "3"))

|               | drug | length | treatment | bdi.pre | subject | time | bdi |
|---------------|------|--------|-----------|---------|---------|------|-----|
| 1.2m          | No   | >6m    | TAU       | 29      | 1       | 2    | 2   |
| 2.2m          | Yes  | >6m    | BtheB     | 32      | 2       | 2    | 16  |
| 3.2m          | Yes  | <6m    | TAU       | 25      | 3       | 2    | 20  |
| 1.4m          | No   | >6m    | TAU       | 29      | 1       | 4    | 2   |
| 2.4m          | Yes  | >6m    | BtheB     | 32      | 2       | 4    | 24  |
| 3.4m          | Yes  | <6m    | TAU       | 25      | 3       | 4    | NA  |
| 1.6m          | No   | >6m    | TAU       | 29      | 1       | 6    | NA  |
| 2 <b>.</b> 6m | Yes  | >6m    | BtheB     | 32      | 2       | 6    | 17  |
| 3 <b>.</b> 6m | Yes  | <6m    | TAU       | 25      | 3       | 6    | NA  |

```
R> data("BtheB", package = "HSAUR")
R> layout(matrix(1:2, nrow = 1))
R> ylim <- range(BtheB[, grep("bdi", names(BtheB))],</pre>
      na.rm = TRUE)
+
R> boxplot(subset(BtheB, treatment == "TAU")[, grep("bdi",
      names(BtheB))], main = "Treated as usual", ylab = "BDI",
+
+
      xlab = "Time (in months)", names = c(0, 2, 4,
          6, 8), ylim = ylim)
+
R> boxplot(subset(BtheB, treatment == "BtheB")[, grep("bdi",
      names(BtheB))], main = "Beat the Blues", ylab = "BDI",
+
      xlab = "Time (in months)", names = c(0, 2, 4,
+
          6, 8), ylim = ylim)
+
```

Treated as usual





Figure 10.1 Boxplots for the repeated measures by treatment group for the BtheB data.

| 1 <b>.</b> 8m | No  | >6m | TAU   | 29 | 1 | 8 | NA |
|---------------|-----|-----|-------|----|---|---|----|
| 2.8m          | Yes | >6m | BtheB | 32 | 2 | 8 | 20 |
| 3.8m          | Yes | <6m | TAU   | 25 | 3 | 8 | NA |

The resulting *data.frame* BtheB\_long contains a number of missing values and in applying the lmer function these will be dropped. But notice it is only the missing values that are removed, *not* participants that have at least one missing value. All the available data is used in the model fitting process. The lmer function is used in a similar way to the lm function met in Chapter ?? with the addition of a random term to identify the source of the repeated

measurements, here subject. We can fit the two models (??) and (??) and test which is most appropriate using

```
R> library("lme4")
R> BtheB_lmer1 <- lmer(bdi ~ bdi.pre + time + treatment +</pre>
      drug + length + (1 | subject), data = BtheB_long,
+
      method = "ML", na.action = na.omit)
+
R> BtheB_lmer2 <- lmer(bdi ~ bdi.pre + time + treatment +</pre>
      drug + length + (time | subject), data = BtheB_long,
+
      method = "ML", na.action = na.omit)
+
R> anova(BtheB_lmer1, BtheB_lmer2)
Data: BtheB_long
Models:
BtheB_lmer1: bdi ~ bdi.pre + time + treatment + drug + length + (1 | subject)
BtheB_lmer2: bdi ~ bdi.pre + time + treatment + drug + length + (time | subject)
          Df AIC BIC logLik Chisq Chi Df
BtheB_lmer1 7 1884.62 1910.07 -935.31
BtheB_lmer2 9 1887.81 1920.52 -934.90 0.8161
                                                       2
            Pr(>Chisq)
BtheB_lmer1
BtheB_lmer2
                  0.665
```

ANALYSING LONGITUDINAL DATA I

# R> summary(BtheB\_lmer1)

Linear mixed-effects model fit by maximum likelihood Formula: bdi ~ bdi.pre + time + treatment + drug + length + (1 | subject) Data: BtheB\_long AIC BIC logLik MLdeviance REMLdeviance 1885 1910 -935.3 1871 1866 Random effects: Groups Name Variance Std.Dev. subject (Intercept) 48.304 6.9501 25.128 5.0127 Residual number of obs: 280, groups: subject, 97 Fixed effects: Estimate Std. Error t value (Intercept) 5.94366 2.24922 2.643 8.225 0.07759 bdi.pre 0.63819 time -0.71702 0.14606 -4.909 1.66375 -1.426 treatmentBtheB -2.37308 drugYes -2.79784 1.72000 -1.627 length>6m 0.25635 1.63219 0.157 Correlation of Fixed Effects: (Intr) bdi.pr time trtmBB drugYs bdi.pre -0.678 time -0.264 0.023 tretmntBthB -0.389 0.121 0.022 -0.071 -0.237 -0.025 -0.323 drugYes length>6m -0.238 -0.242 -0.043 0.002 0.158

Figure 10.2 R output of the linear mixed-effects model fit for the BtheB data.

# Bibliography

- Bates, D. (2005), "Fitting linear mixed models in R," *R News*, 5, 27–30, URL http://CRAN.R-project.org/doc/Rnews/.
- Bates, D. and Sarkar, D. (2006), *lme4: Linear Mixed-Effects Models Using S4 Classes*, URL http://CRAN.R-project.org, R package version 0.9975-1.
- Pinheiro, J. C. and Bates, D. M. (2000), *Mixed-Effects Models in S and S-PLUS*, New York, USA: Springer.

# CHAPTER 11

# Analysing Longitudinal Data II – Generalised Estimation Equations: Treating Respiratory Illness and Epileptic Seizures

# 11.1 Introduction

# 11.2 Generalised Estimating Equations

# 11.3 Analysis Using R

# 11.3.1 Beat the Blues Revisited

To use the gee function, package gee (Carey et al., 2006) has to be installed and attached:

# R> library("gee")

The gee function is used in a similar way to the lme function met in Chapter 10, with the addition of the features of the glm function that specify the appropriate error distribution for the response and the implied link function, and an argument to specify the structure of the working correlation matrix. Here we will fit an independence structure and then an exchangeable structure. The R code for fitting generalised estimation equations to the BtheB\_long data (as constructed in Chapter 10, with idenity working correlation matrix is as follows (note that the gee function assumes the rows of the *data.frame* BtheB\_long to be ordered with respect to subjects)

and with exchangeable correlation matrix

```
R> btb_gee1 <- gee(bdi ~ bdi.pre + treatment + length +
+ drug, data = BtheB_long, id = subject, family = gaussian,
+ corstr = "exchangeable")</pre>
```

The summary method can be used to inspect the fitted models; the results are shown in Figures 11.1 and 11.2

#### 11.3.2 Respiratory Illness

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The baseline status, i.e., the status for month == 0, will enter the models as an explanatory variable and thus we have to rearrange the *data.frame* respiratory in order to create a new variable baseline:

```
R> data("respiratory", package = "HSAUR")
R> resp <- subset(respiratory, month > "0")
R> resp$baseline <- rep(subset(respiratory, month ==
+ "0")$status, rep(4, 111))
R> resp$nstat <- as.numeric(resp$status == "good")</pre>
```

The new variable nstat is simply a dummy coding for a poor respiratory status. Now we can use the data resp to fit a logistic regression model and GEE models with an independent and an exchangeable correlation structure as follows;

```
R> resp_glm <- glm(status ~ centre + treatment + sex +</pre>
+
      baseline + age, data = resp, family = "binomial")
R> resp_gee1 <- gee(nstat ~ centre + treatment + sex +
      baseline + age, data = resp, family = "binomial",
+
      id = subject, corstr = "independence", scale.fix = TRUE,
+
+
      scale.value = 1)
R> resp_gee2 <- gee(nstat ~ centre + treatment + sex +
+
      baseline + age, data = resp, family = "binomial",
+
      id = subject, corstr = "exchangeable", scale.fix = TRUE,
      scale.value = 1)
+
```

# R> summary(btb\_gee)

GEE: GENERALIZED LINEAR MODELS FOR DEPENDENT DATA gee S-function, version 4.13 modified 98/01/27 (1998) Model: Link: Identity Variance to Mean Relation: Gaussian Correlation Structure: Independent Call: gee(formula = bdi ~ bdi.pre + treatment + length + drug, id = subject, data = BtheB\_long, family = gaussian, corstr = "independence") Summary of Residuals: Min 10 Median ЗQ Max -21.6497810 -5.8485100 0.1131663 5.5838383 28.1871039 Coefficients: Estimate Naive S.E. Naive z Robust S.E. 3.5686314 1.4833349 2.405816 2.26947617 (Intercept) 0.5818494 0.0563904 10.318235 0.09156455 bdi.pre treatmentBtheB -3.2372285 1.1295569 -2.865928 1.77459534 length>6m 1.4577182 1.1380277 1.280916 1.48255866 drugYes -3.7412982 1.1766321 -3.179667 1.78271179 Robust z (Intercept) 1.5724472 bdi.pre 6.3545274 treatmentBtheB -1.8242066 0.9832449 length>6m drugYes -2.0986557 Estimated Scale Parameter: 79.25813 Number of Iterations: 1 Working Correlation [,1] [,2] [,3] [,4] [1,] 0 1 0 0 0 0 [2,] 0 1 0 [3,] 0 0 1 0 0 0 1 [4,]

Figure 11.1 R output of the summary method for the btb\_gee model.

ANALYSING LONGITUDINAL DATA II

R> summary(btb\_gee1) GEE: GENERALIZED LINEAR MODELS FOR DEPENDENT DATA gee S-function, version 4.13 modified 98/01/27 (1998) Model: Link: Identity Variance to Mean Relation: Gaussian Correlation Structure: Exchangeable Call: gee(formula = bdi ~ bdi.pre + treatment + length + drug, id = subject, data = BtheB\_long, family = gaussian, corstr = "exchangeable") Summary of Residuals: Min 10 Median 3Q Max -23.955980 -6.643864 -1.109741 4.257688 25.452310 Coefficients: Estimate Naive S.E. Naive z Robust S.E. (Intercept) 3.0231602 2.30390185 1.31219140 2.23204410 0.6479276 0.08228567 7.87412417 0.08351405 bdi.pre treatmentBtheB -2.1692863 1.76642861 -1.22806339 1.73614385 -0.1112910 1.73091679 -0.06429596 1.55092705 length>6m drugYes -2.9995608 1.82569913 -1.64296559 1.73155411 Robust z 1.3544357 (Intercept) 7.7583066 bdi.pre treatmentBtheB -1.2494854 length>6m -0.0717577 drugYes -1.7322940 Estimated Scale Parameter: 81.7349 Number of Iterations: 5 Working Correlation [,1] [,2] [,3] [,4] [1,] 1.0000000 0.6757951 0.6757951 0.6757951 [2,] 0.6757951 1.0000000 0.6757951 0.6757951 [3,] 0.6757951 0.6757951 1.0000000 0.6757951 [4,] 0.6757951 0.6757951 0.6757951 1.0000000

Figure 11.2 R output of the summary method for the btb\_gee1 model.

R> summary(resp\_glm) Call: glm(formula = status ~ centre + treatment + sex + baseline + age, family = "binomial", data = resp) Deviance Residuals: 1Q Median 3Q Min Max 0.8953 -2.3146 -0.8551 0.4336 1.9246 Coefficients: Estimate Std. Error z value Pr(>|z|) -0.900171 0.337653 -2.666 0.00768 \*\* (Intercept) centre2 0.671601 0.239567 2.803 0.00506 \*\* treatmenttreatment 1.299216 0.236841 5.486 4.12e-08 \*\*\* sexmale 0.119244 0.294671 0.405 0.68572 0.241290 7.800 6.20e-15 \*\*\* baselinegood 1.882029 0.008864 -2.049 0.04043 \* -0.018166 age \_\_\_ Signif. codes: 0 '\*\*\*' 0.001 '\*\*' 0.01 '\*' 0.05 '.' 0.1 ' ' 1 (Dispersion parameter for binomial family taken to be 1) Null deviance: 608.93 on 443 degrees of freedom Residual deviance: 483.22 on 438 degrees of freedom AIC: 495.22 Number of Fisher Scoring iterations: 4

Figure 11.3 R output of the summary method for the resp\_glm model.

ANALYSING LONGITUDINAL DATA II

R> summary(resp\_gee1) GEE: GENERALIZED LINEAR MODELS FOR DEPENDENT DATA gee S-function, version 4.13 modified 98/01/27 (1998) Model: Link: Logit Variance to Mean Relation: Binomial Independent Correlation Structure: Call: gee (formula = nstat ~ centre + treatment + sex + baseline + age, id = subject, data = resp, family = "binomial", corstr = "independence", scale.fix = TRUE, scale.value = 1) Summary of Residuals: Min 1Q Median 3Q Max -0.93134415 -0.30623174 0.08973552 0.33018952 0.84307712 Coefficients: Estimate Naive S.E. Naive z -0.90017133 0.337653052 -2.665965 (Intercept) 0.67160098 0.239566599 2.803400 centre2 treatmenttreatment 1.29921589 0.236841017 5.485603 sexmale 0.11924365 0.294671045 0.404667 baselinegood 1.88202860 0.241290221 7.799854 -0.01816588 0.008864403 -2.049306 age Robust S.E. Robust z 0.46032700 -1.9555041 (Intercept) 0.35681913 1.8821889 centre2 treatmenttreatment 0.35077797 3.7038127 sexmale 0.44320235 0.2690501 baselinegood 0.35005152 5.3764332 age 0.01300426 -1.3969169 Estimated Scale Parameter: 1 Number of Iterations: 1 Working Correlation [,1] [,2] [,3] [,4] [1,] 0 0 0 1 [2,] 0 1 0 0 [3,] 0 0 1 0 [4,] 0 0 0 1

Figure 11.4 R output of the summary method for the resp\_gee1 model.

#### R> summary(resp\_gee2) GEE: GENERALIZED LINEAR MODELS FOR DEPENDENT DATA gee S-function, version 4.13 modified 98/01/27 (1998) Model: Link: Logit Variance to Mean Relation: Binomial Correlation Structure: Exchangeable Call: gee (formula = nstat ~ centre + treatment + sex + baseline + age, id = subject, data = resp, family = "binomial", corstr = "exchangeable", scale.fix = TRUE, scale.value = 1) Summary of Residuals: Min 1Q Median ЗQ Max -0.93134415 -0.30623174 0.08973552 0.33018952 0.84307712 Coefficients: Estimate Naive S.E. Naive z -0.90017133 0.47846344 -1.8813796 (Intercept) 0.67160098 0.33947230 1.9783676 centre2 treatmenttreatment 1.29921589 0.33561008 3.8712064 0.11924365 0.41755678 0.2855747 sexmale baselinegood 1.88202860 0.34191472 5.5043802 -0.01816588 0.01256110 -1.4462014 age Robust S.E. Robust z 0.46032700 -1.9555041 (Intercept) 0.35681913 1.8821889 centre2 3.7038127 treatmenttreatment 0.35077797 sexmale 0.44320235 0.2690501 baselinegood 0.35005152 5.3764332 age 0.01300426 -1.3969169 Estimated Scale Parameter: 1 Number of Iterations: 1 Working Correlation [,1] [,2] [,3] [,4] [1,] 1.0000000 0.3359883 0.3359883 0.3359883 [2,] 0.3359883 1.0000000 0.3359883 0.3359883 [3,] 0.3359883 0.3359883 1.0000000 0.3359883 [4,] 0.3359883 0.3359883 0.3359883 1.0000000

Figure 11.5 R output of the summary method for the resp\_gee2 model.

#### ANALYSING LONGITUDINAL DATA II

The estimated treatment effect taken from the exchangeable structure GEE model is 1.299 which, using the robust standard errors, has an associated 95% confidence interval

```
R> se <- summary(resp_gee2)$coefficients["treatmenttreatment",
+ "Robust S.E."]
R> coef(resp_gee2)["treatmenttreatment"] + c(-1, 1) *
+ se * qnorm(0.975)
[1] 0.6117037 1.9867281
```

These values reflect effects on the log-odds scale. Interpretation becomes simpler if we exponentiate the values to get the effects in terms of odds. This gives a treatment effect of 3.666 and a 95% confidence interval of

```
R> exp(coef(resp_gee2)["treatmenttreatment"] + c(-1,
+ 1) * se * qnorm(0.975))
[1] 1.843570 7.291637
```

The odds of achieving a 'good' respiratory status with the active treatment is between about twice and seven times the corresponding odds for the placebo.

# 11.3.3 Epilepsy

Moving on to the count data in epilepsy from Table ??, we begin by calculating the means and variances of the number of seizures for all treatment / period interactions

```
R> data("epilepsy", package = "HSAUR")
R> itp <- interaction(epilepsy$treatment, epilepsy$period)
R> tapply(epilepsy$seizure.rate, itp, mean)
```

```
placebo.1 Progabide.1 placebo.2 Progabide.2 placebo.3
9.357143 8.580645 8.285714 8.419355 8.785714
Progabide.3 placebo.4 Progabide.4
8.129032 7.964286 6.709677
```

R> tapply(epilepsy\$seizure.rate, itp, var)

```
placebo.1 Progabide.1 placebo.2 Progabide.2 placebo.3
102.75661 332.71828 66.65608 140.65161 215.28571
Progabide.3 placebo.4 Progabide.4
193.04946 58.18386 126.87957
```

Some of the variances are considerably larger than the corresponding means, which for a Poisson variable may suggest that overdispersion may be a problem, see Chapter ??. We can now fit a Poisson regression model to the data assuming independence using the glm function. We also use the GEE approach to fit an independence structure, followed by an exchangeable structure using the following R code:

```
R> per <- rep(log(2), nrow(epilepsy))
R> epilepsy$period <- as.numeric(epilepsy$period)</pre>
```

```
ANALYSIS USING R 11

R> layout(matrix(1:2, nrow = 1))

R> ylim <- range(epilepsy$seizure.rate)

R> placebo <- subset(epilepsy, treatment == "placebo")

R> progabide <- subset(epilepsy, treatment == "Progabide")

R> boxplot(seizure.rate ~ period, data = placebo, ylab = "Number of seizures",

+ xlab = "Period", ylim = ylim, main = "Placebo")

R> boxplot(seizure.rate ~ period, data = progabide,

+ main = "Progabide", ylab = "Number of seizures",

+ xlab = "Period", ylim = ylim)
```



Figure 11.6 Boxplots of numbers of seizures in each two-week period post randomisation for placebo and active treatments.

```
R> epilepsy_glm <- glm(seizure.rate ~ base + age +</pre>
+
      treatment + offset(per), data = epilepsy, family = "poisson")
R> epilepsy_gee1 <- gee(seizure.rate ~ base + age +</pre>
      treatment + offset(per), data = epilepsy, family = "poisson",
+
      id = subject, corstr = "independence", scale.fix = TRUE,
+
      scale.value = 1)
R> epilepsy_gee2 <- gee(seizure.rate ~ base + age +</pre>
      treatment + offset(per), data = epilepsy, family = "poisson",
+
      id = subject, corstr = "exchangeable", scale.fix = TRUE,
+
      scale.value = 1)
+
R> epilepsy_gee3 <- gee(seizure.rate ~ base + age +
      treatment + offset(per), data = epilepsy, family = "poisson",
```

```
R> layout(matrix(1:2, nrow = 1))
R> ylim <- range(log(epilepsy$seizure.rate + 1))
R> boxplot(log(seizure.rate + 1) ~ period, data = placebo,
+ main = "Placebo", ylab = "Log number of seizures",
+ xlab = "Period", ylim = ylim)
R> boxplot(log(seizure.rate + 1) ~ period, data = progabide,
+ main = "Progabide", ylab = "Log number of seizures",
+ xlab = "Period", ylim = ylim)
```

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Figure 11.7 Boxplots of log of numbers of seizures in each two-week period post randomisation for placebo and active treatments.

```
+ id = subject, corstr = "exchangeable", scale.fix = FALSE,
+ scale.value = 1)
```

As usual we inspect the fitted models using the summary method, the results are given in Figures 11.8, 11.9, 11.10, and 11.11.

```
R> summary(epilepsy_glm)
Call:
glm(formula = seizure.rate ~ base + age + treatment + offset(per),
   family = "poisson", data = epilepsy)
Deviance Residuals:
              1Q
                  Median
                                 3Q
    Min
                                         Max
-4.4360 -1.4034 -0.5029
                            0.4842 12.3223
Coefficients:
                     Estimate Std. Error z value Pr(>/z/)
                   -0.1306156 0.1356191 -0.963 0.33549
0.0226517 0.0005093 44.476 < 2e-16 ***
(Intercept)
base
                    0.0227401 0.0040240
                                           5.651 1.59e-08 ***
age
treatmentProgabide -0.1527009 0.0478051 -3.194 0.00140 **
____
Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
(Dispersion parameter for poisson family taken to be 1)
    Null deviance: 2521.75 on 235 degrees of freedom
Residual deviance: 958.46 on 232 degrees of freedom
AIC: 1732.5
Number of Fisher Scoring iterations: 5
```

Figure 11.8 R output of the summary method for the epilepsy\_glm model.

ANALYSING LONGITUDINAL DATA II

R> summary(epilepsy\_gee1) GEE: GENERALIZED LINEAR MODELS FOR DEPENDENT DATA gee S-function, version 4.13 modified 98/01/27 (1998) Model: Link: Logarithm Variance to Mean Relation: Poisson Correlation Structure: Independent Call: gee(formula = seizure.rate ~ base + age + treatment + offset(per), id = subject, data = epilepsy, family = "poisson", corstr = "independence", scale.fix = TRUE, scale.value = 1) Summary of Residuals: Min 1Q Median 3Q Max -4.9195387 0.1808059 1.7073405 4.8850644 69.9658560 Coefficients: Estimate Naive S.E. Naive z -0.13061561 0.1356191185 -0.9631062 (Intercept) 0.02265174 0.0005093011 44.4761250 base 0.02274013 0.0040239970 5.6511312 age treatmentProgabide -0.15270095 0.0478051054 -3.1942393 Robust S.E. Robust z (Intercept) 0.365148155 -0.3577058 0.001235664 18.3316325 base 0.011580405 1.9636736 age treatmentProgabide 0.171108915 -0.8924196 Estimated Scale Parameter: 1 Number of Iterations: 1 Working Correlation [,1] [,2] [,3] [,4] [1,] 1 0 0 0 [2,] 0 0 0 1 0 [3,] 0 0 1 0 0 0 1 [4,]

Figure 11.9 R output of the summary method for the epilepsy\_gee1 model.

#### R> summary(epilepsy\_gee2) GEE: GENERALIZED LINEAR MODELS FOR DEPENDENT DATA gee S-function, version 4.13 modified 98/01/27 (1998) Model: Link: Logarithm Variance to Mean Relation: Poisson Correlation Structure: Exchangeable Call: gee(formula = seizure.rate ~ base + age + treatment + offset(per), id = subject, data = epilepsy, family = "poisson", corstr = "exchangeable", scale.fix = TRUE, scale.value = 1) Summary of Residuals: Min 1Q Median ЗQ Max -4.9195387 0.1808059 1.7073405 4.8850644 69.9658560 Coefficients: Estimate Naive S.E. Naive z -0.13061561 0.2004416507 -0.651639 (Intercept) 0.02265174 0.0007527342 30.092612 base 0.02274013 0.0059473665 3.823564 age treatmentProgabide -0.15270095 0.0706547450 -2.161227 Robust S.E. Robust z 0.365148155 -0.3577058 (Intercept) 0.001235664 18.3316325 base 0.011580405 1.9636736 age treatmentProgabide 0.171108915 -0.8924196 Estimated Scale Parameter: 1 Number of Iterations: 1 Working Correlation [,1] [,2] [,3] [,4] [1,] 1.0000000 0.3948033 0.3948033 0.3948033 [2,] 0.3948033 1.0000000 0.3948033 0.3948033 [3,] 0.3948033 0.3948033 1.0000000 0.3948033 [4,] 0.3948033 0.3948033 0.3948033 1.0000000

Figure 11.10 R output of the summary method for the epilepsy\_gee2 model.

ANALYSING LONGITUDINAL DATA II

R> summary(epilepsy\_gee3) GEE: GENERALIZED LINEAR MODELS FOR DEPENDENT DATA gee S-function, version 4.13 modified 98/01/27 (1998) Model: Link: Logarithm Variance to Mean Relation: Poisson Correlation Structure: Exchangeable Call: gee(formula = seizure.rate ~ base + age + treatment + offset(per), id = subject, data = epilepsy, family = "poisson", corstr = "exchangeable", scale.fix = FALSE, scale.value = 1) Summary of Residuals: Min 10 Median 3Q Max -4.9195387 0.1808059 1.7073405 4.8850644 69.9658560 Coefficients: Estimate Naive S.E. Naive z -0.13061561 0.452199543 -0.2888451 (Intercept) 0.02265174 0.001698180 13.3388301 base 0.02274013 0.013417353 1.6948302 age treatmentProgabide -0.15270095 0.159398225 -0.9579840 Robust S.E. Robust z (Intercept) 0.365148155 -0.3577058 base 0.001235664 18.3316325 0.011580405 1.9636736 age treatmentProgabide 0.171108915 -0.8924196 Estimated Scale Parameter: 5.089608 Number of Iterations: 1 Working Correlation [,1] [,2] [,3] [,4] [1,] 1.0000000 0.3948033 0.3948033 0.3948033 [2,] 0.3948033 1.0000000 0.3948033 0.3948033 [3,] 0.3948033 0.3948033 1.0000000 0.3948033 [4,] 0.3948033 0.3948033 0.3948033 1.0000000

Figure 11.11 R output of the summary method for the epilepsy\_gee3 model.

# Bibliography

Carey, V. J., Lumley, T., and Ripley, B. D. (2006), gee: Generalized Estimation Equation Solver, URL http://CRAN.R-project.org, R package version 4.13-11.

# CHAPTER 12

# Meta-Analysis: Nicotine Gum and Smoking Cessation and the Efficacy of BCG Vaccine in the Treatment of Tuberculosis

# 12.1 Introduction

# 12.2 Systematic Reviews and Meta-Analysis

# 12.3 Analysis Using R

The aim in collecting the results from the randomised trials of using nicotine gum to help smokers quit was to estimate the overall *odds ratio*, the odds of quitting smoking for those given the gum, divided by the odds of quitting for those not receiving the gum. The odds ratios and corresponding confidence intervals are computed by means of the meta.MH function for fixed effects meta-analysis as shown here

```
R> library("rmeta")
R> data("smoking", package = "HSAUR")
R> smokingOR <- meta.MH(smoking[["tt"]], smoking[["tc"]],
+ smoking[["qt"]], smoking[["qc"]], names = rownames(smoking))</pre>
```

and the results can be inspected via a summary method – see Figure 12.1. We shall use both the fixed effects and random effects approaches here so

that we can compare results. For the fixed effects model (see Figure 12.1) the estimated overall log-odds ratio is 0.513 with a standard error of 0.066. This leads to an estimate of the overall odds ratio of 1.67, with a 95% confidence interval as given above. For the random effects model

```
R> smokingDSL <- meta.DSL(smoking[["tt"]], smoking[["tc"]],
+ smoking[["qt"]], smoking[["qc"]], names = rownames(smoking))
R> print(smokingDSL)
```

```
Random effects ( DerSimonian-Laird ) meta-analysis
Call: meta.DSL(ntrt = smoking[["tt"]], nctrl = smoking[["tc"]], ptrt = smoking[["qt"
        pctrl = smoking[["qc"]], names = rownames(smoking))
Summary OR= 1.75 95% CI ( 1.48, 2.07 )
Estimated random effects variance: 0.05
```

the corresponding estimate is 1.751. Both models suggest that there is clear evidence that nicotine gum increases the odds of quitting. The random effects confidence interval is considerably wider than that from the fixed effects model;

# R> summary(smokingOR)

|                   | OR   | (lower | 95% upper) |
|-------------------|------|--------|------------|
| Blondal89         |      |        |            |
| Campbell91        | 0.98 | 0.50   | 1.92       |
| Fagerstrom82      | 1.76 | 0.80   | 3.89       |
| Fee82             | 1.53 | 0.77   | 3.05       |
| Garcia89          |      |        |            |
| <i>Garvey00</i>   |      |        |            |
| Gross95           | 2.62 | 1.03   | 6.71       |
| Hall85            | 2.03 | 0.78   | 5.29       |
| Hall87            |      |        |            |
| Hall96            | 0.87 | 0.46   | 1.64       |
| Hjalmarson84      |      |        | 4.28       |
| Huber88           | 6.00 |        |            |
| Jarvis82          | 3.33 | 1.37   | 8.08       |
| Jensen91          |      |        |            |
| Killen84          | 1.33 | 0.43   | 4.15       |
| Killen90          | 1.23 | 0.93   | 1.64       |
| <i>Malcolm80</i>  |      |        |            |
| <i>McGovern92</i> | 1.17 | 0.70   | 1.94       |
| Nakamura90        | 3.82 | 1.15   | 12.71      |
| Niaura94          |      |        |            |
| Pirie92           |      |        |            |
| Puska79           | 1.46 | 0.78   | 2.75       |
| Schneider85       |      |        |            |
| Tonnesen88        |      |        |            |
| Villa99           | 1.76 | 0.55   | 5.64       |
| Zelman92          | 1.46 | 0.68   | 3.14       |

Figure 12.1 R output of the summary method for smokingOR.

here the test of homogeneity of the studies is not significant implying that we might use the fixed effects results. But the test is not particularly powerful and it is more sensible to assume a priori that heterogeneity is present and so we use the results from the random effects model.

# ANALYSIS USING R R> plot(smokingOR, ylab = "")



Figure 12.2 Forest plot of observed effect sizes and 95% confidence intervals for the nicotine gum studies.

#### META-ANALYSIS

#### 12.4 Meta-Regression

The examination of heterogeneity of the effect sizes from the studies in a meta-analysis begins with the formal test for its presence, although in most meta-analyses such heterogeneity can almost be assumed to be present. There will be many possible sources of such heterogeneity and estimating how these various factors affect the observed effect sizes in the studies chosen is often of considerable interest and importance, indeed usually more important than the relatively simplistic use of meta-analysis to determine a single summary estimate of overall effect size. We can illustrate the process using the BCG vaccine data. We first find the estimate of the overall effect size from applying the fixed effects and the random effects models described previously:

```
R> data("BCG", package = "HSAUR")
R> BCG_OR <- meta.MH(BCG[["BCGVacc"]], BCG[["NoVacc"]],
+ BCG[["BCGTB"]], BCG[["NoVaccTB"]], names = BCG$Study)
R> BCG_DSL <- meta.DSL(BCG[["BCGVacc"]], BCG[["NoVacc"]],
+ BCG[["BCGTB"]], BCG[["NoVaccTB"]], names = BCG$Study)</pre>
```

The results are inspected using the summary method as shown in Figures 12.3 and 12.4. To assess how the two covariates, latitude and year,

```
R> summary(BCG_OR)
```

```
Fixed effects ( Mantel-Haenszel ) meta-analysis
Call: meta.MH(ntrt = BCG[["BCGVacc"]], nctrl = BCG[["NoVacc"]], ptrt = BCG[["BCGTB"]]
    pctrl = BCG[["NoVaccTB"]], names = BCG$Study)
     OR (lower 95% upper)
1
   0.39
           0.12
                       1.26
2
   0.19
           0.08
                       0.46
   0.25
3
           0.07
                       0.91
   0.23
           0.18
                       0.31
4
5
   0.80
           0.51
                       1.26
                       0.47
   0.38
           0.32
6
7
   0.20
           0.08
                       0.50
8
   1.01
           0.89
                       1.15
9
  0.62
           0.39
                       1.00
10 0.25
           0.14
                       0.42
11 0.71
           0.57
                       0.89
12 1.56
           0.37
                       6.55
13 0.98
           0.58
                       1.66
Mantel-Haenszel OR =0.62 95% CI ( 0.57,0.68 )
Test for heterogeneity: X^2(12) = 163.94 (p-value 0)
```



relate to the observed effect sizes we shall use multiple linear regression but

 $\mathbf{6}$ 

#### PUBLICATION BIAS

# R> summary(BCG\_DSL)

Random effects ( DerSimonian-Laird ) meta-analysis Call: meta.DSL(ntrt = BCG[["BCGVacc"]], nctrl = BCG[["NoVacc"]], ptrt = BCG[["BCGTB" pctrl = BCG[["NoVaccTB"]], names = BCG\$Study) \_\_\_\_\_ OR (lower 95% upper) 0.12 1 0.39 1.26 0.19 2 0.08 0.46 0.25 0.07 0.91 3 4 0.23 0.18 0.31 5 0.80 0.51 1.26 6 0.38 0.32 0.47 0.08 7 0.20 0.50 8 1.01 0.89 1.15 9 0.62 0.39 1.00 10 0.25 0.14 0.42 11 0.71 0.57 0.89 12 1.56 0.37 6.55 13 0.98 1.66 0.58 SummaryOR= 0.47 95% CI ( 0.32,0.69 ) Test for heterogeneity:  $X^2(12) = 163.16$  (p-value 0)

Estimated random effects variance: 0.37

Figure 12.4 R output of the summary method for BCG\_DSL.

will weight each observation by  $W_i = (\hat{\sigma}^2 + V_i^2)^{-1}, i = 1, ..., 13$ , where  $\hat{\sigma}^2$  is the estimated between-study variance and  $V_i^2$  is the estimated variance from the *i*th study. The required R code to fit the linear model via weighted least squares is:

```
R> studyweights <- 1/(BCG_DSL$tau2 + BCG_DSL$selogs)
R> y <- BCG_DSL$logs
R> BCG_mod <- lm(y ~ Latitude + Year, data = BCG, weights = studyweights)
and the results of the summary method are shown in Figure 12.5. There is
some evidence that latitude is associated with observed effect size, the log-
odds ratio becoming increasingly negative as latitude increases, as we can see
from a scatterplot of the two variables with the added weighted regression fit
seen in Figure 12.6.</pre>
```

# 12.5 Publication Bias

We can construct a funnel plot for the nicotine gum data using the R code depicted with Figure 12.8. There does not appear to be any strong evidence of publication bias here.

#### R> summary(BCG\_mod) Call: $lm(formula = y \sim Latitude + Year, data = BCG, weights = studyweights)$ Residuals: 1Q Median Min ЗQ Max -1.40868 -0.33622 -0.04847 0.25412 1.13362 Coefficients: Estimate Std. Error t value Pr(>/t/) (Intercept) -14.521025 37.178382 -0.391 0.7043 0.0794 . Latitude -0.026463 0.013553 -1.953 0.397 Year 0.007442 0.018755 0.6998 \_\_\_ Signif. codes: 0 '\*\*\*' 0.001 '\*\*' 0.01 '\*' 0.05 '.' 0.1 ' ' 1 Residual standard error: 0.6862 on 10 degrees of freedom Multiple R-Squared: 0.45, Adjusted R-squared: 0.34 F-statistic: 4.091 on 2 and 10 DF, p-value: 0.05033

Figure 12.5 R output of the summary method for BCG\_mod.

PUBLICATION BIAS
R> plot(y ~ Latitude, data = BCG, ylab = "Estimated log-OR")
R> abline(lm(y ~ Latitude, data = BCG, weights = studyweights))



Figure 12.6 Plot of observed effect size for the BCG vaccine data against latitude, with a weighted least squares regression fit shown in addition.



Figure 12.7 Example funnel plots from simulated data. The asymmetry in the lower plot is a hint that a publication bias might be a problem.

# PUBLICATION BIAS

```
R> funnelplot(smokingDSL$logs, smokingDSL$selogs, summ = smokingDSL$logDSL,
+ xlim = c(-1.7, 1.7))
R> abline(v = 0, lty = 2)
```



Figure 12.8 Funnel plot for nicotine gum data.

# CHAPTER 13

# Principal Component Analysis: The Olympic Heptathlon

# 13.1 Introduction

# 13.2 Principal Component Analysis

# 13.3 Analysis Using ${\sf R}$

To begin it will help to score all the seven events in the same direction, so that 'large' values are 'good'. We will recode the running events to achieve this;

```
R> data("heptathlon", package = "HSAUR")
R> heptathlon$hurdles <- max(heptathlon$hurdles) -
+ heptathlon$hurdles
R> heptathlon$run200m <- max(heptathlon$run200m) -
+ heptathlon$run200m
R> heptathlon$run800m <- max(heptathlon$run800m) -
+ heptathlon$run800m</pre>
```

Figure 13.1 shows a scatterplot matrix of the results from the 25 competitors on the seven events. We see that most pairs of events are positively correlated to a greater or lesser degree. The exceptions all involve the javelin event – this is the only really 'technical' event and it is clear that training to become successful in the other six 'power'-based events makes this event difficult for the majority of the competitors. We can examine the numerical values of the correlations by applying the **cor** function

# R> round(cor(heptathlon[, -score]), 2)

|          | hurdles | highjump | shot | run200m | longjump | javelin | run800m |
|----------|---------|----------|------|---------|----------|---------|---------|
| hurdles  | 1.00    | 0.81     | 0.65 | 0.77    | 0.91     | 0.01    | 0.78    |
| highjump | 0.81    | 1.00     | 0.44 | 0.49    | 0.78     | 0.00    | 0.59    |
| shot     | 0.65    | 0.44     | 1.00 | 0.68    | 0.74     | 0.27    | 0.42    |
| run200m  | 0.77    | 0.49     | 0.68 | 1.00    | 0.82     | 0.33    | 0.62    |
| longjump | 0.91    | 0.78     | 0.74 | 0.82    | 1.00     | 0.07    | 0.70    |
| javelin  | 0.01    | 0.00     | 0.27 | 0.33    | 0.07     | 1.00    | -0.02   |
| run800m  | 0.78    | 0.59     | 0.42 | 0.62    | 0.70     | -0.02   | 1.00    |

This correlation matrix demonstrates again the points made earlier. A principal component analysis of the data can be applied using the prcomp function. The result is a list containing the coefficients defining each component (sometimes referred to as *loadings*), the principal component scores, etc. The required code is (omitting the score variable)

# PRINCIPAL COMPONENT ANALYSIS

R> score <- which(colnames(heptathlon) == "score")
R> plot(heptathlon[, -score])



Figure 13.1 Scatterplot matrix for the heptathlon data.

R> heptathlon\_pca <- prcomp(heptathlon[, -score], scale = TRUE)
R> print(heptathlon\_pca)

```
Standard deviations:
[1] 2.1119364 1.0928497 0.7218131 0.6761411 0.4952441 0.2701029
[7] 0.2213617
```

Rotation:

|          | PC1        | PC2         | PC3         | PC4         |
|----------|------------|-------------|-------------|-------------|
| hurdles  | -0.4528710 | 0.15792058  | -0.04514996 | 0.02653873  |
| highjump | -0.3771992 | 0.24807386  | -0.36777902 | 0.67999172  |
| shot     | -0.3630725 | -0.28940743 | 0.67618919  | 0.12431725  |
| run200m  | -0.4078950 | -0.26038545 | 0.08359211  | -0.36106580 |
| longjump | -0.4562318 | 0.05587394  | 0.13931653  | 0.11129249  |

```
javelin -0.0754090 -0.84169212 -0.47156016 0.12079924

run800m -0.3749594 0.22448984 -0.39585671 -0.60341130

PC5 PC6 PC7

hurdles -0.09494792 -0.78334101 0.38024707

highjump 0.01879888 0.09939981 -0.43393114

shot 0.51165201 -0.05085983 -0.21762491

run200m -0.64983404 0.02495639 -0.45338483

longjump -0.18429810 0.59020972 0.61206388

javelin 0.13510669 -0.02724076 0.17294667

run800m 0.50432116 0.15555520 -0.09830963
```

The summary method can be used for further inspection of the details:

#### R> summary(heptathlon\_pca)

```
      Importance of components:
      PC1
      PC2
      PC3
      PC4
      PC5
      PC6

      Standard deviation
      2.112
      1.093
      0.7218
      0.6761
      0.4952
      0.2701

      Proportion of Variance
      0.637
      0.171
      0.0744
      0.0653
      0.0350
      0.0104

      Cumulative Proportion
      0.637
      0.808
      0.8822
      0.9475
      0.9826
      0.9930

      PC7
      Standard deviation
      0.221
      Proportion of Variance
      0.007
      Cumulative Proportion
      1.000
```

The linear combination for the first principal component is

```
R> a1 <- heptathlon_pca$rotation[, 1]
R> a1
```

```
hurdles highjump shot run200m longjump
-0.4528710 -0.3771992 -0.3630725 -0.4078950 -0.4562318
javelin run800m
-0.0754090 -0.3749594
```

We see that the 200m and long jump competitions receive the highest weight but the javelin result is less important. For computing the first principal component, the data need to be rescaled appropriately. The center and the scaling used by prcomp internally can be extracted from the heptathlon\_pca via

```
R> center <- heptathlon_pca$center
R> scale <- heptathlon_pca$scale</pre>
```

Now, we can apply the scale function to the data and multiply with the loadings matrix in order to compute the first principal component score for each competitor

```
R> hm <- as.matrix(heptathlon[, -score])
R> drop(scale(hm, center = center, scale = scale) %*%
+ heptathlon_pca$rotation[, 1])
```

| Joyner-Kersee (USA) | John (GDR)        | Behmer (GDR) |
|---------------------|-------------------|--------------|
| -4.121447626        | -2.882185935      | -2.649633766 |
| Sablovskaite (URS)  | Choubenkova (URS) | Schulz (GDR) |
| -1.343351210        | -1.359025696      | -1.043847471 |

# PRINCIPAL COMPONENT ANALYSIS

| Fleming (AUS)  | Greiner (USA)    | Lajbnerova (CZE)   |
|----------------|------------------|--------------------|
| -1.100385639   | -0.923173639     | -0.530250689       |
| Bouraga (URS)  | Wijnsma (HOL)    | Dimitrova (BUL)    |
| -0.759819024   | -0.556268302     | -1.186453832       |
| Scheider (SWI) | Braun (FRG)      | Ruotsalainen (FIN) |
| 0.015461226    | 0.003774223      | 0.090747709        |
| Yuping (CHN)   | Hagger (GB)      | Brown (USA)        |
| -0.137225440   | 0.171128651      | 0.519252646        |
| Mulliner (GB)  | Hautenauve (BEL) | Kytola (FIN)       |
| 1.125481833    | 1.085697646      | 1.447055499        |
| Geremias (BRA) | Hui-Ing (TAI)    | Jeong-Mi (KOR)     |
| 2.014029620    | 2.880298635      | 2.970118607        |
| Launa (PNG)    |                  |                    |
| 6.270021972    |                  |                    |

or, more conveniently, by extracting the first from all precomputed principal components

# R> predict(heptathlon\_pca)[, 1]

| Joyner-Kersee (USA) | John (GDR)        | Behmer (GDR)       |
|---------------------|-------------------|--------------------|
| -                   |                   | · · · · ·          |
| -4.121447626        | -2.882185935      | -2.649633766       |
| Sablovskaite (URS)  | Choubenkova (URS) | Schulz (GDR)       |
| -1.343351210        | -1.359025696      | -1.043847471       |
| Fleming (AUS)       | Greiner (USA)     | Lajbnerova (CZE)   |
| -1.100385639        | -0.923173639      | -0.530250689       |
| Bouraga (URS)       | Wijnsma (HOL)     | Dimitrova (BUL)    |
| -0.759819024        | -0.556268302      | -1.186453832       |
| Scheider (SWI)      | Braun (FRG)       | Ruotsalainen (FIN) |
| 0.015461226         | 0.003774223       | 0.090747709        |
| Yuping (CHN)        | Hagger (GB)       | Brown (USA)        |
| -0.137225440        | 0.171128651       | 0.519252646        |
| Mulliner (GB)       | Hautenauve (BEL)  | Kytola (FIN)       |
| 1.125481833         | 1.085697646       | 1.447055499        |
| Geremias (BRA)      | Hui-Ing (TAI)     | Jeong-Mi (KOR)     |
| 2.014029620         | 2.880298635       | 2.970118607        |
| Launa (PNG)         |                   |                    |
| 6.270021972         |                   |                    |

The first two components account for 81% of the variance. A barplot of each component's variance (see Figure 13.2) shows how the first two components dominate. A plot of the data in the space of the first two principal components, with the points labelled by the name of the corresponding competitor can be produced as shown with Figure 13.3. In addition, the first two loadings for the events are given in a second coordinate system, also illustrating the special role of the javelin event. This graphical representation is known as *biplot* (?). The correlation between the score given to each athlete by the standard scoring system used for the heptathlon and the first principal component score can be found from

R> cor(heptathlon\$score, heptathlon\_pca\$x[, 1])

ANALYSIS USING R R> plot(heptathlon\_pca)



heptathlon\_pca

Figure 13.2 Barplot of the variances explained by the principal components.

# [1] -0.9910978

This implies that the first principal component is in good agreement with the score assigned to the athletes by official Olympic rules; a scatterplot of the official score and the first principal component is given in Figure 13.4.
PRINCIPAL COMPONENT ANALYSIS

-5 0 5 Hgg<sup>Htnv</sup> 4 Wjns 0.2 Kytl Jn–M  $\sim$ Grnr BoYgong Mlln H-In **Dimtn** longjum Grms 0.0 Schl 0 Ljbn PC2 run2 Bhmr Sblv 2 -0.2 Jy–K Chbn 4 -0.4 ဖျ Laun -0.4 -0.2 0.0 0.2 0.4 0.6 PC1

R> biplot(heptathlon\_pca, col = c("gray", "black"))

Figure 13.3 Biplot of the (scaled) first two principal components.

ANALYSIS USING R R> plot(heptathlon\$score, heptathlon\_pca\$x[, 1])



Figure 13.4 Scatterplot of the score assigned to each athlete in 1988 and the first principal component.

#### CHAPTER 14

## Multidimensional Scaling: British Water Voles and Voting in US Congress

#### 14.1 Introduction

14.2 Multidimensional Scaling

#### 14.3 Analysis Using R

We can apply classical scaling to the distance matrix for populations of water voles using the R function cmdscale. The following code finds the classical scaling solution and computes the two criteria for assessing the required number of dimensions as described above.

```
R> data("watervoles", package = "HSAUR")
R> voles_mds <- cmdscale(watervoles, k = 13, eig = TRUE)
R> voles_mds$eig
[1] 7.359910e-01 2.626003e-01 1.492622e-01 6.990457e-02
[5] 2.956972e-02 1.931184e-02 2.775558e-17 -1.139451e-02
[9] -1.279569e-02 -2.849924e-02 -4.251502e-02 -5.255450e-02
[13] -7.406143e-02
```

Note that some of the eigenvalues are negative. The criterion  $P_2$  can be computed by

R> sum(abs(voles\_mds\$eig[1:2]))/sum(abs(voles\_mds\$eig))

[1] 0.6708889

and the criterion suggested by Mardia et al. (1979) is

R> sum((voles\_mds\$eig[1:2])^2)/sum((voles\_mds\$eig)^2)

[1] 0.9391378

The two criteria for judging number of dimensions differ considerably, but both values are reasonably large, suggesting that the original distances between the water vole populations can be represented adequately in two dimensions. The two-dimensional solution can be plotted by extracting the coordinates from the points element of the voles\_mds object; the plot is shown in Figure 14.1.

We shall now apply non-metric scaling to the voting behaviour shown in Table ??. Non-metric scaling is available with function isoMDS from package MASS (Venables and Ripley, 2002):

```
4 MULTIDIMENSIONAL SCALING
R> x <- voles_mds$points[, 1]
R> y <- voles_mds$points[, 2]
R> plot(x, y, xlab = "Coordinate 1", ylab = "Coordinate 2",
+ xlim = range(x) * 1.2, type = "n")
R> text(x, y, labels = colnames(watervoles))
```



Figure 14.1 Two-dimensional solution from classical multidimensional scaling of distance matrix for water vole populations.

## R> library("MASS") R> data("voting", package = "HSAUR") R> voting\_mds <- isoMDS(voting)</pre>

and we again depict the two-dimensional solution (Figure 14.3). The Figure suggests that voting behaviour is essentially along party lines, although there is more variation among Republicans. The voting behaviour of one of the Republicans (Rinaldo) seems to be closer to his democratic collegues rather than to the voting behaviour of other Republicans.



Figure 14.2 Minimum spanning tree for the watervoles data.



Figure 14.3 Two-dimensional solution from non-metric multidimensional scaling of distance matrix for voting matrix.

# ANALYSIS USING R R> library("MASS") R> voting\_sh <- Shepard(voting[lower.tri(voting)], + voting\_mds\$points) R> plot(voting\_sh, pch = ".", xlab = "Dissimilarity", + ylab = "Distance", xlim = range(voting\_sh\$x), + ylim = range(voting\_sh\$x))

```
R> lines(voting_sh$x, voting_sh$yf, type = "S")
```



Figure 14.4 The Shepard diagram for the voting data shows some discrepancies between the original dissimilarities and the multidimensional scaling solution.

 $\overline{7}$ 

\_\_\_\_| |\_\_\_\_

## Bibliography

- Mardia, K. V., Kent, J. T., and Bibby, J. M. (1979), *Multivariate Analysis*, London, UK: Academic Press.
- Venables, W. N. and Ripley, B. D. (2002), *Modern Applied Statistics with* S, Springer, 4th edition, URL http://www.stats.ox.ac.uk/pub/MASS4/, ISBN 0-387-95457-0.

#### CHAPTER 15

## Cluster Analysis: Classifying the Exoplanets

#### 15.1 Introduction

#### 15.2 Cluster Analysis

#### 15.3 Analysis Using R

Sadly Figure 15.2 gives no completely convincing verdict on the number of groups we should consider, but using a little imagination 'little elbows' can be spotted at the three and five group solutions. We can find the number of planets in each group using

```
R> planet_kmeans3 <- kmeans(planet.dat, centers = 3)
R> table(planet_kmeans3$cluster)
```

1 2 3 28 10 63

The centers of the clusters for the untransformed data can be computed using a small convenience function

```
R> ccent <- function(cl) {
    f <- function(i) colMeans(planets[cl == i, ])
    x <- sapply(sort(unique(cl)), f)
    colnames(x) <- sort(unique(cl))
    return(x)
    + }</pre>
```

which, applied to the three cluster solution obtained by k-means gets
R> ccent(planet\_kmeans3\$cluster)

1 2 3 mass 7.0532143 3.4360 1.6540635 period 839.1644356 2420.5500 311.3897179 eccen 0.5184643 0.2718 0.1777984

for the three cluster solution and, for the five cluster solution using

```
R> planet_kmeans5 <- kmeans(planet.dat, centers = 5)
R> table(planet_kmeans5$cluster)
1 2 3 4 5
```

28 5 7 49 12

R> ccent(planet\_kmeans5\$cluster)

```
CLUSTER ANALYSIS
R> data("planets", package = "HSAUR")
R> library("scatterplot3d")
R> scatterplot3d(log(planets$mass), log(planets$period),
      log(planets$eccen), type = "h", angle = 55,
+
+
      scale.y = 0.7, pch = 16, y.ticklabs = seq(0,
          10, by = 2), y.margin.add = 0.1)
+
```



Figure 15.1 3D scatterplot of the logarithms of the three variables available for each of the exoplanets.

|        | 1           | 2        | 3           | 4           | 5        |
|--------|-------------|----------|-------------|-------------|----------|
| mass   | 2.2617857   | 14.3480  | 2.185714    | 1.6846122   | 8.595    |
| period | 580.6828929 | 659.3976 | 2557.642857 | 282.2685965 | 1335.740 |
| eccen  | 0.4910714   | 0.3268   | 0.199000    | 0.1221082   | 0.473    |

#### ANALYSIS USING R

```
R> rge <- apply(planets, 2, max) - apply(planets, 2,
+ min)
R> planet.dat <- sweep(planets, 2, rge, FUN = "/")
R> n <- nrow(planet.dat)
R> wss <- rep(0, 10)
R> wss[1] <- (n - 1) * sum(apply(planet.dat, 2, var))
R> for (i in 2:10) wss[i] <- sum(kmeans(planet.dat,
+ centers = i)$withinss)
R> plot(1:10, wss, type = "b", xlab = "Number of groups",
+ ylab = "Within groups sum of squares")
```



Figure 15.2 Within-cluster sum of squares for different numbers of clusters for the exoplanet data.

R> plot(planet\_mclust, planet.dat, what = "BIC", col = "black", + ylab = "-BIC")



Figure 15.3 Plot of BIC values for a variety of models and a range of number of clusters.

#### 15.3.1 Model-based Clustering in R

We now proceed to apply model-based clustering to the planets data. R functions for model-based clustering are available in package *mclust* (Fraley et al., 2006, Fraley and Raftery, 2002). Here we use the Mclust function since this selects both the most appropriate model for the data *and* the optimal number of groups based on the values of the BIC computed over several models and a range of values for number of groups. The necessary code is:

R> library("mclust")
R> planet\_mclust <- Mclust(planet.dat)</pre>

and we first examine a plot of BIC values using The resulting diagram is

#### ANALYSIS USING R

shown in Figure 15.3. In this diagram the numbers refer to different model assumptions about the shape of clusters:

- 1. Spherical, equal volume,
- 2. Spherical, unequal volume,
- 3. Diagonal equal volume, equal shape,
- 4. Diagonal varying volume, varying shape,
- 5. Ellipsoidal, equal volume, shape and orientation,
- 6. Ellipsoidal, varying volume, shape and orientation.

The BIC selects model 4 (diagonal varying volume and varying shape) with three clusters as the best solution as can be seen from the **print** output:

#### R> print(planet\_mclust)

best model: VVI with 3 components

This solution can be shown graphically as a scatterplot matrix The plot is shown in Figure 15.4. Figure 15.5 depicts the clustering solution in the threedimensional space. The number of planets in each cluster and the mean vectors of the three clusters for the untransformed data can now be inspected by using

```
R> table(planet_mclust$classification)
```

1 2 3 19 41 41

R> ccent(planet\_mclust\$classification)

1 2 3 mass 1.16652632 1.5797561 6.0761463 period 6.47180158 313.4127073 1325.5310048 eccen 0.03652632 0.3061463 0.3704951

Cluster 1 consists of planets about the same size as Jupiter with very short periods and eccentricities (similar to the first cluster of the k-means solution). Cluster 2 consists of slightly larger planets with moderate periods and large eccentricities, and cluster 3 contains the very large planets with very large periods. These two clusters do not match those found by the k-means approach.

R> x <- clPairs(planet.dat, classification = planet\_mclust\$classification, + symbols = 1:3, col = "black")



#### ANALYSIS USING R

R> scatterplot3d(log(planets\$mass), log(planets\$period),

- + log(planets\$eccen), type = "h", angle = 55,
- + scale.y = 0.7, pch = planet\_mclust\$classification,
- + y.ticklabs = seq(0, 10, by = 2), y.margin.add = 0.1)



Figure 15.5 3D scatterplot of planets data showing a three cluster solution from Mclust.

\_\_\_\_| |\_\_\_\_

## Bibliography

- Fraley, C. and Raftery, A. E. (2002), "Model-based clustering, discriminant analysis, and density estimation," *Journal of the American Statistical Association*, 97, 611–631.
- Fraley, C., Raftery, A. E., and Wehrens, R. (2006), *mclust: Model-based Cluster Analysis*, URL http://www.stat.washington.edu/mclust, R package version 3.0-0.

#### CHAPTER 16

### Errata

The document gives a list of typos, errors, inconsistencies etc. which have been spotted. Moreover, small numeric output differences which are due to updated packages are reported here. To get a full list of differences run R CMD check HSAUR on the source package.

#### Preface

Typo in name of vignette for Chapter 1, should read

```
R> vignette("Ch_introduction_to_R", package = "HSAUR")
and
```

```
R> edit(vignette("Ch_introduction_to_R", package = "HSAUR"))
As of version 1.0-3, only the correctly named vignette is available.
```

#### 16.1 Introduction to R

Typo at page 20 (Ex. 1.5): number of companies, not number of countries.

#### 16.2 Simple Inference

Typo at page 31, code line 4: use argument varwidth = TRUE, not var.width = TRUE.

#### 16.3 Conditional Inference

- The names of the test statistics in the output have been changed from T to Z or chi-squared throughout the chapter.
- Reference Hothorn et al. (2006a) updated

#### 16.4 Analysis of Variance

-nothing known-

#### 16.5 Multiple Linear Regression

Page 83: both fitted and predict can be used to compute fitted values, the later on can be applied to new unseen data as well.

#### ERRATA

#### 16.6 Logistic Regression and Generalised Linear Models

Function myplot (page 100): the vfont argument in text has been changed to family = "HersheySerif" (the resulting plots remain the same).

#### 16.7 Density Estimation

- Page 121: small numeric differences for the output of optim
- update to *mclust* version 3.0-0 (new names of parameters in mclust objects)

#### 16.8 Recursive Partitioning

- Page 139: small differences in predtab
- Page 140: small differences in table at bottom of this page
- Reference Hothorn et al. (2006b) updated

#### 16.9 Survival Analysis

The name of the test statistic in the output of surv\_test has been changed to chi-squared.

#### 16.10 Analysing Longitudinal Data I

Page 168, Figure 10.2: summary does not provide degrees of freedom and p-values in newer versions of *lme4*.

#### 16.11 Analysing Longitudinal Data II

-nothing known-

#### 16.12 Meta-Analysis

-nothing known-

#### 16.13 Principal Component Analysis

-nothing known-

#### 16.14 Multidimensional Scaling

-nothing known-

#### 16.15 Cluster Analysis

update to *mclust* version 3.0-0 (new plot method)

#### CLUSTER ANALYSIS

#### Thanks

We would like to thank the following people for pointing out errors, typos etc and for making suggestions for improvements:

- Tobias Verbeke
- Brian D. Ripley

\_\_\_\_| |\_\_\_\_

## Bibliography

- Hothorn, T., Hornik, K., van de Wiel, M. A., and Zeileis, A. (2006a), "A Lego system for conditional inference," *The American Statistician*, 60, 257-263, URL http://statmath.wu-wien.ac.at/~zeileis/papers/ Hothorn+Hornik+VanDeWiel-2006.pdf.
- Hothorn, T., Hornik, K., and Zeileis, A. (2006b), "Unbiased recursive partitioning: A conditional inference framework," *Journal of Computational and Graphical Statistics*, 15, 651–674, URL http://statmath.wu-wien.ac.at/ ~zeileis/papers/Hothorn+Hornik+Zeileis-2006.pdf.

## **The HSAUR Package**

November 2, 2006

Title A Handbook of Statistical Analyses Using R

Date \$Date: 2006/10/21 16:18:55 \$

Version 1.0-6

Author Brian S. Everitt and Torsten Hothorn

Maintainer Torsten Hothorn <Torsten.Hothorn@R-project.org>

- **Description** Functions, data sets, analyses and examples from the book 'A Handbook of Statistical Analyses Using R' (Brian S. Everitt and Torsten Hothorn, Chapman & Hall/CRC, 2006). The first chapter of the book, which is entitled 'An Introduction to R', is completely included in this package, for all other chapters, a vignette containing all data analyses is available.
- URL The publishers web page is http://www.crcpress.com/shopping\_cart/products/product\_detail.asp?sku=C5394

**Depends** R ( $\geq$  2.2.0), lattice, MASS, scatterplot3d ( $\geq$  0.3-23)

**Suggests** ape (>= 1.6), coin (>= 0.3-3), flexmix (>= 1.1-0), gee (>= 4.13-10), ipred (>= 0.8-3), lme4 (>= 0.98-1), mclust (>= 3.0-0), party (>= 0.2-8), randomForest (>= 4.5-12), rmeta (>= 2.12), vcd (>= 0.9-3), survival

LazyData yes

License GPL

#### **R** topics documented:

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BCG

BCG Vaccine Data

#### Description

A meta-analysis on the efficacy of BCG vaccination against tuberculosis (TB).

#### Usage

data("BCG")

#### **BtheB**

#### Format

A data frame with 13 observations on the following 7 variables.

**Study** an identifier of the study.

**BCGTB** the number of subjects suffering from TB after a BCG vaccination.

**BCGVacc** the number of subjects with BCG vaccination.

**NoVaccTB** the number of subjects suffering from TB without BCG vaccination.

**NoVacc** the total number of subjects without BCG vaccination.

Latitude geographic position of the place the study was undertaken.

Year the year the study was undertaken.

#### Details

Bacille Calmette Guerin (BCG) is the most widely used vaccination in the world. Developed in the 1930s and made of a live, weakened strain of Mycobacterium bovis, the BCG is the only vaccination available against tuberculosis today. Colditz et al. (1994) report data from 13 clinical trials of BCG vaccine each investigating its efficacy in the treatment of tuberculosis. The number of subjects suffering from TB with or without BCG vaccination are given here. In addition, the data contains the values of two other variables for each study, namely, the geographic latitude of the place where the study was undertaken and the year of publication. These two variables will be used to investigate and perhaps explain any heterogeneity among the studies.

#### Source

G. A. Colditz, T. F. Brewer, C. S. Berkey, M. E. Wilson, E. Burdick, H. V. Fineberg and F. Mosteller (1994), Efficacy of BCG vaccine in the prevention of tuberculosis. Meta-analysis of the published literature. *Journal of the American Medical Association*, **271**(2), 698–702.

#### Examples

BtheB

Beat the Blues Data

#### Description

Data from a clinical trial of an interactive multimedia program called 'Beat the Blues'.

#### Usage

data("BtheB")

#### Format

A data frame with 100 observations of 100 patients on the following 8 variables.

**drug** did the patient take anti-depressant drugs (No or Yes).

- **length** the length of the current episode of depression, a factor with levels <6m (less than six months) and >6m (more than six months).
- treatment treatment group, a factor with levels TAU (treatment as usual) and BtheB (Beat the Blues)

bdi.pre Beck Depression Inventory II before treatment.

bdi.2m Beck Depression Inventory II after two months.

bdi.4m Beck Depression Inventory II after four months.

bdi.6m Beck Depression Inventory II after six months.

bdi.8m Beck Depression Inventory II after eight months.

#### Details

Longitudinal data from a clinical trial of an interactive, multimedia program known as "Beat the Blues" designed to deliver cognitive behavioural therapy to depressed patients via a computer terminal. Patients with depression recruited in primary care were randomised to either the Beating the Blues program, or to "Treatment as Usual (TAU)".

Note that the data are stored in the wide form, i.e., repeated measurments are represented by additional columns in the data frame.

#### Source

J. Proudfoot, D. Goldberg and A. Mann (2003). Computerised, interactive, multimedia CBT reduced anxiety and depression in general practice: A RCT. *Psychological Medicine*, **33**, 217–227.

#### Examples

CYGOB1

#### Description

Energy output and surface termperature for Star Cluster CYG OB1.

#### Usage

```
data("CYGOB1")
```

#### Format

A data frame with 47 observations on the following 2 variables.

**logst** log survface termperature of the star.

logli log light intensity of the star.

#### Details

The Hertzsprung-Russell (H-R) diagram forms the basis of the theory of stellar evolution. The diagram is essentially a plot of the energy output of stars plotted against their surface temperature. Data from the H-R diagram of Star Cluster CYG OB1, calibrated according to VanismaGreve1972 are given here.

#### Source

F. Vanisma and J. P. De Greve (1972), Close binary systems before and after mass transfer. *Astro-physics and Space Science*, **87**, 377–401.

D. J. Hand, F. Daly, A. D. Lunn, K. J. McConway and E. Ostrowski (1994). *A Handbook of Small Datasets*, Chapman and Hall/CRC, London.

#### Examples

```
data("CYGOB1", package = "HSAUR")
plot(logst ~ logli, data = CYGOB1)
```

Forbes2000

#### Description

The Forbes 2000 list is a ranking of the world's biggest companies, measured by sales, profits, assets and market value.

#### Usage

data("Forbes2000")

#### Format

A data frame with 2000 observations on the following 8 variables.

rank the ranking of the company.

name the name of the company.

country a factor giving the country the company is situated in.

category a factor describing the products the company produces.

sales the amount of sales of the company in billion USD.

profits the profit of the company in billion USD.

assets the assets of the company in billion USD.

marketvalue the market value of the company in billion USD.

#### Source

http://www.forbes.com, assessed on November 26th, 2004.

#### Examples

```
data("Forbes2000", package = "HSAUR")
summary(Forbes2000)
### number of countries
length(levels(Forbes2000$country))
### number of industries
length(levels(Forbes2000$category))
```

HSAURtable

#### Produce LaTeX Tables

#### Description

Generate longtable LaTeX environments.

#### Usage

#### Arguments

| object     | an object of table or data.frame.   |
|------------|---|
| xname      | the name of the object.   |
| pkg        | the package object comes from, optionally.                                    |
| nrows      | the number of rows actually printed for a data.frame.                         |
| caption    | the (optional) caption of the table without label.                            |
| label      | the (optional) label to be defined for this table.                            |
| pcol       | the number of parallel columns.   |
| rownames   | logical, should the rownames be printed in the first row without column name? |
| topcaption | logical, should the captions be placed on top (default) of the table?         |
| index      | logical, should an index entry be generated?                                  |
|            | additional arguments, currently ignored.                                      |

#### Details

Based on the data in object, an object from which a Latex table (in a longtable environment) may be constructed (via toLatex) is generated.

#### Value

An object of class tabtab or dftab for which toLatex methods are available.

toLatex produces objects of class Latex, a character vector, essentially.

#### Examples

Lanza

Prevention of Gastointestinal Damages

#### Description

Data from four randomised clinical trials on the prevention of gastointestinal damages by Misoprostol reported by Lanza et al. (1987, 1988a,b, 1989).

#### Usage

```
data("Lanza")
```

#### Format

A data frame with 198 observations on the following 3 variables.

**study** a factor with levels I, II, III, and IV describing the study number.

treatment a factor with levels Misoprostol Placebo

**classification** an ordered factor with levels 1 < 2 < 3 < 4 < 5 describing an ordered response variable.

#### Details

The response variable is defined by the number of haemorrhages or erosions.

#### Source

F. L. Lanza (1987), A double-blind study of prophylactic effect of misoprostol on lesions of gastric and duodenal mucosa induced by oral administration of tolmetin in healthy subjects. *British Journal of Clinical Practice*, May suppl, 91–101.

F. L. Lanza, R. L. Aspinall, E. A. Swabb, R. E. Davis, M. F. Rack, A. Rubin (1988a), Double-blind, placebo-controlled endoscopic comparison of the mucosal protective effects of misoprostol versus cimetidine on tolmetin-induced mucosal injury to the stomach and duodenum. *Gastroenterology*, **95**(2), 289–294.

#### aspirin

F. L. Lanza, K. Peace, L. Gustitus, M. F. Rack, B. Dickson (1988b), A blinded endoscopic comparative study of misoprostol versus sucralfate and placebo in the prevention of aspirin-induced gastric and duodenal ulceration. *American Journal of Gastroenterology*, **83**(2), 143–146.

F. L. Lanza, D. Fakouhi, A. Rubin, R. E. Davis, M. F. Rack, C. Nissen, S. Geis (1989), A doubleblind placebo-controlled comparison of the efficacy and safety of 50, 100, and 200 micrograms of misoprostol QID in the prevention of ibuprofen-induced gastric and duodenal mucosal lesions and symptoms. *American Journal of Gastroenterology*, **84**(6), 633–636.

#### Examples

```
aspirin
```

Aspirin Data

#### Description

Efficacy of Aspirin in preventing death after a myocardial infarct.

#### Usage

data("aspirin")

#### Format

A data frame with 7 observations on the following 4 variables.

**dp** number of deaths after placebo.

- tp total number subjects treated with placebo.
- da number of deaths after Aspirin.
- ta total number of subjects treated with Aspirin.

#### Details

The data were collected for a meta-analysis of the effectiveness of Aspirin (versus placebo) in preventing death after a myocardial infarction.

#### Source

J. L. Fleiss (1993), The statistical basis of meta-analysis. *Statistical Methods in Medical Research* 2, 121–145.

#### Examples

```
data("aspirin", package = "HSAUR")
aspirin
```

birthdeathrates Birth and Death Rates Data

#### Description

Birth and death rates for 69 countries.

#### Usage

data("birthdeathrates")

#### Format

A data frame with 69 observations on the following 2 variables.

birth birth rate.

death death rate.

#### Source

J. A. Hartigan (1975), Clustering Algorithms. John Wiley & Sons, New York.

#### Examples

```
data("birthdeathrates", package = "HSAUR")
plot(birthdeathrates)
```

bladdercancer Bladder Cancer Data

#### Description

Data arise from 31 male patients who have been treated for superficial bladder cancer, and give the number of recurrent tumours during a particular time after the removal of the primary tumour, along with the size of the original tumour.

#### Usage

```
data("bladdercancer")
```

#### clouds

#### Format

A data frame with 31 observations on the following 3 variables.

time the duration.

tumorsize a factor with levels <=3cm and >3cm.

number number of recurrent tumours.

#### Details

The aim is the estimate the effect of size of tumour on the number of recurrent tumours.

#### Source

G. U. H. Seeber (1998), Poisson Regression. In: *Encyclopedia of Biostatistics* (P. Armitage and T. Colton, eds), John Wiley & Sons, Chichester.

#### Examples

```
data("bladdercancer", package = "HSAUR")
mosaicplot(xtabs(~ number + tumorsize, data = bladdercancer))
```

clouds

Cloud Seeding Data

#### Description

Data from an experiment investigating the use of massive amounts of silver iodide (100 to 1000 grams per cloud) in cloud seeding to increase rainfall.

#### Usage

data("clouds")

#### Format

A data frame with 24 observations on the following 7 variables.

seeding a factor indicating whether seeding action occured (no or yes).

time number of days after the first day of the experiment.

cloudcover the percentage cloud cover in the experimental area, measured using radar.

sne suitability criterion.

**prewetness** the total rainfall in the target area one hour before seeding (in cubic metres times 1e+8).

echomotion a factor showing whether the radar echo was moving or stationary.

rainfall the amount of rain in cubic metres times 1e+8.

#### Details

Weather modification, or cloud seeding, is the treatment of individual clouds or storm systems with various inorganic and organic materials in the hope of achieving an increase in rainfall. Introduction of such material into a cloud that contains supercooled water, that is, liquid water colder than zero Celsius, has the aim of inducing freezing, with the consequent ice particles growing at the expense of liquid droplets and becoming heavy enough to fall as rain from clouds that otherwise would produce none.

The data available in cloud were collected in the summer of 1975 from an experiment to investigate the use of massive amounts of silver iodide 100 to 1000 grams per cloud) in cloud seeding to increase rainfall. In the experiment, which was conducted in an area of Florida, 24 days were judged suitable for seeding on the basis that a measured suitability criterion (SNE).

#### Source

W. L. Woodley, J. Simpson, R. Biondini and J. Berkeley (1977), Rainfall results 1970-75: Florida area cumulus experiment. *Science* **195**, 735–742.

#### Examples

```
data("clouds", package = "HSAUR")
layout(matrix(1:2, nrow = 2))
boxplot(rainfall ~ seeding, data = clouds, ylab = "Rainfall")
boxplot(rainfall ~ echomotion, data = clouds, ylab = "Rainfall")
```

epilepsy Epilepsy Data

#### Description

A randomised clinical trial investigating the effect of an anti-epileptic drug.

#### Usage

```
data("epilepsy")
```

#### Format

A data frame with 236 observations on the following 6 variables.

treatment the treatment group, a factor with levels placebo and Progabide.

**base** the number of seizures before the trial.

**age** the age of the patient.

seizure.rate the number of seizures (response variable).

period treatment period, an ordered factor with levels 1 to 4.

**subject** the patient ID, a factor with levels 1 to 59.

#### foster

#### Details

In this clinical trial, 59 patients suffering from epilepsy were randomized to groups receiving either the anti-epileptic drug Progabide or a placebo in addition to standard chemotherapy. The numbers of seizures suffered in each of four, two-week periods were recorded for each patient along with a baseline seizure count for the 8 weeks prior to being randomized to treatment and age. The main question of interest is whether taking progabide reduced the number of epileptic seizures compared with placebo.

#### Source

P. F. Thall and S. C. Vail (1990), Some covariance models for longitudinal count data with overdispersion. *Biometrics*, **46**, 657–671.

#### Examples

foster

Foster Feeding Experiment

#### Description

The data are from a foster feeding experiment with rat mothers and litters of four different genotypes. The measurement is the litter weight after a trial feeding period.

#### Usage

data("foster")

#### Format

A data frame with 61 observations on the following 3 variables.

litgen genotype of the litter, a factor with levels A, B, I, and J.

motgen genotype of the mother, a factor with levels A, B, I, and J.

weight the weight of the litter after a feeding period.

#### Details

Here the interest lies in uncovering the effect of genotype of mother and litter on litter weight.
# Source

D. J. Hand, F. Daly, A. D. Lunn, K. J. McConway and E. Ostrowski (1994). A Handbook of Small Datasets, Chapman and Hall/CRC, London.

## Examples

```
data("foster", package = "HSAUR")
plot.design(foster)
```

gardenflowers Garden Flowers

# Description

The dissimilarity matrix of 18 species of garden flowers.

#### Usage

```
data("gardenflowers")
```

#### Format

An object of class dist.

# Details

The dissimilarity was computed based on certain characteristics of the flowers.

# Source

L. Kaufman and P. J. Rousseeuw (1990), *Finding groups in data: an introduction to cluster analysis*, John Wiley & Sons, New York.

```
data("gardenflowers", package = "HSAUR")
gardenflowers
```

heptathlon

# Description

Results of the olympic heptathlon competition, Seoul, 1988.

# Usage

```
data("heptathlon")
```

# Format

A data frame with 25 observations on the following 8 variables.

hurdles results 100m hurdles.

highjump results high jump.

**shot** results shot.

run200m results 200m race.

longjump results long jump.

javelin results javelin.

run800m results 800m race.

score total score.

## Details

The first combined Olympic event for women was the pentathlon, first held in Germany in 1928. Initially this consisted of the shot putt, long jump, 100m, high jump and javelin events held over two days. The pentathlon was first introduced into the Olympic Games in 1964, when it consisted of the 80m hurdles, shot, high jump, long jump and 200m. In 1977 the 200m was replaced by the 800m and from 1981 the IAAF brought in the seven-event heptathlon in place of the pentathlon, with day one containing the events-100m hurdles, shot, high jump, 200m and day two, the long jump, javelin and 800m. A scoring system is used to assign points to the results from each event and the winner is the woman who accumulates the most points over the two days. The event made its first Olympic appearance in 1984.

In the 1988 Olympics held in Seoul, the heptathlon was won by one of the stars of women's athletics in the USA, Jackie Joyner-Kersee. The results for all 25 competitors are given here.

# Source

D. J. Hand, F. Daly, A. D. Lunn, K. J. McConway and E. Ostrowski (1994). A Handbook of Small Datasets, Chapman and Hall/CRC, London.

# Examples

```
data("heptathlon", package = "HSAUR")
plot(heptathlon)
```

mastectomy

Survival Times after Mastectomy of Breast Cancer Patients

# Description

Survival times in months after mastectomy of women with breast cancer. The cancers are classified as having metastized or not based on a histochemical marker.

# Usage

```
data("matectomy")
```

## Format

A data frame with 42 observations on the following 3 variables.

time survival times in months.

event a logical indicating if the event was observed (TRUE) or if the survival time was censored (FALSE).

metastized a factor at levels yes and no.

# Source

B. S. Everitt and S. Rabe-Hesketh (2001), *Analysing Medical Data using S-PLUS*, Springer, New York, USA.

## Examples

```
data("mastectomy", package = "HSAUR")
table(mastectomy$metastized)
```

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meteo

# Description

Several meteorological measurements for a period between 1920 and 1931.

## Usage

```
data("meteo")
```

# Format

A data frame with 11 observations on the following 6 variables.

year the years.

rainNovDec rainfall in November and December (mm).

temp average July temperature.

rainJuly rainfall in July (mm).

radiation radiation in July (millilitres of alcohol).

yield average harvest yield (quintals per hectare).

# Details

Carry out a principal components analysis of both the covariance matrix and the correlation matrix of the data and compare the results. Which set of components leads to the most meaningful interpretation?

## Source

B. S. Everitt and G. Dunn (2001), Applied Multivariate Data Analysis, 2nd edition, Arnold, London.

```
data("meteo", package = "HSAUR")
meteo
```

orallesions

# Description

The distribution of the oral lesion site found in house-to-house surveys in three geographic regions of rural India.

# Usage

```
data("orallesions")
```

# Format

A two-way classification, see table.

# Source

Cyrus R. Mehta and Nitin R. Patel (2003), *StatXact-6: Statistical Software for Exact Nonparametric Inference*, Cytel Software Cooperation, Cambridge, USA.

# Examples

```
data("orallesions", package = "HSAUR")
mosaicplot(orallesions)
```

phosphate

Phosphate Level Data

# Description

Plasma inorganic phosphate levels from 33 subjects.

# Usage

data("phosphate")

## pistonrings

# Format

A data frame with 33 observations on the following 9 variables.

group a factor with levels control and obese.

- t0 baseline phosphate level,
- t0.5 phosphate level after 1/2 an hour.
- t1 phosphate level after one an hour.
- t1.5 phosphate level after 1 1/2 hours.
- t2 phosphate level after two hours.
- **t3** phosphate level after three hours.
- t4 phosphate level after four hours.
- **t5** phosphate level after five hours.

# Source

C. S. Davis (2002), *Statistical Methods for the Analysis of Repeated Measurements*, Springer, New York.

## Examples

```
data("phosphate", package = "HSAUR")
plot(t0 ~ group, data = phosphate)
```

pistonrings Piston Rings Failures

## Description

Number of failures of piston rings in three legs of four steam-driven compressors.

#### Usage

```
data("pistonrings")
```

## Format

A two-way classification, see table.

## Details

The data are given in form of a table. The table gives the number of piston-ring failures in each of three legs of four steam-driven compressors located in the same building. The compressors have identical design and are oriented in the same way. The question of interest is whether the two classification variables (compressor and leg) are independent.

# Source

S. J. Haberman (1973), The analysis of residuals in cross-classificed tables. *Biometrics* **29**, 205–220.

# Examples

```
data("pistonrings", package = "HSAUR")
mosaicplot(pistonrings)
```

planets

#### Exoplanets Data

# Description

Data on planets outside the Solar System.

#### Usage

```
data("planets")
```

## Format

A data frame with 101 observations from 101 exoplanets on the following 3 variables.

mass Jupiter mass of the planet.

period period in earth days.

eccen the radial eccentricity of the planet.

## Details

From the properties of the exoplanets found up to now it appears that the theory of planetary development constructed for the planets of the Solar System may need to be reformulated. The exoplanets are not at all like the nine local planets that we know so well. A first step in the process of understanding the exoplanets might be to try to classify them with respect to their known properties.

# Source

M. Mayor and P. Frei (2003). *New Worlds in the Cosmos: The Discovery of Exoplanets*. Cambridge University Press, Cambridge, UK.

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# plasma

# Examples

plasma

#### Blood Screening Data

# Description

The erythrocyte sedimentation rate and measurements of two plasma proteins (fibrinogen and globulin).

# Usage

data("plasma")

# Format

A data frame with 32 observations on the following 3 variables.

fibrinogen the fibrinogen level in the blood.

**globulin** the globulin level in the blood.

**ESR** the erythrocyte sedimentation rate, either less or greater 20 mm / hour.

#### Details

The erythrocyte sedimentation rate (ESR) is the rate at which red blood cells (erythrocytes) settle out of suspension in blood plasma, when measured under standard conditions. If the ESR increases when the level of certain proteins in the blood plasma rise in association with conditions such as rheumatic diseases, chronic infections and malignant diseases, its determination might be useful in screening blood samples taken form people suspected to being suffering from one of the conditions mentioned. The absolute value of the ESR is not of great importance rather it is whether it is less than 20mm/hr since lower values indicate a healthy individual.

The question of interest is whether there is any association between the probability of an ESR reading greater than 20mm/hr and the levels of the two plasma proteins. If there is not then the determination of ESR would not be useful for diagnostic purposes.

## Source

D. Collett and A. A. Jemain (1985), Residuals, outliers and influential observations in regression analysis. *Sains Malaysiana*, **4**, 493–511.

# Examples

```
data("plasma", package = "HSAUR")
layout(matrix(1:2, ncol = 2))
boxplot(fibrinogen ~ ESR, data = plasma, varwidth = TRUE)
boxplot(globulin ~ ESR, data = plasma, varwidth = TRUE)
```

polyps

#### Familial Andenomatous Polyposis

# Description

Data from a placebo-controlled trial of a non-steroidal anti-inflammatory drug in the treatment of familial andenomatous polyposis (FAP).

# Usage

```
data("polyps")
```

## Format

A data frame with 20 observations on the following 3 variables.

**number** number of colonic polyps at 12 months.

treat treatment arms of the trail, a factor with levels placebo and drug.

**age** the age of the patient.

## Details

Giardiello et al. (1993) and Piantadosi (1997) describe the results of a placebo-controlled trial of a non-steroidal anti-inflammatory drug in the treatment of familial andenomatous polyposis (FAP). The trial was halted after a planned interim analysis had suggested compelling evidence in favour of the treatment. Here we are interested in assessing whether the number of colonic polyps at 12 months is related to treatment and age of patient.

#### Source

F. M. Giardiello, S. R. Hamilton, A. J. Krush, S. Piantadosi, L. M. Hylind, P. Celano, S. V. Booker, C. R. Robinson and G. J. A. Offerhaus (1993), Treatment of colonic and rectal adenomas with sulindac in familial adenomatous polyposis. *New England Journal of Medicine*, **328**(18), 1313–1316.

S. Piantadosi (1997), Clinical Trials: A Methodologic Perspective. John Wiley & Sons, New York.

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## pottery

# Examples

```
data("polyps", package = "HSAUR")
plot(number ~ age, data = polyps, pch = as.numeric(polyps$treat))
legend(40, 40, legend = levels(polyps$treat), pch = 1:2, bty = "n")
```

pottery

#### Romano-British Pottery Data

## Description

Chemical composition of Romano-British pottery.

# Usage

data("pottery")

#### Format

A data frame with 45 observations on the following 9 chemicals.

Al2O3 aluminium trioxide.

Fe2O3 iron trioxide.

MgO magnesium oxide.

CaO calcium oxide.

Na2O natrium oxide.

K2O calium oxide.

TiO2 titanium oxide.

- MnO mangan oxide.
- **BaO** barium oxide.

#### Details

The data gives the chemical composition of specimens of Romano-British pottery, determined by atomic absorption spectrophotometry, for nine oxides.

#### Source

A. Tubb and N. J. Parker and G. Nickless (1980), The analysis of Romano-British pottery by atomic absorption spectrophotometry. *Archaeometry*, **22**, 153–171.

```
data("pottery", package = "HSAUR")
plot(pottery)
```

rearrests

## Description

Rearrests of juventile felons by type of court in which they were tried.

# Usage

```
data("rearrests")
```

#### Format

A two-way classification, see table.

# Details

The data (taken from Agresti, 1996) arise from a sample of juveniles convicted of felony in Florida in 1987. Matched pairs were formed using criteria such as age and the number of previous offences. For each pair, one subject was handled in the juvenile court and the other was transferred to the adult court. Whether or not the juvenile was rearrested by the end of 1988 was then noted. Here the question of interest is whether the true proportions rearrested were identical for the adult and juvenile court assignments?

#### Source

A. Agresti (1996). An Introduction to Categorical Data Analysis. Wiley, New York.

# Examples

```
data("rearrests", package = "HSAUR")
rearrests
```

respiratory Respiratory Illness Data

# Description

The respiratory status of patients recruited for a randomised clinical multicenter trial.

# Usage

```
data("respiratory")
```

#### roomwidth

# Format

A data frame with 555 observations on the following 7 variables.

**centre** the study center, a factor with levels 1 and 2.

**treatment** the treatment arm, a factor with levels placebo and treatment.

**sex** a factor with levels female and male.

**age** the age of the patient.

status the respiratory status (response variable), a factor with levels poor and good.

month the month, each patient was examined at months 0, 1, 2, 3 and 4.

**subject** the patient ID, a factor with levels 1 to 111.

## Details

In each of two centres, eligible patients were randomly assigned to active treatment or placebo. During the treatment, the respiratory status (categorised poor or good) was determined at each of four, monthly visits. The trial recruited 111 participants (54 in the active group, 57 in the placebo group) and there were no missing data for either the responses or the covariates. The question of interest is to assess whether the treatment is effective and to estimate its effect.

Note that the data are in long form, i.e, repeated measurments are stored as additional rows in the data frame.

## Source

C. S. Davis (1991), Semi-parametric and non-parametric methods for the analysis of repeated measurements with applications to clinical trials. *Statistics in Medicine*, **10**, 1959–1980.

# Examples

```
data("respiratory", package = "HSAUR")
mosaicplot(xtabs( ~ treatment + month + status, data = respiratory))
```

roomwidth Student

Students Estimates of Lecture Room Width

#### Description

Lecture room width estimated by students in two different units.

#### Usage

data("roomwidth")

# Format

A data frame with 113 observations on the following 2 variables.

unit a factor with levels feet and metres.

width the estimated width of the lecture room.

# Details

Shortly after metric units of length were officially introduced in Australia, each of a group of 44 students was asked to guess, to the nearest metre, the width of the lecture hall in which they were sitting. Another group of 69 students in the same room was asked to guess the width in feet, to the nearest foot. The data were collected by Professor T. Lewis and are taken from Hand et al (1994). The main question is whether estimation in feet and in metres gives different results.

# Source

D. J. Hand, F. Daly, A. D. Lunn, K. J. McConway and E. Ostrowski (1994). *A Handbook of Small Datasets*, Chapman and Hall/CRC, London.

# Examples

```
data("roomwidth", package = "HSAUR")
convert <- ifelse(roomwidth$unit == "feet", 1, 3.28)
boxplot(I(width * convert) ~ unit, data = roomwidth)</pre>
```

schizophrenia Age of Onset of Schizophrenia Data

## Description

Data on sex differences in the age of onset of schizophrenia.

#### Usage

data("schizophrenia")

# Format

A data frame with 251 observations on the following 2 variables.

age age at the time of diagnosis.

gender a factor with levels female and male

#### schizophrenia2

## Details

A sex difference in the age of onset of schizophrenia was noted by Kraepelin (1919). Subsequently epidemiological studies of the disorder have consistently shown an earlier onset in men than in women. One model that has been suggested to explain this observed difference is know as the subtype model which postulates two type of schizophrenia, one characterised by early onset, typical symptoms and poor premorbid competence, and the other by late onset, atypical symptoms, and good premorbid competence. The early onset type is assumed to be largely a disorder of men and the late onset largely a disorder of women.

#### Source

E. Kraepelin (1919), Dementia Praecox and Paraphrenia. Livingstone, Edinburgh.

#### Examples

data("schizophrenia", package = "HSAUR")
boxplot(age ~ gender, data = schizophrenia)

schizophrenia2 Schizophrenia Data

#### Description

Though disorder and early onset of schizophrenia.

# Usage

```
data("schizophrenia2")
```

# Format

A data frame with 220 observations on the following 4 variables.

**subject** the patient ID, a factor with levels 1 to 44.

onset the time of onset of the disease, a factor with levels < 20 yrs and > 20 yrs.

disorder whether thought disorder was absent or present, the response variable.

month month after hospitalisation.

## Details

The data were collected in a follow-up study of women patients with schizophrenia. The binary response recorded at 0, 2, 6, 8 and 10 months after hospitalisation was thought disorder (absent or present). The single covariate is the factor indicating whether a patient had suffered early or late onset of her condition (age of onset less than 20 years or age of onset 20 years or above). The question of interest is whether the course of the illness differs between patients with early and late onset?

#### Source

Davis (2002), Statistical Methods for the Analysis of Repeated Measurements, Springer, New York.

#### Examples

```
data("schizophrenia2", package = "HSAUR")
mosaicplot(xtabs( ~ onset + month + disorder, data = schizophrenia2))
```

schooldays

## Days not Spent at School

# Description

Data from a sociological study, the number of days absent from school is the response variable.

# Usage

data("schooldays")

## Format

A data frame with 154 observations on the following 5 variables.

race race of the child, a factor with levels aboriginal and non-aboriginal.

sex the sex of the child, a factor with levels female and male.

**school** the school type, a factor with levels F0 (primary), F1 (first), F2 (second) and F3 (third form).

**learner** how good is the child in learning things, a factor with levels average and slow.

absent number of days absent from school.

# Details

The data arise from a sociological study of Australian Aboriginal and white children reported by Quine (1975).

In this study, children of both sexes from four age groups (final grade in primary schools and first, second and third form in secondary school) and from two cultural groups were used. The children in age group were classified as slow or average learners. The response variable was the number of days absent from school during the school year. (Children who had suffered a serious illness during the years were excluded.)

# Source

S. Quine (1975), Achievement Orientation of Aboriginal and White Adolescents. Doctoral Dissertation, Australian National University, Canberra.

# skulls

# Examples

```
data("schooldays", package = "HSAUR")
plot.design(schooldays)
```

skulls

Egyptian Skulls

## Description

Measurements made on Egyptian skulls from five epochs.

# Usage

data("skulls")

# Format

A data frame with 150 observations on the following 5 variables.

- **epoch** the epoch the skull as assigned to, a factor with levels c4000BC c3300BC, c1850BC, c200BC, and cAD150, where the years are only given approximately, of course.
- mb maximum breaths of the skull.
- **bh** basibregmatic heights of the skull.
- **bl** basialiveolar length of the skull.
- nh nasal heights of the skull.

# Details

The question is whether the measurements change over time. Non-constant measurements of the skulls over time would indicate interbreeding with immigrant populations.

#### Source

D. J. Hand, F. Daly, A. D. Lunn, K. J. McConway and E. Ostrowski (1994). *A Handbook of Small Datasets*, Chapman and Hall/CRC, London.

```
pairs(means,
    panel = function(x, y) {
        text(x, y, levels(skulls$epoch))
    })
```

smoking

## Nicotine Gum and Smoking Cessation

## Description

Data from a meta-analysis on nicotine gum and smoking cessation

## Usage

data("smoking")

# Format

A data frame with 26 observations (studies) on the following 4 variables.

- **qt** the number of treated subjetcs who stopped smoking.
- tt the totla number of treated subjects.
- **qc** the number of subjetcs who stopped smoking without being treated.
- tc the total number of subject not being treated.

## Details

Cigarette smoking is the leading cause of preventable death in the United States and kills more Americans than AIDS, alcohol, illegal drug use, car accidents, fires, murders and suicides combined. It has been estimated that 430,000 Americans die from smoking every year. Fighting tobacco use is, consequently, one of the major public health goals of our time and there are now many programs available designed to help smokers quit. One of the major aids used in these programs is nicotine chewing gum, which acts as a substitute oral activity and provides a source of nicotine that reduces the withdrawal symptoms experienced when smoking is stopped. But separate randomized clinical trials of nicotine gum have been largely inconclusive, leading Silagy (2003) to consider combining the results studies found from an extensive literature search. The results of these trials in terms of numbers of people in the treatment arm and the control arm who stopped smoking for at least 6 months after treatment are given here.

# Source

C. Silagy (2003), Nicotine replacement therapy for smoking cessation (Cochrane Review). *The Cochrane Library*, **4**, John Wiley & Sons, Chichester.

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## students

# Examples

students

Student Risk Taking

# Description

Students were administered two parallel forms of a test after a random assignment to three different treatments.

## Usage

data("students")

# Format

A data frame with 35 observations on the following 3 variables.

treatment a factor with levels AA, C, and NC.

**low** the result of the first test.

high the result of the second test.

# Details

The data arise from a large study of risk taking (Timm, 2002). Students were randomly assigned to three different treatments labelled AA, C and NC. Students were administered two parallel forms of a test called low and high. The aim is to carry out a test of the equality of the bivariate means of each treatment population.

# Source

N. H. Timm (2002), Applied Multivariate Analysis. Springer, New York.

```
data("students", package = "HSAUR")
layout(matrix(1:2, ncol = 2))
boxplot(low ~ treatment, data = students, ylab = "low")
boxplot(high ~ treatment, data = students, ylab = "high")
```

suicides

# Description

Data from a study carried out to investigate the causes of jeering or baiting behaviour by a crowd when a person is threatening to commit suicide by jumping from a high building.

# Usage

```
data("suicides")
```

#### Format

A two-way classification, see table.

# Source

L. Mann (1981), The baiting crowd in episodes of threatened suicide. *Journal of Personality and Social Psychology*, **41**, 703–709.

## Examples

```
data("suicides", package = "HSAUR")
mosaicplot(suicides)
```

toothpaste Toothpaste Data

# Description

Meta-analysis of studies comparing two different toothpastes.

# Usage

data("toothpaste")

## voting

# Format

A data frame with 9 observations on the following 7 variables.

**Study** the identifier of the study.

nA number of subjects using toothpaste A.

meanA mean DMFS index of subjects using toothpaste A.

sdA standard deviation of DMFS index of subjects using toothpaste A.

nB number of subjects using toothpaste B.

meanB mean DMFS index of subjects using toothpaste B.

sdB standard deviation of DMFS index of subjects using toothpaste B.

# Details

The data are the results of nine randomised trials comparing two different toothpastes for the prevention of caries development. The outcomes in each trial was the change, from baseline, in the decayed, missing (due to caries) and filled surface dental index (DMFS).

## Source

B. S. Everitt and A. Pickles (2000), *Statistical Aspects of the Design and Analysis of Clinical Trials*, Imperial College Press, London.

## Examples

data("toothpaste", package = "HSAUR")
toothpaste

voting

House of Representatives Voting Data

# Description

Voting results for 15 congressmen from New Jersey.

# Usage

```
data("voting")
```

## Format

A 15 times 15 matrix.

# Details

Romesburg (1984) gives a set of data that shows the number of times 15 congressmen from New Jersey voted differently in the House of Representatives on 19 environmental bills. Abstentions are not recorded.

## Source

H. C. Romesburg (1984), *Cluster Analysis for Researchers*. Lifetime Learning Publications, Belmont, Canada.

# Examples

```
data("voting", package = "HSAUR")
require("MASS")
voting_mds <- isoMDS(voting)
plot(voting_mds$points[,1], voting_mds$points[,2],
    type = "n", xlab = "Coordinate 1", ylab = "Coordinate 2",
    xlim = range(voting_mds$points[,1])*1.2)
text(voting_mds$points[,1], voting_mds$points[,2],
    labels = colnames(voting))
voting_sh <- Shepard(voting[lower.tri(voting]], voting_mds$points)</pre>
```

water

Mortality and Water Hardness

# Description

The mortality and drinking water hardness for 61 cities in England and Wales.

#### Usage

```
data("water")
```

## Format

A data frame with 61 observations on the following 4 variables.

location a factor with levels North and South indicating whether the town is as north as Derby.

town the name of the town.

mortality averaged annual mortality per 100.000 male inhabitants.

hardness calcium concentration (in parts per million).

#### watervoles

## Details

The data were collected in an investigation of environmental causes of disease. They show the annual mortality per 100,000 for males, averaged over the years 1958-1964, and the calcium concentration (in parts per million) in the drinking water for 61 large towns in England and Wales. The higher the calcium concentration, the harder the water. Towns at least as far north as Derby are identified in the table. Here there are several questions that might be of interest including, are mortality and water hardness related, and do either or both variables differ between northern and southern towns?

## Source

D. J. Hand, F. Daly, A. D. Lunn, K. J. McConway and E. Ostrowski (1994). *A Handbook of Small Datasets*, Chapman and Hall/CRC, London.

# Examples

watervoles

# Description

Percentage incidence of the 13 characteristics of water voles in 14 areas.

Water Voles Data

## Usage

```
data("watervoles")
```

# Format

A dissimilarity matrix for the following 14 variables, i.e, areas: Surrey, Shropshire, Yorkshire, Perthshire, Aberdeen, Elean Gamhna, Alps, Yugoslavia, Germany, Norway, Pyrenees I, Pyrenees II, North Spain, and South Spain.

## Details

Corbet et al. (1970) report a study of water voles (genus Arvicola) in which the aim was to compare British populations of these animals with those in Europe, to investigate whether more than one species might be present in Britain. The original data consisted of observations of the presence or absence of 13 characteristics in about 300 water vole skulls arising from six British populations and eight populations from the rest of Europe. The data are the percentage incidence of the 13 characteristics in each of the 14 samples of water vole skulls.

# Source

G. B. Corbet, J. Cummins, S. R. Hedges, W. J. Krzanowski (1970), The taxonomic structure of British water voles, genus *Arvicola. Journal of Zoology*, **61**, 301–316.

## Examples

```
data("watervoles", package = "HSAUR")
watervoles
```

waves

Electricity from Wave Power at Sea

# Description

Measurements of root mean square bending moment by two different mooring methods.

# Usage

data("waves")

#### Format

A data frame with 18 observations on the following 2 variables.

method1 Root mean square bending moment in Newton metres, mooring method 1method2 Root mean square bending moment in Newton metres, mooring method 2

## Details

In a design study for a device to generate electricity from wave power at sea, experiments were carried out on scale models in a wave tank to establish how the choice of mooring method for the system affected the bending stress produced in part of the device. The wave tank could simulate a wide range of sea states and the model system was subjected to the same sample of sea states with each of two mooring methods, one of which was considerably cheaper than the other. The question of interest is whether bending stress differs for the two mooring methods.

## Source

D. J. Hand, F. Daly, A. D. Lunn, K. J. McConway and E. Ostrowski (1994). *A Handbook of Small Datasets*, Chapman and Hall/CRC, London.

```
data("waves", package = "HSAUR")
plot(method1 ~ method2, data = waves)
```

weightgain

# Description

The data arise from an experiment to study the gain in weight of rats fed on four different diets, distinguished by amount of protein (low and high) and by source of protein (beef and cereal).

# Usage

```
data("weightgain")
```

## Format

A data frame with 40 observations on the following 3 variables.

source source of protein given, a factor with levels Beef and Cereal.

type amount of protein given, a factor with levels High and Low.

weightgain weigt gain in grams.

# Details

Ten rats are randomized to each of the four treatments. The question of interest is how diet affects weight gain.

# Source

D. J. Hand, F. Daly, A. D. Lunn, K. J. McConway and E. Ostrowski (1994). A Handbook of Small Datasets, Chapman and Hall/CRC, London.

womensrole

## Description

Data from a survey from 1974 / 1975 asking both female and male responders about their opinion on the statement: Women should take care of running their homes and leave running the country up to men.

# Usage

```
data("womensrole")
```

# Format

A data frame with 42 observations on the following 4 variables.

education years of education.

**sex** a factor with levels Male and Female.

agree number of subjects in agreement with the statement.

disagree number of subjects in disagreement with the statement.

## Details

The data are from Haberman (1973) and also given in Collett (2003). The questions here are whether the response of men and women differ.

#### Source

S. J. Haberman (1973), The analysis of residuals in cross-classificed tables. *Biometrics*, **29**, 205–220.

D. Collett (2003), Modelling Binary Data. Chapman and Hall / CRC, London. 2nd edition.

```
data("womensrole", package = "HSAUR")
summary(subset(womensrole, sex == "Female"))
summary(subset(womensrole, sex == "Male"))
```

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