# Learn R

As a Language

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# **Preface**

"Suppose that you want to teach the 'cat' concept to a very young child. Do you explain that a cat is a relatively small, primarily carnivorous mammal with retractible claws, a distinctive sonic output, etc.? I'll bet not. You probably show the kid a lot of different cats, saying 'kitty' each time, until it gets the idea. To put it more generally, generalizations are best made by abstraction from experience."

R. P. Boas Can we make mathematics intelligible?, 1981

Why the title "Learn R: As a Language"? This book is based on exploration and practice that aims at teaching how to express various operations on data using the R language. It focuses on the language, rather than on specific types of data analysis, and exposes the reader to current usage and does not spare the quirks of the language. When we use our native language in everyday life, we do not think about grammar rules or sentence structure, except for the trickier or unfamiliar situations. My aim is for this book to help readers grow to use R in this same way, i.e., to become fluent in R. The book is structured around the elements of languages with chapter titles that highlight the parallels between natural languages like English and the R language.

Learn R: As a Language is different to other books about R in that it emphasizes learning of the language itself, rather than how to use R to address specific data analysis tasks. The aim is to enable readers to use R to implement original solutions to the data analysis and data visualization tasks they encounter. Use of quantitative methods and data analysis has become more frequent in fields with a limited long-term tradition in their use, like humanities, or, the complexity of the methods used has dramatically increased in recent years, like in Biology. Such trends can be expected to continue in the future.

Nowadays, many students of biological and environmental sciences learn R in courses about statistics or data analysis. However, frequently not in enough depth to effectively use it in scripts for automating data analyses or documenting the whole data analysis workflow to ensure reproducibility. Students in the humanities and also in other fields, may find it easier to learn the R language separately from data analysis and statistics. There are also many who are already familiar with statistical principles and wiling to switch from other software to R. *Learn R: As a* 

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*Language* is written with these readers in mind to serve both as a text book and as a reference.

A language is a system of communication. Basic concepts and operations are based on abstractions that are shared across programming languages and relevant to programs of all sizes and complexities; these abstractions are explained in the book together with their implementation in the R language. Other abstractions and programming concepts, outside the scope of this book, are relevant to large and complex pieces of software meant to be widely distributed. In other words, *Learn R: As a Language* aims at teaching and supporting *programming in the small*: the use of R to automate the drudgery of data manipulation, including the different steps spanning from data input and exploration to the production of publication-quality illustrations and their documentation.

Using a language actively is the most efficient way of learning it. By using it, I mean actually reading, writing, and running scripts or programs. Learn R: As a Language supports learning the R language in a way comparable to how children learn to speak: they work out what the rules are, simply by listening to people speak and trying to utter what they want to tell their parents. Of course, small children also receive guidance through feedback, but they are not taught a prescriptive set of rules like when learning a second language at school. Instead of listening, readers will read and run code, and instead of speaking, readers will write and try to execute R code statements on a computer. I do provide explanations and guidance, as understanding how R works greatly helps with its use. However, the approach I encourage in this book is for readers to play with the numerous examples and variations upon them, to find out by themselves the patterns behind the R language. Instead of parents being the sounding board for the first utterances of readers new to R, the computer will play this role. Although working through the examples in Learn R: As a Language in a group of peers or in class is beneficial, the book is designed to be useful also in the absence of such support.

This revised second edition reflects changes that took place in R and packages described. Very few code chunks from the first edition had stopped working but deprecations meant that some examples triggered messages or warnings, and will eventually fail. Recent (> 4.0.0) versions of R have significant enhancements such as the new pipe operator. Packages have also evolved acquiring new features. Feedback from readers and reviewers has highlighted some gaps in the contents and unclear explanations.

An additional change is in my view about some of the packages in the 'tidyverse'. This change is reflected most strongly in Chapter 8. I have realized by my own experience and from advising other users, including students in the life sciences, that the rate of development and the frequency of code-breaking changes can make some of the *tidyverse* packages difficult for users for whom data analysis is just one aspect of their occupation. In other words, those current and future users to whom this book is targeted. It seems to me that except for packages like 'ggplot2' and 'stringr', much of the current development effort from Posit (formerly RStudio) aims at professional data analysts rather than occasional users of R. There is nothing wrong with this, but it is necessary to be aware that for occasional users learning base R can be a better investment of their time.

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Re-reading myself the book after some time allowed me to think of other improvements. I have updated the book accordingly making it more accessible to readers with no previous experience in computer programming. I have added diagrams and flowcharts to facilitate comprehension of common programming abstractions. I also edited the text from the first edition to fix all errors and outdated examples or explanations known to me.

### Acknowledgements

I thank Jaakko Heinonen for introducing me to the then new R. Along the way many well known and not so famous experts have answered my questions in usenet and more recently in StackOverflow. I wish to warmly thank members of my own research group, students participating in the courses I have taught, colleagues I have collaborated with, authors of the books I have read and people I have only met online or at conferences. All of them have made it possible for me to write this book. I am indebted to Tarja Lehto, Titta Kotilainen, Tautvydas Zalnierius, Fang Wang, Yan Yan, Neha Rai, Markus Laurel, Brett Cooper, Viivi Lindholm, Zuzana Svarna, colleagues, students and anonymous reviewers for many very helpful comments on the draft manuscript and/or the published first edition. Rob Calver, editor of both editions, provided encouragement with great patience, Shashi Kumar, Lara Spieker, Vaishali Singh, Sherry Thomas, and Paul Boyd for their help with different aspects of this project.

I was able to work intensively for a few months on the writing of this 2nd edition thanks to a sabbatical granted by my employer, the Faculty of Biological and Environmental Sciences of the University of Helsinki, Finland. I thank Prof. Kurt Fagerstedt for his support.

In many ways this text owes much more to people who are not authors than to myself. However, as I am the one who has written *Learn R: As a Language* and decided what to include and exclude, I take full responsibility for any errors and inaccuracies.

Helsinki, September 28, 2023

# Using the Book to Learn R

The important part of becoming a programmer is learning to think like a programmer. You don't need to know the details of a programming language by heart, you can just look that stuff up.

The treasure is in the structure, not the nails.

P. Burns Tao Te Programming, 2012

# 1.1 Aims of this chapter

In this chapter I describe how I imagine the book can be used most effectively to learn the R language. Learning R and remembering what one has previously learnt and forgotten makes it also necessary to use this book and other sources as reference. Learning to use R effectively, also involves learning how search for information and learning how to ask questions from other users, for example, through on-line forums. Thus, I also give advice on how to find answers to R-related questions and how to use the available documentation.

# 1.2 Approach and structure

Depending on previous experience, reading *Learn R: As a Language* will be about exploring a new world or revisiting a familiar one. In both cases *Learn R: As a Language* aims to be a travel guide, neither a traveler's account, nor a cookbook of R recipes. It can be used as a course book, supplementary reading or for self instruction, and also as a reference. My hope is that as a guide to the use of R, this

book will remain useful to readers' as they gain experience and develop skills. I encourage readers to approach R like a child approaches his or her mother tongue when learning to speak: do not struggle, just play, and fool around with R! If the

going gets difficult and frustrating, take a break! If you get a new insight, take a break to enjoy the victory!

In R, like in most "rich" languages, there are multiple ways of coding the same operations. I have included code examples that aim to strike a balance between execution speed and readability. One could write equivalent R books using substantially different code examples. Keep this is mind when reading the book and using R. Keep also in mind that it is impossible to remember everything about R and as a user you will frequently need to consult the documentation, even while doing the exercises in this book. The R language, in a broad sense, is vast because it can be expanded with independently developed packages. Learning to use R mainly consists of learning the basics plus developing the skill of finding your way in R, its documentation and on-line question and answer forums.

Readers should not aim at remembering all the details presented in the book, this is impossible for most of us. Later use of this and other books, and documentation effectively as references, depends on a good grasp of a broad picture of how R works and on learning how to navigate the documentation; i.e., it is more important to remember abstractions and in what situations they are used, and function names, than the details of how to use them. Developing a sense of when one needs to be careful not to fall in a "language trap" is also important.

The book can be used both as a text book for learning R and as a reference. It starts with simple concepts and language elements progressing towards more complex language structures and uses. Along the way readers will find, in each chapter, descriptions and examples for the common (usual) cases and the exceptions. Some books hide the exceptions and counterintuitive features from learners to make the learning easier, I instead have included these but marked them using icons and marginal bars. There are two reasons for choosing this approach. First, the boundary between boringly easy and frustratingly challenging is different for each of us, and varies depending on the subject dealt with. So, I hope the marks will help readers predict what to expect, how much effort to put in each section and even what to read and what to skip. Second, if I had hidden the tricky bits of the R language, I would have made reader's later use of R more difficult. It would have also made the book less useful as a reference.

The book contains many code examples as well as exercises. I expect readers will run code examples and try as many variations of them as needed to develop an understanding of the "rules" of the R language, e.g., how the function or feature exemplified works. This is what long-time users of R do when facing an unfamiliar feature or a gap in their understanding.

Readers new to R should read at least chapters 2 to 6 sequentially. Possibly, skipping parts of the text and exercises marked as advanced. However, I expect to be most useful to these readers, not to completely skip the description of unusual features and special cases, but rather to skim enough from them so as to get an idea of what special situations they may face as R users. Exercises should not be skipped, as they are a key component of the didactic approach used.

Readers already familiar with R will be able to read the chapters in the book in any order, as the need arises. Marginal bars and icons, and the backwards and for-

ward cross references among sections, make possible for readers to *select suitable path* within the book both when learning R and when using the book as a reference.

I expect *Learn R: As a Language* to remain useful as a reference to those readers who use it to learn R. It will be also useful as a reference to readers already familiar with R. To support the use of the book as a reference, I have been thorough with indexing, including many carefully chosen terms, their synonyms and the names of all R objects and constructs discussed, collecting them in three alphabetical indexes: *General index*, *Index of R names by category*, and *Alphabetic index of R names* starting at pages 416, 432 and 424, respectively. I have also included back and forward cross references linking related sections throughout the whole book.

### 1.3 Typographic and naming conventions

#### 1.3.1 Call outs

Marginal bars and icons are used in the book to inform about what content is advanced or included with a specific aim. The following icons and colours are used.

Signals in-depth explanations of specific R features or general programming concepts. Several of these explanations make reference to programming concepts or features of the R language that are explained later in the book. Readers new to R and computer programming can safely skip these call outs on first reading of the book. To become proficient in the use of R these readers are expected to return at a later time without hurry, preferably with a cup of coffee or tea to these call outs. Readers with more experience, like those possibly reading individual chapters or using the book as a reference, will find these in-depth explanations useful.

A Signals important bits of information that must be remembered when using R—i.e., explanations of some unusual, but important, feature of the language or concepts that in my experience are easily missed by those new to R.

# **3** Frequently asked question

Signals my answer to a question that I expect to be useful to readers based on the popularity of similar or related questions posted in on-line forums. When reading through the book, they highlight things that are worth special attention. When using the book as a reference, they help find solutions to frequently encountered difficulties.

1.1 Signals *playgrounds* containing open-ended exercises—ideas and pieces of R code to play with at the R console. I expect readers to run these examples both as is and after creating variations by editing the code, studying the output, or diagnosis messages, returned by R in each case. Numbered by chapter for easy reference.

1.2 Signals *advanced playgrounds* sections that require more time to play with before grasping concepts than regular *playground* sections. Numbered by chapter together with other playgrounds.

#### 1.3.2 Code conventions and syntax highlighting

Small sections of program code interspersed within the main text, receive the name of *code chunks*. In this book R code chunks are typeset in a typewriter font, using colour to highlight the different elements of the syntax, such as variables, functions, constant values, etc. R code elements embedded in the text are similarly typeset but always black. For example in the code chunk below mean() and print() are functions; 1, 5 and 3 are constant numeric values, and z is the name of a variable where the result of the computation done in the first line of code is stored. The line starting with ## shows what is printed or shown when executing the second statement: [1] 1. In the book ## is used as a marker to signal output from R, it is not part of the output. As # is the marker for comments in the R language, prepending # to the output makes it possible to copy and pasted into the R console the whole contents of the code chunks as they appear in the book.

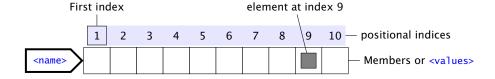
```
z <- mean(1, 5, 3)
print(z)
## [1] 1</pre>
```

When explaining general concepts I use short abstract names, while for real-life examples I use descriptive names. Although not required, for clarity, I use abstract names that hint at the structure of objects stored, such as mat1 for a matrix, vct4 for a vector and df3 for a data frame. This convention resembles that followed by the base R documentation.

Code in playgrounds either works in isolation or if it depends on objects created in the examples in the main text, this is mentioned within the playground. In playgrounds I use names in capital letters so that they are distinct. The code outside playgrounds does reuse objects created earlier in the same section, and occasionally in earlier sections of the same chapter.

#### 1.3.3 Diagrams

To describe data objects I use diagrams inspired in Joseph N. Hall's PEGS (Perl Graphical Structures) (Hall and Schwartz 1997). I use colour fill to highlight the type of the stored objects. I use the "signal" sign for the names of whole objects and of their component members, the former with a thicker border. Below is an example from chapter 3.



For code structure I use diagrams based on boxes and arrows, and to describe the flow of code execution, the usual flow charts.

In the different diagrams, I use the notation <value>, <statement>, <name>, etc., as generic placeholders indicating *any valid value*, *any valid R statement*, *any valid R name*, etc.

## 1.4 Findings answers to problems

#### 1.4.1 What are the options

First of all do not panic! Every programmer, even those with decades of experience, get stuck with problems from time to time, and can run out of ideas for a while. This is normal, and happens to all of us.

It is important to learn how to find answers as part of the routine of using R. First of all one can read the documentation of the function or object that one is trying to use, which in many cases also includes use examples. R's help pages tell how to use individual functions or objects. In contrast, R's manual *An Introduction to R* and books describe what functions or overall approaches to use for different tasks.

Reading the documentation and books not always helps. Sometimes one can become blind to the obvious, by being too familiar with a piece of code, as it also happens when writing in a natural language like English. A second useful step is, thus, looking at the code with "different eyes", those of a friend or workmate, or your own eyes a day or a week later.

One can also seek help in specialized on-line forums or from peers or "local experts". If searching in forums for existing questions and answers fails to yield a useful answer, one can write a new question in a forum.

When searching for answers, asking for advice or reading books, one can be confronted with different ways of approaching the same tasks. Do not allow this to overwhelm you; in most cases it will not matter which approach you use as many computations can be done in R, as in any computer language, in several different ways, still obtaining the same result. Use the alternative that you find easier to understand.

#### 1.4.2 R's built-in help

Every object available in base R or exported by an R extension package (functions, methods, classes, data) is documented in R's help system. Sometimes a single help page documents several R objects. Not only help pages are always available, but they are structured consistently with a title, short description, and frequently also a detailed description. In the case of functions, parameter names, their purpose and expected arguments are always described, as well as the returned value. Usually at the bottom of help pages, several examples of the use of the objects or functions are given. How to access R help is described in section 2.3 on page 12.

In addition to help pages, R's distribution includes useful manuals as PDF or HTML files. These manuals are also available at https://rstudio.github.io/r-manuals/restyled for easier reading in web browsers. In addition to help pages, many packages, contain *vignettes* such as User Guides or articles describing the algorithms used and/or containing use case examples. In the case of some packages, a web site with documentation in HTML format is also available. Package documentation can be also accessed through CRAN. The DESCRIPTION of packages provides

contact information for the maintainer, links to web sites, and instructions on how to report bugs. Similar information plus a short description are frequently also available in a README file.

Error messages tend to be terse in R, and may require some lateral thinking and/or "experimentation" to understand the real cause behind problems. Learning to interpret error messages is necessary to become a proficient user of R, so forcing errors and warnings with purposely written "bad" code is a useful exercise.

#### 1.4.3 Online forums

#### Netiquette

When posting requests for help, one needs to abide by what is usually described as "netiquette", which in many respects also applies to asking in person or by email help from a peer or local expert. Preference among sources of information depends on what one finds easier to use. Consideration towards others' time is necessary but has to be shalanced against wasting too much of one's own time.

In most internet forums, a certain behavior is expected from those asking and answering questions. Some types of misbehavior, like use of offensive or inappropriate language, will usually result in the user losing writing rights in a forum. Occasional minor misbehavior, usually results in the original question not being answered and instead the problem highlighted in a comment. In general following the steps listed below will greatly increase your chances of getting a detailed and useful answer.

- Do your homework: first search for existing answers to your question, both online and in the documentation. (Do mention that you attempted this without success when you post your question.)
- Provide a clear explanation of the problem, and all the relevant information. The version of R, operating system, and any packages loaded and their versions can be important.
- If at all possible, provide a simplified and short, but self-contained, code example that reproduces the problem (sometimes called a *reprex*).
- Be polite.
- Contribute to the forum by answering other users' questions when you know the answer.

Carefully preparing a reproducible example ("reprex") is crucial. A *reprex* is a self-contained and as simple as possible piece of computer code that triggers (and so demonstrates) a problem. If possible, when data are needed, a data set included in base R or artificial data generated within the reprex code should be used. If the problem can only be reproduced with one's own data, then one needs to provide a minimal subset of it that still triggers the problem.

While preparing a *reprex* one has to simplify the code, and sometimes this step makes clear the nature of the problem. Always, before posting a reprex online,

check it with the latest versions of R and any package being used. If sharing data, be careful about confidential information and either remove or mangle it.

I must say that about two out of three times I prepare a *reprex*, it allows me to find the root of the problem and a solution or a work-around on my own. Preparing a *reprex* takes some effort but it is worthwhile even if it ends up not being posted on-line.

R package 'reprex' and its RStudio add-in simplify the creation of reproducible code examples, by creating and copying to the clipboard a reprex encoded in Markdown and ready to be pasted into a question at StackOverflow or into an issue at GitHub. See https://reprex.tidyverse.org/ for details.

#### StackOverflow

Nowadays, StackOverflow (http://stackoverflow.com/) is the best question-and-answer (Q&A) support site for R. Within the StackOverflow site there is an R collective. In most cases, searching for existing questions and their answers, will be all that you need to do. If asking a question, make sure that it is really a new question. If there is some question that looks similar, make clear how your question is different.

StackOverflow has a user-rights system based on reputation, and questions and answers can be up- and down-voted. Questions with the most up-votes are listed at the top of searches, and the most voted answers to each question are also displayed first. Who asks a question is expected to accept correct answers. If the questions or answers one writes are up-voted one gains reputation (expressed as number). As one accumulates reputation, gets badges and additional rights, such as editing other users' questions and answers or later on, even deleting wrong answers or off-topic questions from the system. This sounds complicated, but works extremely well at ensuring that the base of questions and answers is relevant and correct, without relying heavily on nominated *moderators*. When using StackOverflow, do contribute by accepting correct answers, up-voting questions and answers that you find useful, down-voting those you consider poor, and flagging or correcting errors you may discover.

Being careful in the preparation of a reproducible example is important both when asking a question at StackOverflow and when reporting a bug to the maintainer of any piece of software. For the question to be reliably answered or the problem to be fixed, the person answering a question, needs to be able to reproduce the problem, and after modifying the code, needs to be able to test if the problem has been solved or not. However, even if you are facing a problem caused by your misunderstanding of how R works, the simpler the example, the more likely that someone will quickly realize what your intention was when writing the code that produces a result different from what you expected. Even when it is not possible to create a reprex, one needs to ask clearly only one thing per question.

The code of conduct (https://stackoverflow.com/conduct) and help that explains expected behavior (https://stackoverflow.com/help) are available at the site and worthwhile reading before using the site actively for the first time.

#### Contacting the author

The best way to get in contacting with me about this book is by rasing an issue at https://github.com/aphalo/learnr-book-crc/issues. Issues can be used both to ask for support questions related to the book, report mistakes and suggest changes to the text, diagrams and/or example code. Edits to the manuscript of this book can be submitted as pull requests.

Issues are raised by filling-in an on-line form, at a web page that also contains brief instructions. Git issues are a very efficient way of keeping track of corrections that need to be done. As support questions usually reveal unclear explanations or other problems, raising issues to ask them facilitates the tasks of improving and keeping the book up-to-date.

## 1.5 Further reading

At the end of each chapter a section like this one gives suggestions for further reading on related subjects. To understand what programming as an activity is you can read *Tao Te Programming* (Burns 2012). It will make easier the learning of programming in R, both practically and emotionally. In Burns's words "This is a book about what goes on in the minds of programmers".

# R: the Language and the Program

In a world of ... relentless pressure for more of everything, one can lose sight of the basic principles—simplicity, clarity, generality—that form the bedrock of good software.

Brian W. Kernighan and Rob Pike *The Practice of Programming*, 1999

## 2.1 Aims of this chapter

I share some facts about the history and design of the R language so that you can gain a good vantage point from which to grasp the logic behind R's features, making it easier to understand and remember them. You will learn the distinction between the R program itself and the front-end programs, like RStudio, frequently used together with R.

You will also learn how to interact with R when sitting at a computer. You will learn the difference between typing commands interactively and reading each partial result from R on the screen as you enter them, versus using R scripts containing multiple commands stored in a file to execute or run a "job" that saves results to another file for later inspection.

I describe the steps taken in a typical scientific or technical study, including the data analysis work flow and the roles that R can play in it. I share my views on the advantages and disadvantages of textual command languages such as R compared to menu-driven user interfaces, frequently used in other statistics software. I discuss the role of textual languages and *literate programming* in the very important question of reproducibility of data analyses and mention how I have used them while writing and typesetting this book.

#### **2.2** What is **R**?

#### 2.2.1 R as a language

R is a computer language designed for data analysis and data visualization, however, in contrast to some other scripting languages, it is, from the point of view of computer programming, a complete language—it is not missing any important feature. In other words, no fundamental operations or data types are lacking (Chambers 2016). I attribute much of its success to the fact that its design achieves a very good balance between simplicity, clarity and generality. R excels at generality thanks to its extensibility at the cost of only a moderate loss of simplicity, while clarity is ensured by enforced documentation of extensions and support for both object-oriented and functional approaches to programming. The same three principles can be also easily followed by user code written in R.

In the case of languages like C++, C, Pascal and FORTRAN multiple software implementations exist (different compilers and interpreters, i.e., pieces of software that translate programs encoded in these languages into *machine code* instructions for computer processors to run). So in addition to different flavours of each language stemming from different definitions, e.g., versions of international standards, different implementations of the same standard may have, usually small, unintentional and intentional differences.

Most people think of R as a computer program, similar to SAS or SPPS. R is indeed a computer program—a piece of software— but it is also a computer language, implemented in the R program. At the moment, differently to most other computer languages, this difference is not important as the R program is the only widely used implementation of the R language.

R started as a partial implementation of the then relatively new S language (Becker and Chambers 1984; Becker et al. 1988). When designed, S, developed at Bell Labs in the U.S.A., provided a novel way of carrying out data analyses. S evolved into S-Plus (Becker et al. 1988). S-Plus was available as a commercial program, most recently from TIBCO, U.S.A. R started as a poor man's home-brewed implementation of S, for use in teaching, developed by Robert Gentleman and Ross Ihaka at the University of Auckland, in New Zealand (Ihaka and Gentleman 1996). Initially R, the program, implemented a subset of the S language. The R program evolved until only relatively few differences between S and R remained. These remaining differences are intentional—thought of as significant improvements. In more recent times R overtook S-Plus in popularity. The R language is not standardised, and no formal definition of its grammar exists. Consequently, the R language is defined by the behavior of its implementation in the R program.

What makes R different from SPSS, SAS, etc., is that S was designed from the start as a computer programming language. This may look unimportant for someone not actually needing or willing to write software for data analysis. However, in reality it makes a huge difference because R is easily extensible, both using the R language for implementation and by calling from R functions and routines written in other computer programming languages such as C, C++, FORTRAN, Python or

What is R?

Java. This flexibility means that new functionality can be easily added, and easily shared with a consistent R-based user interface. In other words, instead of having to switch between different pieces of software to do different types of analyses or plots, one can usually find a package that will make new tools seamlessly available within R.

The name "base R" is used to distinguish R itself, as in the R executable included in the R distribution and its default packages, from R in a broader sense, which includes contributed packages. A few packages are included in the R distribution, but most R packages are independently developed extensions and separately distributed. The number of freely available open-source R packages available is huge, in the order of 20 000.

The most important advantage of using a language like R is that instructions to the computer are given as text. This makes it easy to repeat or *reproduce* a data analysis. Textual instructions serve to communicate to other people what has been done in a way that is unambiguous. Sharing the instructions themselves avoids a translation from a set of instructions to the computer into text readable to humans—say the materials and methods section of a paper.

Readers with programming experience, will notice that some features of R differ from those in other programming languages. R does not have the strict type checks of Pascal or C++. It has operators that can take vectors and matrices as operands. Reliable and fast R code, tends to rely on different *idioms* than well-written Pascal or C++ code.

#### 2.2.2 R as a computer program

The R program itself is open-source, i.e., its source code is available for anybody to inspect, modify and use. A small fraction of users will directly contribute improvements to the R program itself, but it is possible, and those contributions are important in making R extremely reliable. The executable, the R program we actually use, can be built for different operating systems and computer hardware. The members of the R developing team aim to keep the results obtained from calculations done on all the different builds and computer architectures as consistent as possible. The idea is to ensure that computations return consistent results not only across updates to R but also across different operating systems like Linux, Unix (including OS X), and MS-Windows, and computer hardware.

The R program does not have a full-fledged graphical user interface (GUI), or menus from which to start different types of analyses. Instead, the user types the commands at the R console and the result is displayed starting on the next line (Figure 2.1). The same textual commands can also be saved into a text file, line by line, and such a file, called a "script" can substitute for the direct typing of the same sequence of commands at the console (writing and use of R scripts are explained in chapter 5 on page 125). When we work at the console, typing-in commands one by one, we use R *interactively*. When we run a script, we may say that we run a "batch job." The two approaches described above are available in the R program itself.

```
R Console

> print("hello")
[1] "hello"

> |
```

#### FIGURE 2.1

The R console where the user can type textual commands one by one. Here the user has typed print("Hello") and *entered* it by ending the line of text by pressing the "enter" key. The result of running the command is displayed below the command. The character at the head of the input line, a ">" in this case, is called the command prompt, signaling where a command can be typed in. Commands entered by the user are displayed in red, while results returned by R are displayed in blue. "[1]" can be ignored here, its meaning is explained on page 28

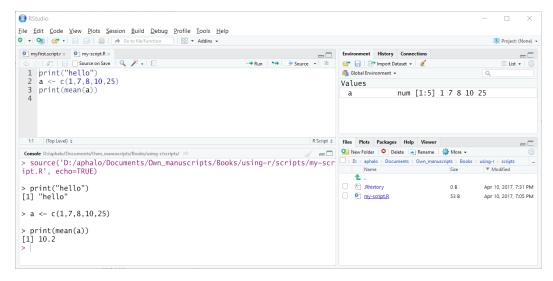
As R is essentially a command-line application, it can be used on what nowadays are frugal computing resources, equivalent to a personal computer of three decades ago. R can run even on the Raspberry Pi, a micro-controller board with the processing power of a modest smart phone (see https://r4pi.org/). At the other end of the spectrum, on really powerful servers, R can be used for the analysis of big data sets with millions of observations. How powerful a computer is needed for a given data analysis task depends on the size of the data sets, on how patient one is, on the ability to select efficient algorithms and on writing "good" code.

#### 2.3 Using R

#### 2.3.1 Editors and IDEs

Integrated Development Environments (IDEs) are normally used when developing computer programs. IDEs provide a centralized user interface from within which the different tools used to create and test a computer program can be accessed and used in coordination. Most IDEs include a dedicated editor capable of syntax highlighting (automatically colouring "code words" based on their role in the programming language), and even able to report some mistakes in advance of running the code. One could describe such an editor as the equivalent of a word processor with spelling and grammar checking, that can alert about spelling and syntax errors for a computer language like R instead of for a natural language like English. IDEs frequently add other features that help navigation of the programme source code and make easy the access to documentation.

It is nowadays very common to use an IDE as a front-end or middleman between the user and the R program. Computations are still done in the R program, which Using R



#### FIGURE 2.2

The RStudio interface after running the script that is visible in tab my-script.R of the editor pane (top left). Here I used the "Source" button to run the script and R printed the results to the R console in the lower left pane. The lower right pane shows a list of files, including the script open in the editor. The upper right pane displays a list of the objects currently visible in the user workspace, object a, which was created by the code in the second line of the R script.

is *not* built-in in the IDEs. Of the available IDEs for R, RStudio is currently the most popular by a wide margin. Recent versions of RStudio support Python in addition to R.

Readers with programming experience may be already familiar with Microsoft's free Visual Studio Code or the open-source Eclipse IDEs for which add-ons supporting R are available.

The main window of IDEs is in most cases divided into windows or panes, possibly with tabs. In RStudio one has access to the R console, a text editor, a file-system browser, a pane for graphical output, and access to several additional tools such as for installing and updating extension packages. Although RStudio supports very well the development of large scripts and packages, it is currently, in my opinion, also the best possible way of using R at the console as it has the R help system very well integrated both in the editor and R console. Figure 2.2 shows the main window displayed by RStudio after running the same script as shown at the R console (Figure 2.5) and at the operating system command prompt (Figure 2.6). By comparing these three figures it is clear that RStudio is really only a software layer between the user and an unmodified R executable. In RStudio the script was sourced by pressing the "Source" button at the top of the editor panel. RStudio, in response to this, generated the code needed to source the file and "entered" it at the console (2.2, lower left screen panel, text in purple), the same console where we can directly type this same R command if we wish.

When a script is run, if an error is triggered, RStudio automatically finds the location of the error, a feature you will find useful when running code from exercises in this book. Other features are beyond what one needs for simple everyday data analysis and aimed at package development and report generation. Tools for debugging, code profiling, bench marking of code and unit tests, make it possible to analyze and improve performance as well help with quality assurance and certification of R packages, and exceed what you will needed for this book's exercises and simple data analysis. RStudio also integrates support for file version control, which is not only useful for package development, but also for keeping track of the progress or concurrent work with collaborators in the analysis of data.

The "desktop" version of RStudio that one installs and uses locally, runs on most modern operating systems, such as Linux, Unix, OS X, and MS-Windows. There is also a server version that runs on Linux, as well as a cloud service (https://posit.cloud/) providing shared access to such a server. The RStudio server is used remotely through a web browser. The user interface is almost the same in all cases. Desktop and server versions are both distributed as unsupported free software and as supported commercial software.

RStudio and other IDEs support saving of their state and some settings per working folder under the name of *project*, so that work on a data analysis can be interrupted and later continued, even on a different computer. As mentioned in section 2.3.2 on page 14, when working with R we keep related files in a folder.

In this book I provide only a minimum of guidance on the use of RStudio, and no guidance for other IDEs. To learn more about RStudio, please, read the documentation available through RStudio's help menu and keep at hand a printed copy of the RStudio cheat sheet while learning how to use it. This and other useful R-related cheatsheets can be downloaded at https://posit.co/resources/cheatsheets/. Additional instructions on the use of RStudio, including a video, are available through the Resources menu entry at the book website at https://www.learnr-book.info/.

#### 2.3.2 R sessions and workspaces

We use *session* to describe the interactive execution from start to finish of one running instance of the R program. We use *workspace* to name the imaginary space were all objects currently available in an R session are stored. In R the whole workspace can be stored in a single file on disk at the end or during a session and restored later into another session, possibly on a different computer. Usually when working with R we dedicate a folder in disk storage to store all files from a given data analysis project. We normally keep in this folder files with data to read in, scripts, a file storing the whole contents of the workspace, named by default .Rdata and a text file with the history of commands entered interactively, named by default .Rhistory. The user's files within this folder can be located in nested folders. There are no strict rules on how the files should be organised or on their number. The recommended practice is to avoid crowded folders and folders containing unrelated files. It is a good idea to keep in a given folder and workspace the work in progress for a single data-analysis project or experiment, so that the

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workspace can be saved and restored easily between sessions and work continued from where one left it independently of work done in other workspaces. The folder where files are currently read and saved is in R documentation called the *current working directory*. When opening an .Rdata file the current working directory is automatically set to the location where the .Rdata file was read from.

RStudio projects are implemented as a folder with a name ending in .Rprj, located under the same folder where scripts, data, .Rdata and .Rhistory are stored. This folder is managed by RStudio and should be not modified or deleted by the user. Only in the very rare case of its corruption, it should be deleted, and the RStudio project created again from scratch. Files .Rdata and .Rhistory should not be deleted by the user, except to reset the R workspace. However, this is unnecessary as it can be also easily achieved from within R.

#### 2.3.3 Using R interactively

Decades ago users communicated with computers through a physical terminal (keyboard plus text-only screen) that was frequently called a *console*. A text-only interface to a computer program, in most cases a window or a pane within a graphical user interface, is still called a console. In our case, the R console (Figure 2.1). This is the native user interface of R.

Typing commands at the R console is useful when one is playing around, rather aimlessly exploring things, or trying to understand how an R function or operator we are not familiar with works. Once we want to keep track of what we are doing, there are better ways of using R, which allow us to keep a record of how an analysis has been carried out. The different ways of using R are not exclusive of each other, so most users will use the R console to test individual commands and plot data during the first stages of exploration. As soon as we decide how we want to plot or analyze the data, it is best to start using scripts. This is not enforced in any way by R, but scripts are what really brings to light the most important advantages of using a programming language for data analysis. In Figure 2.1 we can see how the R console looks. The text in red has been typed in by the user, except for the prompt >, and the text in blue is what R has displayed in response. It is essentially a dialogue between user and R. The console can *look* different when displayed within an IDE like RStudio, but the only difference is in the appearance of the text rather than in the text itself (cf. Figures 2.1 and 2.3).

The two previous figures showed the result of entering a single command. Figure 2.4 shows how the console looks after the user has entered several commands, each as a separate line of text.

The examples in this book require only the console window for user input. Menu-driven programs are not necessarily bad, they are just unsuitable when there is a need to set very many options and choose from many different actions. They are also difficult to maintain when extensibility is desired, and when independently developed modules of very different characteristics need to be integrated. Textual languages also have the advantage, to be addressed in later chapters, that command sequences can be stored in human- and computer-readable text files. Such files constitute a record of all the steps used, and in most cases, makes it trivial to

```
Console D:/aphalo/Documents/Own_manuscripts/Books/using-r/ 

> print("Hello")

[1] "Hello"

> |
```

#### FIGURE 2.3

The R console embedded in RStudio. The same commands have been typed in as in Figure 2.1. Commands entered by the user are displayed in purple, while results returned by R are displayed in black.

```
> print("hello")
[1] "hello"
> mean(c(1,5,6,2,3,4))
[1] 3.5
> a <- c(1,7,8,10,25)
> mean(a)
[1] 10.2
> sd(a)
[1] 8.927486
> b <- factor(c("trea", "trea", "ctrl", "ctrl"))
```

#### FIGURE 2.4

The R console after several commands have been entered. Commands entered by the user are displayed in red, while results returned by R are displayed in blue.

manually reproduce the same steps at a later time. Scripts are a very simple and handy way of communicating to other users how a given data analysis has been done or can be done.

In the console one types commands at the > prompt. When one ends a line by pressing the return or enter key, if the line can be interpreted as an R command, the result will be printed at the console, followed by a new > prompt. If the command is incomplete, a + continuation prompt will be shown, and you will be able to type in the rest of the command. For example if the whole calculation that you would like to do is 1 + 2 + 3, if you enter in the console 1 + 2 + 1 in one line, you will get a continuation prompt where you will be able to type 3. However, if you type 1 + 2, the result will be calculated, and printed.

For example, one can search for a help page at the R console.

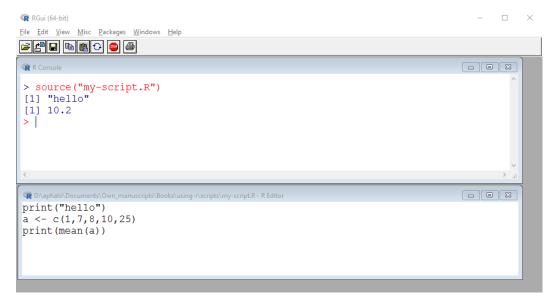
Below are the first code example and first playground in the book. This first example is for illustration only, and you can return to them later as only in page 20 I discuss how to install or get access to the R program.

```
help("sum")
?sum
```

2.1 Look at help for some other functions like mean(), var(), plot() and, why not, help() itself!

```
help(help)
```

Using R



#### FIGURE 2.5

Screen capture of the R console and editor just after running a script. The upper pane shows the R console, and the lower pane, the script file in an editor.

When trying to access help related to R extension packages trough R's built in help, make sure the package is loaded into the current R session, as described on page 179, before calling help().

When using RStudio there are easier ways of navigating to a help page than calling function help() by typing its name, for example, with the cursor on the name of a function in the editor or console, pressing the F1 key opens the corresponding help page in the help pane. Letting the cursor hover for a few seconds over the name of a function at the R console will open "bubble help" for it. If the function is defined in a script or another file that is open in the editor pane, one can directly navigate from the line where the function is called to where it is defined. In RStudio one can also search for help through the graphical interface. The R manuals can also be accessed most easily through the Help menu in RStudio or RGUI.

#### 2.3.4 Using R in a "batch job"

To run a script we need first to prepare a script in a text editor. Figure 2.5 shows the console immediately after running the script file shown in the text editor. As before, red text, the command <code>source("my-script.R")</code>, was typed by the user, and the blue text in the console is what was displayed by R as a result of this action. The title bar of the console, shows "R-console," while the title bar of the editor shows the <code>path</code> to the script file that is open and ready to be edited followed by "R-editor."

Mhen working at the command prompt, most results are printed by default.

```
D:\aphalo\Documents\Own_manuscripts\Books\using-r\scripts>Rscript my-script.R
Using libraries at paths:
- C:/Users/aphalo/Documents/R/win-library/3.3
- C:/Program Files/R/R-3.3.3/library
[1] "hello"
[1] 10.2

D:\aphalo\Documents\Own_manuscripts\Books\using-r\scripts>
```

#### FIGURE 2.6

Screen capture of the MS-Windows command console just after running the same script. Here we use Rscript to run the script; the exact syntax will depend on the operating system in use. In this case, R prints the results at the operating system console or shell, rather than in its own R console.

However, within scripts one needs to use function print() explicitly when a result is to be displayed.

A true "batch job" is not run at the R console but at the operating system command prompt, or shell. The shell is the console of the operating system—Linux, Unix, OS X, or MS-Windows. Figure 2.6 shows how running a script at the Windows command prompt looks. A script can be run at the operating system prompt to do time-consuming calculations with the output saved to a file. One may use this approach on a server, say, to leave a large data analysis job running overnight or even for several days.

Within RStudio desktop it is possible to access the operating system shell through the tab named "Terminal" and through the menu. It is also possible to run jobs in the background in tab "Background jobs", i.e., while simultaneously using the R console. This is made possible by concurrently running two or more instances of the R program.

# 2.4 Reproducible data analysis with R

Statistical concepts and procedures are not only important after data are collected but also crucial at the design stage of any data-based study. Rather frequently, we deal with existing data from the real world or from model simulations already at the planning stage of an experiment or survey. Statistics provides the foundation for the design of experiments and surveys, data analysis and data visualization.

This is similar to the role played by grammar and vocabulary to communication in a natural language like English. Statistics makes possible decision-making based on partial evidence (or samples), but it is also a means of communication. Data visualization also plays a key role in the written and oral communication of study conclussions. R is useful throughout all stages of the research process, from design of studies to communication of the results.

During recent years the lack of reproducibility in scientific research, frequently described as a *reproducibility crisis*, has been broadly discussed and analysed (Gandrud 2015). One of the problems faced when attempting to reproduce scientific and technical studies, is reproducing the data analysis. More generally, under any situation where accountability is important, from scientific research to decision making in commercial enterprises, industrial quality control and safety, and environmental impact assessments, being able to reproduce a data analysis reaching the same conclusions from the same data is crucial. Thus, an unambiguous description of the steps taken for an analysis is a requirement. Currently, most approaches to reproducible data analysis are based on automating report generation and including, as part of the report, all the computer commands used.

A reliable record of what commands have been run on which data is especially difficult to keep when issuing commands through menus and dialogue boxes in a graphical user interface or by interactively typing commands as text at a console. Even working interactively at the R console using copy and paste to include commands and results in a report typed in a word processor is error prone, and laborious. The use and archiving of R scripts alleviates this difficulty.

However, a further requirement to achieve reproducibility is the consistency between the saved and reported output and the R commands reported as having been used to produce them, saved separately when using scripts. This creates an error-prone step between data analysis and reporting. To solve this problem an approach to data analysis inspired in what is called *literate programming* (Knuth 1984), was developed: running an especially formatted script that produces a document, used to report the analysis, that includes the R code used for the analysis, the results of running this code and any explanatory text needed to describe the methodology used and interpret the results of the analysis.

Although a system capable of producing such reports with R, called 'Sweave' (Leisch 2002), has been available for a couple decades, it was rather limited and not supported by an IDE, making its use rather tedious. Package 'knitr' (Xie 2013) further developed the approach and together with its integration into RStudio made the use of this type of reports much easier. Less sophisticated reports, called R *notebooks*, formatted as HTML files can be created directly from ordinary R scripts containing no especial formatting. Notebooks are HTML files that show as text the code used interspersed with the results, and can contain embedded the actual source script used to generate them.

Package 'knitr' supports the writing of reports with the textual explanations encoded using either Markdown or Las markup for text-formatting instructions. While Markdown (https://daringfireball.net/projects/markdown/) is an easy to learn and use text markup approach, Las Lamport1994 is based on Tex@Knuth, the most powerful typesetting engine freely available. There are dif-

ferent flavours of Markdown, including R markdown (see https://rmarkdown.rstudio.com/) with special support for R code. Quarto (see https://quarto.org/) was recently released as an enhancement of R markdown (see https://rmarkdown.rstudio.com/), improving typesetting and styling and providing a single system capable of generating a broad selection of outputs. When used together with R, Quarto relies on package 'knitr' for the key step in the conversion, so in a strict sense Quarto does not replace it.

Because of the availability of these approaches to the generation of reports, the R language is extremely useful when reproducibility is important. Both 'knitr' and Quarto are powerful and flexible enough to write whole books, such as this very book you are now reading, produced with R, 'knitr' and LTFX. All pages in the book are generated directly, all plots and other R output included are generated by R and included automatically in the typeset version. All diagrams are generated by LTFXduring the typesetting step. The only exception are the figures in this chapter that have been manually captured from the computer screen. Why am I using this approach? First because I want to make sure that every bit of code as you will see printed, runs without error. In addition, I want to make sure that the output displayed below every line or chunk of R language code is exactly what R returns. Furthermore, it saves a lot of work for me as author, as I can just update R and all the packages used to their latest version, and build the book again, after any changes needed to keep it up to date and free of errors. By using these tools and markup in plain text files, the indices, cross-references, citations and list of references are all generated automatically.

Although the use of these tools is very important, they are outside the scope of this book and well described in other books dedicated to them (Gandrud 2015; Xie 2013). When using R in this way, a good command of R as a language for communication with both humans and computers is very useful.

### 2.5 Getting ready to use R

As the book is designed with the expectation that readers will run code examples as the read the text, you have to ensure access to the R before reading the next chapter. It is likely that your school, employer or teacher has already enabled access to R. If not, or if you are reading the book on your own, you should install R or secure access to an on-line service. Using RStudio or another IDE can facilitate the use of R, but all the code in the remaining chapters makes only use of R and packages available through CRAN. Chapters

I have written an R package, named 'learnrbook', containing original data and computer-readable listings for all code examples and exercises in the book. It also contains code and data that makes it easier to instal the packages used in later chapters. Its name is 'learnrbook' and is available through CRAN. It is not necessary for you to install this or any other packages until section 6.4.2 on page 179, where I explain how to install and use R R packages.

Further reading 21

Are there any resources to support the *Learn R: As a Language* book? Please, visit https://www.learnr-book.info/ to find additional material related to this book, including additional free chapters. Up-to-date instructions for software installation are provided on-line at this and other sites, as these instructions are likely to change after the publication of the book.

# • How to install the R program in my computer?

Installation of R varies depending on the operating system and computer hardware, and is in general similar to that of other software under a given operating system distribution. For most types of computer hardware the current version of R is available through the Comprehensive R Archive Network (CRAN) at https://cran.r-project.org/. Especially in the case of Linux distributions, R can frequently be installed as a component of the operating system distribution. There are some exceptions, such as the *R4Pi* distribution of R for the Raspberry Pi, which is maintained independently (https://r4pi.org/).

Installers for Linux, Windows and MacOS are available through CRAN (https://cran.r-project.org/) together with brief but up-to-date installation instructions.

# **1** How to install the **RStudio** IDE in my computer?

RStudio installers are available at Posit's web site (https://posit.co/products/open-source/rstudio/) of which the free version is suitable for running the code examples and exercises in the book. In many cases the IT staff at your employer or school will install them, or they may be already included in the default computer setup.

# **9** How to get access to RStudio as a cloud service?

An alternative, that is very well suited for courses or learning as part of a group is the RStudio cloud service, recently renamed Posit cloud (https://posit.co/products/cloud/cloud/). For individual use a free account is in many cases enough and for groups a low cost teacher's account works very well.

# 2.6 Further reading

Suggestions for further reading are dependent on how you plan to use R. If you envision yourself running batch jobs under Linux or Unix, you would profit from learning to write shell scripts. Because bash is widely used nowadays, *Learning the bash Shell* (Newham and Rosenblatt 2005) can be recommended. If you aim at writing R code that is going to be reused, and have some familiarity with C, C++ or Java, reading *The Practice of Programming* (Kernighan and Pike 1999) will provide a mostly language-independent view of programming as an activity and help you master the all-important tricks of the trade. The history of R, and its relation or S, is best told by those who were involved at early stages of its development, Chambers (2016, Chapter 2, and Ihaka (1998).

# Base R: "Words" and "Sentences"

The desire to economize time and mental effort in arithmetical computations, and to eliminate human liability to error, is probably as old as the science of arithmetic itself.

Howard Aiken *Proposed automatic calculating machine*, 1937; reprinted 1964

### 3.1 Aims of this chapter

In my experience, for those not familiar with computer programming languages, the best first step in learning the R language is to use it interactively by typing textual commands at the R *console*. This teaches not only the syntax and grammar rules, but also gives a glimpse at the advantages and flexibility of this approach to data analysis. In this chapter I focus on the different simple values or items that can be stored and manipulated in R, as well as the role of computer program statements, the equivalent of "sentences" in natural languages.

In the first part of the chapter we will use R to do everyday calculations that should be so easy and familiar that you will not need to think about the operations themselves. This easy start will give you a chance to focus on learning how to issue textual commands at the command prompt.

Later in the chapter, you will gradually need to focus more on the R language and its grammar and less on how commands are entered. By the end of the chapter you will be familiar with most of the kinds of simple "words" used in the R language and you will be able to read and write simple R statements.

Along the chapter, I will occasionally show the equivalent of the R code in mathematical notation. If you are not familiar with the mathematical notation, you can safely ignore the mathematics, as long as you understand the diagrams and the R code.

#### 3.2 Natural and computer languages

Computer languages have strict rules and interpreters and compilers that translate these languages into machine code are unforgiving about errors. They will issue error messages, but in contrast to human readers or listeners, will not guess your intentions and continue. However, computer languages have a much smaller set of words than natural languages, such as English. If you are new to computer programming, understanding the parallels between computer and natural languages may be useful.

One can think of constant values and variables (values stored under a name) as nouns and of operators and functions as verbs. A complete command, or statement, is the equivalent of a natural language sentence: "a comprehensible utterance." The simple statement a+1 has three components: a, a variable, +, an operator and 1 a constant. The statement sqrt(4) has two components, a function sqrt() and a numerical constant 4. We say that "to compute  $\sqrt{4}$  we *call* sqrt() with 4 as its *argument*."

Although all values manipulated in a digital computer are stored as *bits* in memory, multiple interpretations are possible. Numbers, letters, logical values, etc., can be encoded into bits and decoded as long as their type or mode is known. The concept of class is not directly related to how values are encoded when stored in computer memory, but instead on their interpretation as part of a computer program. We can have, for example, RGB color values, stored as three numbers such as 0, 0, 255, as hexadecimal numbers stored as characters #0000FF, or even use fancy names stored as character strings like "blue". We could create a class for colors using any of these representations, based on two different modes: numeric and character.

#### 3.3 Numeric values and arithmetic

When working in R with arithmetic expressions, the normal mathematical precedence rules are followed and parentheses can be used to alter this order. Parentheses can be nested, but in contrast to the usual practice in mathematics, the same parenthesis symbol is used at all nesting levels.

Both in mathematics and programming languages *operator precedence rules* determine which subexpressions are evaluated first and which later. Contrary to primitive electronic calculators, R evaluates numeric expressions containing operators according to the rules of mathematics. In the expression  $1 + 2 \times 3$ , the product  $2 \times 3$  has precedence over the addition, and is evaluated first, yielding as the result of the whole expression, 7. Similar rules apply to other operators, even those taking as operands non-numeric values.

The equivalent of the math expression

$$\frac{3+e^2}{\cos\pi}$$

is, in R, written as follows:

```
(3 + exp(2)) / cos(pi)
## [1] -10.38906
```

Where constant pi ( $\pi = 3.1415...$ ) and function cos() (cosine) are defined in base R. Many trigonometric and mathematical functions are available in addition to operators like +, -, \*, /, and ^.

In R angles are expressed in radians, thus  $\cos(\pi) = 1$  and  $\sin(\pi) = 0$ , according to trigonometry. Degrees can be converted into radians taking into account that the circle corresponds to  $2 \times \pi$  when expressed in radians and to  $360^{\circ}$  when expressed in degrees. Thus the cosine of an agle of  $45^{\circ}$  can be computed as follows.

```
sin(45/180 * pi)
## [1] 0.7071068
```

One thing to remember when translating fractions into R code is that in arithmetic expressions the bar of the fraction generates a grouping that alters the normal precedence of operations. In contrast, in an R expression this grouping must be explicitly signaled with additional parentheses.

If you are in doubt about how precedence rules work, you can add parentheses to make sure the order of computations is the one you intend. Redundant parentheses have no effect.

```
1 + 2 * 3

## [1] 7

1 + (2 * 3)

## [1] 7

(1 + 2) * 3

## [1] 9
```

The number of opening (left side) and closing (right side) parentheses must be balanced, and they must be located so that each enclosed term is a valid mathematical expression, i.e., code that can be evaluated to return a value, a value that can be inserted in place of the expression enclosed in parenthesis before evaluating the remaining of the expression. For example, (1 + 2) \* 3 after evaluating (1 + 2) becomes 3 \* 3 yielding 9. In contrast, (1 +) 2 \* 3 is a syntax error as 1 + is incomplete and does not yield a number.

3.1 In *playgrounds* the output from running the code in R are not shown, as these are exercises for you to enter at the R console and run. In general you should not skip them as in most cases playgrounds aim to teach or demonstrate concepts or features that I have *not* included in full-detail in the main text. You are strongly encouraged to *play*, in other words, create new variations of the examples and execute them to explore how R works.

```
1 + 1

2 * 2

2 + 10 / 5

(2 + 10) / 5

10^2 + 1

sqrt(9)

pi

sin(pi)

log(100)

log10(100)

log2(8)

exp(1)
```

Variables are used to store values. After we *assign* a value to a variable, we can use in our code the name of the variable in place of the stored value. The "usual" assignment operator is <-. In R, all names, including variable names, are case sensitive. Variables a and A are two different variables. Variable names can be long in R although it is not a good idea to use very long names. Here I am using very short names, something that is usually also a very bad idea. However, in the examples in this chapter where the stored values have no connection to the real world, simple names emphasize their abstract nature. In the chunk below, vct1 and vct2 are arbitrarily chosen variable names; I should have used names like height.cm or outside.temperature.c if they had been useful to convey information.

In the book, I use variable names that help recognize the kind of object stored, as this is most relevant when learning R. Here I use vct1 because in R, as we will see in page 28, numeric objects are always vectors, even when of length one.

```
vct1 <- 1
vct1 + 1
## [1] 2
vct1
## [1] 1
vct2 <- 10
vct2 <- vct1 + vct2
vct2
## [1] 11</pre>
```

Entering the name of a variable *at the R console* implicitly calls function print() displaying the stored value on the console. The same applies to any other statement entered *at the R console*: print() is implicitly called with the result of executing the statement as its argument.

```
vct1
## [1] 1
print(vct1)
## [1] 1
vct1 + 1
## [1] 2
print(vct1 + 1)
## [1] 2
```

3.2 There are some syntactically legal assignment statements that are not very frequently used, but you should be aware that they are valid, as they will not trigger error messages, and may surprise you. The most important thing is to write code consistently. The "backwards" assignment operator -> and resulting code like 1 -> vct1 are valid but less frequently used. The use of the equals sign (=) for assignment in place of <- although valid is discouraged. Chaining assignments as in the first statement below can be used to signal to the human reader that vct1, vct2 and vct3 are being assigned the same value.

```
VCT1 <- VCT2 <- VCT3 <- 0
VCT1
VCT2
VCT3
1 -> VCT1
VCT1
VCT1 = 3
VCT1
remove(VCT1, VCT2, VCT3) # cleanup
```

In R, all numbers belong to mode numeric (we will discuss the concepts of *mode* and *class* in section 3.8 on page 59). We can query if the mode of an object is numeric with function is.numeric(). The returned values are either TRUE or FALSE. These are logical values that will be discussed in section 3.5 on page 49.

```
mode(1)
## [1] "numeric"
vct1 <- 1
is.numeric(vct1)
## [1] TRUE</pre>
```

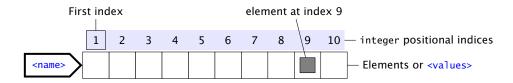
Because numbers can be stored in different formats, most computing languages implement several different types of numbers. In most cases R's numeric values can be used everywhere that a number is expected. However, in some cases it has advantages to explicitly indicate that we will store or operate on whole numbers, in which case we can use class integer, with integer constants indicated by a trailing capital "L," as in 32L.

```
is.numeric(1L)
## [1] TRUE
is.integer(1L)
## [1] TRUE
is.double(1L)
## [1] FALSE
```

Real numbers are a mathematical abstraction, and do not have an exact equivalent in computers. Instead of Real numbers, computers store and operate on numbers that are restricted to a broad but finite range of values and have a finite resolution. They are called, *floats* (or *floating-point* numbers); in R they go by the name of double and can be created with the constructor double().

```
is.numeric(1)
## [1] TRUE
is.integer(1)
## [1] FALSE
is.double(1)
## [1] TRUE
```

Vectors are one-dimensional in structure, of varying length and used to store similar values, e.g., numbers. They are different to the vectors, commonly used in Physics when describing directional forces, which are symbolized with an arrow as an "accent," such as  $\vec{\mathbf{F}}$ . In R numeric values and other atomic values are always vector s that can contain zero, one or more elements. The diagram below exemplifies a vector containing ten elements, also called members. These elements can be extracted using integer numbers as positional indices, and manipulated as described in more detail in section 3.10 on page 64.



Vectors, in mathematical notation, are similarly represented using positional indexes as subscripts,

$$a_{1...n} = a_1, a_2, \dots a_i, \dots, a_n,$$
 (3.1)

where  $a_{1...n}$  is the whole vector and  $a_1$  its first member. The length of  $a_{1...n}$  is n as it contains n members. In the diagram above n = 10.

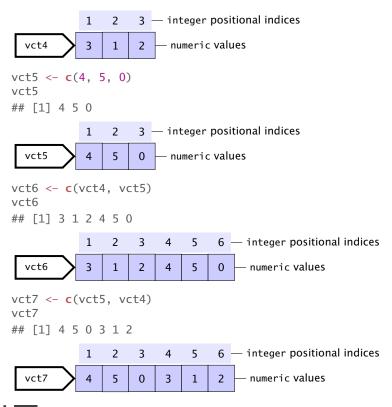
As you have seen above, the results of calculations were printed preceded with [1]. This is the index or position in the vector of the first number (or other value) displayed at the head of the current line. As in R single values are vectors of length one, when they are printed, they are also preceded with [1].

One can use function c() "concatenate" to create a vector from other vectors, including vectors of length 1, or even vectors of length 0, such as the numeric constants in the statements below. The first example shows an anonymous vector created, printed, and then automatically discarded.

```
c(3, 1, 2)
## [1] 3 1 2
```

To be able to reuse the vector, we assign it to a variable, giving a name to it. The length of a vector can be queried with function length(). We show below R code followed by diagrams depicting the structure of the vectors created.

```
vct4 <- c(3, 1, 2)
length(vct4)
## [1] 3
vct4
## [1] 3 1 2</pre>
```



# **?** How to create an empty vector?

```
numeric()
## numeric(0)
```

Next I show concatenation with a vector of the same class with length zero.

```
c(vct7, numeric())
## [1] 4 5 0 3 1 2
```

Function c() accepts as arguments two or more vectors and concatenates them, one after another. Quite frequently we may need to insert one vector in the middle of another. For this operation, c() is not useful by itself. One could use indexing combined with c(), but this is not needed as R provides a function capable of directly doing this operation. Although it can be used to "insert" values, it is named append(), and by default, it indeed appends one vector at the end of another.

```
append(vct4, vct5)
## [1] 3 1 2 4 5 0
```

The output above is the same as for c(a, b), however, append() accepts as an argument an index position after which to "append" its second argument. This results in an *insert* operation when the index points at any position different from the end of the vector.

```
append(vct4, values = vct5, after = 2)
## [1] 3 1 4 5 0 2
```

3.3 One can create sequences using function seq() or the operator:, or repeat values using function rep(). In this case, I leave to the reader to work out the rules by running these and his/her own examples, with the help of the documentation, available through help(seq) and help(rep).

```
-1:5
5:-1
seq(from = -1, to = 1, by = 0.1)
rep(-5, times = 4)
rep(1:2, length.out = 4)
```

**8** How to create a vector of zeros?

```
numeric(length = 10)
## [1] 0 0 0 0 0 0 0 0 0 0

or
rep(0, times = 10)
## [1] 0 0 0 0 0 0 0 0 0 0
```

Next, something that makes R different from most other programming languages: vectorized arithmetic. Operators and functions that are vectorized accept, as arguments, vectors of arbitrary length, in which case the result returned is equivalent to having applied the same function or operator individually to each element of the vector.

```
log10(100)
## [1] 2
log10(c(10, 5, 100, 200))
## [1] 1.00000 0.69897 2.00000 2.30103
```

Function sum() accepts vectors of different lengths as input but is not vectorized, as it always returns a vector of length one as result.

```
sum(100)
## [1] 100
sum(c(10, 5, 100, 200))
## [1] 315
```

A vectorized sum, also called a parallel sum of vectors, to differentiate it from obtaining the sum of the members of a vector, as computed above with function sum(), is the usual way in which operators like + and other arithmetic operators and functions work in R.

```
c(3, 1, 2) + c(1, 2, 31) ## [1] 4 3 33
```

Vectorized functions and operators that operate on more than one vector simultaneously, in many cases accept vectors of mismatched length as arguments or operands. When two or more vectors are of different length these functions and operators recycle the shorter vector(s) to match the length of the longest one. The two statements below are equivalent, in the first statement, the short vector 1 is recycled into c(1, 1, 1) and then the vectorized addition is done of the members at the same positions in the two vectors.

```
c(3, 1, 2) + 1
## [1] 4 2 3
c(3, 1, 2) + c(1, 1, 1)
## [1] 4 2 3
```

In the second code statement (line) below, vct4 is of length 3, but the numeric constant 2 is a vector of length 1, this short constant vector is extended, by recycling (replicating) its value, into a longer vector of ones—i.e., a vector of the same length as the longest vector in the statement, a.

```
vct4 <- c(3, 1, 2)
(vct4 + 1) * 2
## [1] 8 4 6
vct4 * 0:1
## Warning in vct4 * 0:1: longer object length is not a multiple of shorter
object length
## [1] 0 1 0
vct4 - vct4
## [1] 0 0 0</pre>
```

Make sure you understand what calculations are taking place in the chunk above, and also the one below. Vectorization and vector recycling are key features of the R language.

```
vct8 <- rep(1, 6)
vct8
## [1] 1 1 1 1 1 1 1
vct8 + 1:2
## [1] 2 3 2 3 2 3
vct8 + 1:3
## [1] 2 3 4 2 3 4
vct8 + 1:4
## warning in vct8 + 1:4: longer object length is not a multiple of shorter
object length
## [1] 2 3 4 5 2 3</pre>
```

- 3.4 Create further variants of the statements in the code chunk above to work out when a warning is issue and if in any case an error is triggered because of the length of the operands.
- Most functions defined in base R apply recycling to vectors passed as argument to at least some of their parameters. When recycling is supported, the conditions triggering warnings or errors are consistent with those you discovered in the playground above. However, if and how recycling is applied depends on how functions have been defined. Thus, there is variation, especially, but not only, in the case of functions and operators defined in contributed extension packages. For example, package 'tibble' and some other packages in the 'tidyverse' support recycling but some boundary cases that trigger a warning in base R functions, trigger an error in functions defined in these packages. See section 8.4.2 on page 245 about package 'tibble'.

As mentioned above, a vector can have a length of zero or more member values. Vectors of length zero may seem at first sight quite useless, but in fact they are very useful. They allow the handling of "no input" or "nothing to do" cases as normal cases, which in the absence of vectors of length zero would require to be treated as special cases. Constructors for R classes like numeric() return vectors of a length given by their first argument, which defaults to zero.

```
vct9 <- numeric(length = 0) # named argument
vct9
## numeric(0)
length(vct8)
## [1] 6
numeric() # default argument
## numeric(0)</pre>
```

Vectors of length zero, behave in most cases, as expected—e.g., they can be concatenated as shown here.

```
length(c(vct4, vct9, vct5))
## [1] 6
length(c(vct4, vct5))
## [1] 6
```

Many functions, such as R's maths functions and operators, will accept numeric vectors of length zero as valid input, returning also a vector of length zero, issuing neither a warning nor an error message. In other words, *these are valid operations* in R.

```
log(numeric(0))
## numeric(0)
5 + numeric(0)
## numeric(0)
```

Even when of length zero, vectors do have to belong to a class acceptable for the operation: 5 + character(0) is an error (character values are described in section 3.4 on page 41).

Passing as argument to parameter length a value larger than zero creates a longer vector filled with zeros in the case of numeric().

```
numeric(length = 5)
## [1] 0 0 0 0 0
```

The length of a vector can be explicitly increased, with missing values filled automatically with NA, the marker for not available.

```
vct10 <- 1:5
length(vct10) <- 10
vct10
## [1] 1 2 3 4 5 NA NA NA NA NA</pre>
```

If the length is decreased, the values in the *tail* of the vector are discarded.

```
vct11 <- 1:10
vct11
## [1] 1 2 3 4 5 6 7 8 9 10
length(vct11) <- 5
vct11
## [1] 1 2 3 4 5</pre>
```

There are some special values available for numbers. NA meaning "not available" is used for missing values. (NA) values play a very important role in the analysis of data, as frequently some observations are missing from an otherwise complete data set due to "accidents" during the course of an experiment or survey. It is important to understand how to interpret NA values: They are placeholders for something that is unavailable, in other words, whose value is *unknown*. NA values propagate when used, so that numerical computations yield NA when one or more input of the values is unknown.

```
vct12 <- c(NA, 5)
vct12
## [1] NA 5
vct12 + 1
## [1] NA 6
```

Calculations can also yield the following values NaN "not a number", Inf and -Inf for  $\infty$  and  $-\infty$ . As you will see below, calculations yielding these values do **not** trigger errors or warnings, as they are arithmetically valid. Inf and -Inf are also valid numerical values for input and constants.

```
vct12 + Inf
## [1] NA Inf
Inf / vct12
## [1] NA Inf
-1 / 0
## [1] -Inf
1 / 0
## [1] Inf
Inf / Inf
## [1] NaN
Inf + 4
## [1] Inf
-Inf * -1
## [1] Inf
```

3.5 When to use vectors of length zero, and when NAS? Make sure you understand the logic behind the different behavior of functions and operators with respect to NA and numeric() or its equivalent numeric(0). What do they represent? Why NA s are not ignored, while vectors of length zero are?

```
123 + numeric()
123 + NA
```

*Model answer:* NA values are used to signal a value that "was lost" or "was expected" but is unavailable because of some accident. A vector of length zero, represents no values, but within the normal expectations. In particular, if vectors are

expected to have a certain length, or if index positions along a vector are meaningful, then using NA is a must.

Any operation, even tests of equality, involving one or more NA's return an NA. In other words, when one input to a calculation is unknown, the result of the calculation is unknown. This means that a special function is needed for testing for the presence of NA values.

```
is.na(c(NA, 1))
## [1] TRUE FALSE
```

In the example above, we can also see that is.na() is vectorized, and that it applies the test to each of the elements of the vector individually, returning the result as TRUE or FALSE.

One thing to be aware of are the consequences of the fact that numbers in computers are almost always stored with finite precision and/or range: the expectations derived from the mathematical definition of Real numbers are not always fulfilled. See the box on page 35 for an in-depth explanation.

```
1 - 1e-20
## [1] 1
```

When using integer values these problems do not exist, as integer arithmetic is not affected by loss of precision in calculations restricted to integers. Because of the way integers are stored in the memory of computers, within the representable range, they are stored exactly. One can think of computer integers as a subset of whole numbers restricted to a certain range of values.

```
1L + 3L
## [1] 4
1L * 3L
## [1] 3
```

Using the "usual" division operator yields a floating-point double result, while the integer division operator %/% yields an integer result, and the modulo operator %% returns the remainder from the integer division.

```
1L / 3L

## [1] 0.33333333

1L %/% 3L

## [1] 0

1L %% 3L

## [1] 1
```

If as a result of an operation the result falls outside the range of representable values, the returned value is NA.

```
1000000L * 1000000L * 1000000L * 1000000L: NAs produced by integer overflow ## [1] NA
```

Both doubles and integers are considered numeric. In most situations, conversion is automatic and we do not need to worry about the differences between these two types of numeric values. The functions in the next chunk return TRUE or FALSE, i.e., logical values (see section 3.5 on page 49).

```
is.numeric(1L)
## [1] TRUE
is.integer(1L)
## [1] TRUE
is.double(1L)
## [1] FALSE
is.double(1L / 3L)
## [1] TRUE
is.numeric(1L / 3L)
## [1] TRUE
```

3.6 Study the variations of the previous example shown below, and explain why the two statements return different values. Hint: 1 is a double constant. You can use is.integer() and is.double() in your explorations.

```
1 * 1000000L * 1000000L
1000000L * 1000000L * 1
```

The usual way to store numerical values in computers is to reserve a fixed amount of space in memory for each value, which imposes limits on which numbers can be represented or not, and the maximum precision that can be achieved. The difference between integer amd double is explained on page 27. Integers, or "whole numbers", like R integer values are stored always with the same resolution such that the smallest difference between two integer values is 1. The amount of memory available to store an individual value creates a limit for the size of largest and smallest values that can be represented. Thus integers in R behave like Integers or whole numbers as defined in mathematics, but constrained to a restricted finite range of values. In computing languages like C different types of integer numbers are available short and long, these differ in the size of the space reserved for them in memory. R integer type is equivalent to long in C, thus the use of L for integer constant values like 5L.

Floating point numbers like R double values are stored in two parts: an integer *significand* and an integer *exponent*, each part using a fixed amount of space in memory. The relative resolution is constrained by the number of digits that can be stored in the significand while the absolute size of the largest and smallest numbers that can be represented is limited by the largest and smallest values that fit in the memory reserved for the exponent. In computing languages like C different types of floating point numbers are available, these differ in the size of the space reserved for them in memory. The properties of Real numbers as defined in mathematics differ from floating point numbers in assuming unlimited resolution and unlimited range of representable values.

In R, numbers that are not integers are stored as *double-precision floats*. Precision of numerical values in computers is usually symbolized by "epsilon" ( $\epsilon$ ), commonly abbreviated *eps*, defined as the largest value of  $\epsilon$  for which  $1 + \epsilon = 1$ . The finite resolution of floats can lead to unexpected results when testing for equality or inequality. Test for equality is done with operator ==. Use of this and other comparison operators is explained in section 3.6 on page 52.

```
1e20 == 1 + 1e20

## [1] TRUE

1 == 1 + 1e-20

## [1] TRUE

0 == 1e-20

## [1] FALSE
```

Another way of revealing the limited precision is during conversion to character.

```
format(5.123, digits = 16) # near maximun resolution
## [1] "5.123"
format(5.123, digits = 22) # more digits than in resolution
## [1] "5.123000000000000220268"
```

More likely to be a problem in real use of R is the accumulation of successive small losses in precision from multiple operations on R double values. Thus when computations involve both very large and very small numbers, the returned value can depend on the order of the operations. In practice ordinary users rarely need to be concerned about losses in precision except when testing for equality and inequality. On the other hand, finite resolution of double numerical values can explain why sometimes returned values for equivalent computations differ, and why some computation algorithms may be preferable, and others even fail, in specific cases.

As the R program can be used on different types of computer hardware, the actual machine limits for storing numbers in memory may vary depending on the type of processor and even the compiler used to build the R program executable. However, it is possible to obtain these values at run time, i.e., while the R is being used, from the variable .Machine, which is part of the R language. Please see the help page for .Machine for a detailed and up-to-date description of the available constants. Beware that when you run the examples below, the values returned by R in your own computer can differ from those returned in the computer I have used to typeset the book as you are reading it here.

```
.Machine$double.eps
## [1] 2.220446e-16
.Machine$double.neg.eps
## [1] 1.110223e-16
.Machine$double.max
## [1] 1024
.Machine$double.min
## [1] -1022
.Machine$double.base
## [1] 2
```

The last two values refer to the exponents of a base number or *radix*, 2, rather than the maximum and minimum size of numbers that can be handled as objects of class double. The maximum size of normalized double values, given by .Machine\$double.xmax, is much larger than the maximum value of integer values, given by .Machine\$integer.max.

```
.Machine$double.xmax
## [1] 1.797693e+308
.Machine$integer.max
## [1] 2147483647
```

As integer values are stored in machine memory without loss of precision, epsilon is not defined for integer values. In R not all out-of-range numeric values behave in the same way: while off-range double values are stored as -Inf or Inf and enter arithmetic as infinite values according the mathematical rules, off-range integer values become NA with a warning.

```
1e1026

## [1] Inf

1e-1026

## [1] 0

2147483699L

## [1] 2147483699
```

2147483600L + 99L

In those statements in the chunk below where at least one operand is double the integer operands are *promoted* to double before computation. A similar promotion does not take place when operations are among integer values, resulting in *overflow*, meaning numbers that are too big to be represented as integer values.

```
## Warning in 2147483600L + 99L: NAs produced by integer overflow
## [1] NA
2147483600L + 99
## [1] 2147483699
2147483600L * 2147483600L
## warning in 2147483600L * 2147483600L: NAs produced by integer overflow
## [1] NA
2147483600L * 2147483600
## [1] 4.611686e+18
```

The exponentiation operator ^ forces the promotion of its arguments to double, resulting in no overflow. In contrast, as seen above, the multiplication operator \* operates on integer values resulting in overflow.

```
2147483600L * 2147483600L * 2147483600L: NAs produced by integer overflow ## [1] NA 2147483600L^2L ## [1] 4.611686e+18
```

Both for display or as part of computations, we may want to decrease the number of significant digits or the number of digits after the decimal marker. Be aware that in the examples below, even if printing is being done by default, these functions return numeric values that are different from their input and can be stored and used in computations. Function round() is used to round numbers to a certain number of decimal places after or before the decimal marker, with a positive

or negative value for digits, respectively. In contrast, function signif() rounds to the requested number of significant digits, i.e., ignoring the position of the decimal marker.

```
round(0.0124567, digits = 3)
## [1] 0.012
signif(0.0124567, digits = 3)
## [1] 0.0125
round(1789.1234, digits = -1)
## [1] 1790
round(1789.1234, digits = 3)
## [1] 1789.123
signif(1789.1234, digits = 3)
## [1] 1790
vct13 <- 0.12345
vct14 <- round(vct13, digits = 2)</pre>
vct13 == vct14
## [1] FALSE
vct13 - vct14
## [1] 0.00345
vct14
## [1] 0.12
```

Functions are described in detail in section 6.2 on page 169. Here I describe them briefly in relation to their use. Functions are objects containing R code that can be used to perform an operation on data passed as argument to its parameters. They return the result of the operation as a single R object, or less frequently, as a side effect. Functions have a name like any other R object. If the name of a function followed by parentheses () and included in a code statement, it becomes a function *call* or a "request" for the code stored in the function object to be run. Many functions, accept R objects and/or constant values as *arguments* to their *formal parameters*. Formal parameters are placeholder names in the code stored in the function object, or the *definition* of the function. In a function call the code in its definition is evaluated (or run) with formal-parameter names taking the values passed as arguments to them.

In a function definition formal parameters can be assigned default values, which are used if no explicit argument is passed in the call. Arguments can be passed to formal parameters by name or by position. In most cases, passing arguments by name makes the code easier to understand and more robust against coding mistakes. In the examples in the book I most frequently pass arguments by name, except for the first parameter.

Being digits, the second parameter, its argument can also be passed by position.

```
round(0.0124567, digits = 3)
## [1] 0.012
round(0.0124567, 3)
## [1] 0.012
```

Functions trunc() and ceiling() return the non-fractional part of a numeric

value as a new numeric value. They differ in how they handle negative values, and neither of them rounds the returned value to the nearest whole number. Hint: you can use help(trunc) or trunc? at the R console, or the help tab of RStudio to find out the answer.

- 3.7 What does value truncation mean? Function trunc() truncates a numeric value, but it does not return an integer.
- Explore how trunc() and ceiling() differ. Test them both with positive and negative values.
- **Advanced** Use function abs() and operators + and to reproduce the output of trunc() and ceiling() for the different inputs.
- Can trunc() and ceiling() be considered type conversion functions in R?
- R supports complex numbers and arithmetic operations with class complex. As complex numbers rarely appear in user-written scripts I give only one example of their use. Complex numbers as defined in mathematics, have two parts, a real component and an imaginary one. Complex numbers can be used, for example, to describe the result of  $\sqrt{-1} = 1i$ .

```
cmp1 <- complex(real = c(-1, 1), imaginary = c(0, 0))
cmp1
## [1] -1+0i  1+0i
cmp2 <- sqrt(cmp1)
cmp2
## [1] 0+1i 1+0i
cmp2A2
## [1] -1+0i  1+0i</pre>
```

Instants in time and periods of time in computers are usually encoded as classes derived from integer, and thus considered in R as atomic classes and the objects vectors. Some of these encodings are standardized and supported by R classes POSIX1t and POSIXct. The computations based on times and dates are difficult because the relationship between local time at a given location and Universal Time Coordinates (UTC) has changed in time, as well as with changes in national borders. Packages 'lubridate' and 'anytime' support operations among time-related data and conversions between character strings and time and date classes easier and less error prone than when using base R functions. Thus I describe classes and operations related to dates and times in chapter 8 on page 241.

It is good to *remove* from the workspace objects that are no longer needed. We use function remove() to delete objects stored in the current workspace.

Arguments passed to remove() can be bare object names as shown here.

```
an.object <- 1:4
remove(an.object) # using a bare name</pre>
```

Function remove() also accepts the names of the objects as character strings. In spite of the name, the argument passed to parameter list must be a vector rather than a list (see section 3.4 on character and section 4.3 on list on pages 41 and 86).

```
an.object <- 5:2
remove(list = "an.object") # using a character vector</pre>
```

Function objects() returns a character vector containing the names of all objects visible in the current environment, or by passing an argument to parameter pattern, only the objects with names matching it.

In RStudio all objects are listed in the **Environment** tab and the search box of this tab can be used to find a given object.

Function remove() accepts both bare names of objects as in the chunk above and character strings corresponding to object names like in remove("any.object"). However, While objects() accept patterns to be matched to object names, remove() does not. Because of this, these two functions have to be used together for removing all objects with names that match a pattern. The pattern can be given as a regular expression (see section 3.4 on page 46).

Both functions have are available under short names matching those used in Linux and Unix for managing files: 1s() is a synonym of objects() and rm() of remove().

Using a simple pattern we obtain the names of all objects with names "vct1", "vct2", and so on. When using a pattern to remove objects, it is good to first use objects() on its own to get a list of the objects that would be deleted by calling remove() passing the names returned by objects() as argument for parameter list.

```
objects(pattern = "^vec.*")
## character(0)
```

The code below removes all objects with names "vct1", "vct2", and so on. We do this at the end of the section before reusing the same names in the code examples of the next section.

```
remove(list = objects(pattern = "^vct[[:digit:]]?"))
```

Similar code chunks are included at the end of each section throughout the book to ensure that code examples are self-contained by section. The chunk about is shown above as an example, but kept hidden in later sections.

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#### 3.4 Character values

In spite of the name character, values of this mode, are vectors of *character strings*". Character constants are written by enclosing characters strings in quotation marks, i.e., "this is a character string". There are three types of quotation marks in the ASCII character set, double quotes ", single quotes ', and back ticks `. The first two types of quotes can be used as delimiters of character constants.

```
vct1 <- "A"
vct1
## [1] "A"
vct2 <- 'A'
vct2
## [1] "A"
vct1 == vct2 # two variables holding character values, or named objects
## [1] TRUE
"A" == 'A' # two constant character values, or anonymous objects
## [1] TRUE</pre>
```

In many computer languages, vectors of characters are distinct from vectors of character strings. In these languages, character vectors store at each index position a single character, while vectors of character strings store at each index position strings of characters of various lengths, such as words or sentences. If you are familiar with C or C++, you need to keep in mind that C's char and R's character are not equivalent and that in R. In contrast to these other languages, in R there is no predefined class for vectors of individual characters and character constants enclosed in double or single quotes are not different.

Concatenating character vectors of length one does not yield a longer character string, it yields instead a longer vector of character strings.

```
vct3 <- 'ABC'
vct4 <- "bcdefg"
vct5 <- c("123", "xyz")
c(vct3, vct4, vct5)
## [1] "ABC" "bcdefg" "123" "xyz'</pre>
```

Having two different delimiters available makes it possible to choose the type of quotation marks used as delimiters so that other quotation marks can be easily included in a string.

```
"He said 'hello' when he came in"
## [1] "He said 'hello' when he came in"
'He said "hello" when he came in'
## [1] "He said \"hello\" when he came in"
```

The outer quotes are not part of the string, they are "delimiters" used to mark the boundaries. As you can see when b is printed special characters can be represented using "escape codes". There are several of them, and here we will show just four, new line  $(\n)$  and tab  $(\t)$ , " the escape code for a quotation mark within a string and the escape code for a single backslash  $\.$  We also show here the dif-

ferent behavior of print() and cat(), with cat() *interpreting* the escape sequences and print() displaying them as entered.

```
vct6 <- "abc\ndef\tx\"yz\"\\tm"
print(vct6)
## [1] "abc\ndef\tx\"yz\"\\tm"
cat(vct6)
## abc
## def x"yz"\ m</pre>
```

The *escape codes* work only in some contexts, as when using cat() to generate the output.

## **3** How to find the length of a character string?

While function length() returns the number of member character strings in a vector, function nchar() returns the number of characters in each string in the vector (see below for examples).

In the example below, function nchar() returns the number of characters in each member string.

```
nchar(x = "abracadabra")
## [1] 11
nchar(x = c("abracadabra", "workaholic", ""))
## [1] 11 10 0
```

To convert a string into upper case or lower case we use functions toupper() and tolower(), respectively.

```
toupper(x = "aBcD")
## [1] "ABCD"
tolower(x = "aBcD")
## [1] "abcd"
```

Function strtrim() trims a string to a maximum number of characters or width.

```
strtrim(x = "abracadabra", width = 6)
## [1] "abraca"
strtrim(x = "abra", width = 6)
## [1] "abra"
strtrim(x = c("abracadabra", "workaholic"), 6)
## [1] "abraca" "workah"
strtrim(x = c("abracadabra", "workaholic"), c(6, 3))
## [1] "abraca" "wor"
```

# **8** How to wrap long character strings?

Use R function strwrap() (see below for examples).

Function strwrap() edits a string to a maximum number of characters or width, by splitting it into a vector of shorter character strings. It can additionally insert a character string at the start or end of each of these new shorter strings.

```
strwrap(x = "This is a long sentence used to show how line wrap-
ping works.", width = 20)
## [1] "This is a long" "sentence used to" "show how line" "wrapping works."
```

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3.8 Function cat() prints a character vector respecting the embedded special characters such new line (encoded as \n) in character strings) and without issuing any additional new lines. Study the code below and the output it generates, consult the documentation of the two functions, and modify the example code until you are confident that you understand in detail how these tow functions work.

How to create a single character string from multiple shorter strings? While function c() is used to concatenate character vectors into longer vectors, function paste() is used to concatenate character strings into a single longer string (see below for examples).

Pasting together character strings has many uses, e.g., assembling informative messages to be printed, programmatically creating file names or file paths, etc. If we pass numbers, they are converted to character before pasting. The default separator is a space character, but this can be changed by passing a character string as argument for sep.

```
paste("n =", 3)
## [1] "n = 3"
paste("n", 3, sep = " = ")
## [1] "n = 3"
```

Pasting constants, as shown above, is of little practical use. In contrast, combining values stored in different variables is a very frequent operation when working with data. A simple use example follows. Assuming vector friends contains the names of friends and vector fruits the fruits they like to eat we can paste these values together into short sentences.

```
friends <- c("John ", "Yan ", "Juana ", "Mary ")
fruits <- c("apples", "lichees", "oranges", "strawberries")
paste(friends, "likes to eat ", fruits, ".", sep = "")
## [1] "John likes to eat apples." "Yan likes to eat lichees."
## [3] "Juana likes to eat oranges." "Mary likes to eat strawberries."</pre>
```

3.9 Why was necessary to pass sep = "" in the call to paste() in the example above? First try to predict what will happen and then remove, sep = "" from the statement above and run it to learn the answer. Try your own variations of the code until you understand the role of the separator string.

We can pass an additional argument to tell that the vector resulting from the paste operation is to be collapsed into a single character string. The argument passed to collapse is used as the separator. I use here cat() so that the newline character is obeyed in the display of the single character string.

```
cat(paste(friends, "likes to eat ", fruits, collapse = ".\n", sep = ""))
## John likes to eat apples.
```

```
## Yan likes to eat lichees.
## Juana likes to eat oranges.
## Mary likes to eat strawberries
```

When the vectors are of different length, the shorter one is recycled as many times as needed, which is not always what we want. In this case we need to first collapse the members of the long vector fruits to change this vector into a vector of length one. We can achieve this by nesting two calls to paste(), and passing an argument to collapse in the inner function call.

```
collapsed_fruits <- paste(fruits, collapse = ", ")
paste("My friends like to eat", collapsed_fruits, "and other fruits.")
## [1] "My friends like to eat apples, lichees, oranges, strawberries and other fruits."</pre>
```

Nesting of function calls is explained in section 5.5 on page 134. However, as the two statements above would in most cases be written as nested function calls, I add this example for reference.

```
paste("My friends like to eat", paste(fruits, col-
lapse = ", "), "and other fruits.")
## [1] "My friends like to eat apples, lichees, oranges, strawberries and other fruits."
```

Function strrep() repeats and pastes character strings, while rep() repeats character strings into vectors.

```
rep(x = "ABC", times = 3)
## [1] "ABC" "ABC" "ABC"
strrep(x = "ABC", times = 3)
## [1] "ABCABCABC"
strrep(x = "ABC", times = c(2, 4))
## [1] "ABCABC" "ABCABCABCABCABC"
strrep(x = c("ABC", "X"), times = 2)
## [1] "ABCABC" "XX"
strrep(x = c("ABC", "X"), times = c(2, 5))
## [1] "ABCABC" "XXXXXX"
```

How to trim leading and/or trailing white space in character strings? Use function trimws() (see below for examples).

Trimming leading and trailing white space is a frequent operation. R function trimws() implements this operation as shown below.

```
trimws(x = " two words ")
## [1] "two words"
trimws(x = c(" eight words and a newline at the end\n", " two words "))
## [1] "eight words and a newline at the end"
## [2] "two words"
```

3.10 Function trimws() has additional parameters that make it possible to select which end of the string is trimmed and which characters are considered whitespace. Use help(trimws) to access the help and study this documentation. Modify the example above so that only trailing white space is removed, and so that the newline character \n is not considered whitespace, and thus not trimmed away.

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Within character strings, substrings can be extracted and replaced *by position* using substring() or substr().

For extraction we can pass to x a constant as shown below or a variable.

```
substr(x = "abracadabra", start = 5, stop = 9)
## [1] "cadab"
substr(x = c("abracadabra", "workaholic"), start = 5, stop = 11)
## [1] "cadabra" "aholic"
```

Replacement is done *in place*, by having function substr() on the left hand side (lhs) of the assignment operator <-. Thus, the argument passed to parameter x of substr() must in this case be a variable rather than a constant. This is a substitution character by character, not insertion, so the number of characters in the string passed as argument to x remains unchanged, i.e., the value returned by nchar() does not change.

```
vct7 <- c("abracadabra", "workaholic")
substr(x = vct7, start = 5, stop = 9) <- "xxx"
vct7
## [1] "abraxxxabra" "workxxxlic"</pre>
```

If we pass values to both start and stop then only part of the value on the *rhs* of the assignment operator <- may be used.

```
vct8 <- c("abracadabra", "workaholic")
substr(x = vct8, start = 5, stop = 6) <- "xxx"
vct8
## [1] "abraxxdabra" "workxxolic"</pre>
```

3.11 Frequently, a very effective way of learning how a function behaves, is to experiment. In the example below, we set start and stop delimiting more characters than those in "xxx". In this case, is "xxx" extended, or start or stop ignored? Run this "toy example" to find out the answer.

```
VCT1 <- c("abracadabra", "workaholic")
substr(x = VCT1, start = 5, stop = 11) <- "xxx"
VCT1
remove(VCT1) # clean up</pre>
```

As in R each character value is a string comprised by zero to many characters, in addition to comparisons based on whole strings or values, partial matches among them are of interest.

To substitute part of a character string *by matching a pattern*, we can use functions sub() or gsub(). The first example uses three character constants, but values stored in variables can also be passed as arguments.

```
sub(pattern = "ab", replacement = "AB", x = "about")
## [1] "ABout"
```

The difference between sub() (substitution) and gsub() (global substitution) is that the first replaces only the first match found while the second replaces all matches.

```
sub(pattern = "ab", replacement = "x", x = "abracadabra")
## [1] "xracadabra"
gsub(pattern = "ab", replacement = "x", x = "abracadabra")
## [1] "xracadxra"
```

3.12 Functions sub() or gsub() accept character vectors as argument for parameter x. Run the two statements below and study how the values returned differ.

```
sub(pattern = "ab", replacement = "x", x = c("abra", "cadabra"))
gsub(pattern = "ab", replacement = "x", x = c("abra", "cadabra"))
```

Function grep() returns indices to the values in a vector matching a pattern, or alternatively, the matching values themselves.

```
grep(pattern = "C", x = c("R", "C++", "C", "Perl", "Pascal"))
## [1] 2 3
grep(pattern = "C", x = c("R", "C++", "C", "Perl", "Pascal"), value = TRUE)
## [1] "C++" "C"
grep(pattern = "C", x = c("R", "C++", "C", "Perl", "Pascal"), ignore.case = TRUE)
## [1] 2 3 5
```

Function grep1() is a variation of grep() that returns a vector of logical values instead of numeric indices to the matching values in x.

```
grepl(pattern = "C", x = c("R", "C++", "C", "Perl", "Pascal"))
## [1] FALSE TRUE TRUE FALSE FALSE
grepl(pattern = "C", x = c("R", "C++", "C", "Perl", "Pascal"), ignore.case = TRUE)
## [1] FALSE TRUE TRUE FALSE TRUE
```

In the examples above the arguments for pattern strings matched exactly their targets. In R and other languages *regular expressions* are used to concisely describe more elaborate and conditional patterns. Regular expressions themselves are encoded as character strings, where some characters and character sequences have special meaning. This means that when a pattern should be interpreted literally rather than specially, fixed = TRUE should be passed in the call. This in addition, ensures faster computation. In the examples above, the patterns used contained no characters with special meaning, thus, the returned value is not affect by passing fixed = TRUE as done here.

```
sub(pattern = "ab", replacement = "AB", x = "about", fixed = TRUE)
## [1] "ABout"
```

Regular expressions are used in Unix and Linux shell scripts and programs, and are part of Perl, C++ and other languages in addition to R. This means that variations exist on the same idea, with R supporting two variations of the syntax. A description of R regular expressions can be accessed with help(regex). We here describe R's default syntax.

Regular expressions are concise, terse and extremely powerful. They are a language in themselves. However, the effort needed to learn their use more than pays back. I will show examples of the use, rather than systematically describe them. I will use gsub() for these examples, but several other R functions including grep() and grep1() accept regular expressions as patterns.

In a regular expression | separates alternative matching patterns.

```
gsub(pattern = "ab|t", replacement = "123", x = "about")
## [1] "123ou123"
```

Within a regular expression we can group characters within [ ] as alternative, e.g, [0123456789], or [0–9] matches any digit.

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Character ^ indicates that the match must be at the "head" of the string, and \$ that the match should be at its "tail".

```
gsub(pattern = "^a[0123456789]",
    replacement = "ab",
    x = c("alout", "a9out", " a3out"))
## [1] "about" "about" " a3out"
```

The replacement can be an empty string.

A dot (.) matches any character. In this example we replace the last character with "".

3.13 How would you modify the last code example above to edit c("about", "axout", "a3outx") into c("about", "axout", "a3out")? Think of different ways of doing this using regular expressions.

The number of matching characters can be indicated with + (match 1 or more times), ? (match 0 or 1 times), \* (match 0 or more times) or even numerically. Matching is in most cases "greedy".

Several named classes of characters are predefined, for example [:lower:] for lower case alphabetic characters according to the current locale (see page 48). In the regular expression in the example below, [:lower:] replaces only a-z, thus we need to keep the outer square brackets. While a-z includes only the unaccented letters, [:lower:] does include additional characters such as ä, ö, or é if they are in use in the current locale. In the case of [:digit:] and 0-9, they are equivalent.

With parentheses we can isolate part of the matched string and reuse it in the replacement with a numeric back-reference. Up to a maximum of nine pairs of parentheses can be used.

```
gsub(pattern = "\land.([0-9])[a-z]*$",
replacement = "gone with \1",
```

3.14 Run the two statements below, study the returned values by creating variations of the patterns and explain why the returned values differ.

Splitting of character strings based on pattern matching is a frequently used operation, e..g., treatment labels containing information about two different treatment factors need to be split into their components before data analysis. Function strsplit() has an interface consistent with grep(). In the examples we will split strings containing date and time of day information in different ways.

```
strsplit(x = "2023-07-29 10:30", split = " ")
## [[1]]
## [1] "2023-07-29" "10:30"
```

Using a simple regular expression we can extract individual strings representing the numbers.

```
strsplit(x = "2023-07-29 10:30", split = " |-|:")
## [[1]]
## [1] "2023" "07" "29" "10" "30"
```

The argument to split is by default interpreted as a regular expression, but as discussed above we can pass fixed = TRUE to prevent this.

One needs to be aware that the part of the string matched by the regular expression is not included in the returned vectors. If the regular expression matches more than what we consider a separator, the returned values may be surprising.

```
strsplit(x = "2023-07-29", split = "-[0-9]+$")
## [[1]]
## [1] "2023-07"
```

When the argument passed to x is a vector with multiple member strings, the returned value is a list of character vectors. This list contains as many character vectors as members had the vector passed as argument to x, each vector the result of splitting one character string in the input. (Lists are described in section 4.3 on page 86.)

```
strsplit(x = c("2023-07-29 10:30", "2023-07-29 19:17"), split = " ")
## [[1]]
## [1] "2023-07-29" "10:30"
##
## [[2]]
## [1] "2023-07-29" "19:17"
```

The ASCII character set is the oldest and simplest in use. In contains only 128 characters including non-printable characters. These characters support the English language. Several different extended versions with 256 characters pro-

vided support for other languages, mostly by adding accented letters and some symbols. The 128 ASCII characters were for a long time the only consistently available across computers set up for different languages and countries (or *locales*). Recently the use of much larger character sets like UTF8 has become common. Since R version 4.2.0 support for UTF8 is available under Windows 10. This makes it possible the processing of text data for many more languages than in the past. Even though now it is possible to use non-ASCII characters as part of object names, it is anyway safer to use only ASCII characters as this support is recent.

The extended character sets include additional characters, that are distinct but may produce glyphs that look very similar to those in the ASCII set. One case are em-dash (—), en-dash (-), minus sign (—) and regular dash (-) which are all different characters, with only the last one recognized by R as the minus operator. For those copying and pasting text from a word-processor into R or RStudio, a frequent difficulty is that even if one types in an ASCII quote character ("), the opening and closing quotes in many languages are automatically replaced with non-ASCII ones ("and") which R does not accept as character string delimiters. The best solution is to use a plain text editor instead of a word processor when writing scripts or editing text files containing data to be read as code statements or numerical data.

A locale definition determines not only the language, and character set, but also date, time, and currency formats.

## 3.5 Logical values and Boolean algebra

What in Mathematics are usually called Boolean values, are called logical values in R. They can have only two values true and false, in addition to NA (not available). Logical values true and false should not be confused with text strings, they are names for the two conditions that can be stored. Logical values are always vectors as all other atomic types in R (by *atomic* we mean that each value is not composed of "parts").

Logical values are rarely used to store data from experiments or surveys. They are used mostly to keep track of binary conditions, like results from comparisons in a script and to operate on them. Most frequent uses of logical values do not involve their storage in user-created variables. Most comparisons or tests return a logical value and Boolean algebra makes it possible to combine the results from multiple tests or conditions into a single combined outcome or binary decision, i.e., TRUE or False, Yes or No. (See section 3.6 on page 52 for examples.)

In mathematics, Boolean algebra provides the rules of the logic used to combine multiple logical values. Boolean operators like AND and OR take as operands logical values and return a logical value as a result. In R there are two "families" of Boolean operators, vectorized and not vectorized. Vectorized operators accept logical vectors of any length as operands, while non vectorized ones accept only log-

ical vectors of length one as operands. In the chunk below we use non-vectorized operators with two logical vectors of length one, a and b, as operands.

```
vct1 <- TRUE
mode(vct1)
## [1] "logical"
vct1
## [1] TRUE
!TRUE # negation
## [1] FALSE
TRUE && FALSE # logical AND
## [1] FALSE
TRUE || FALSE # logical OR
## [1] TRUE
xor(TRUE, FALSE) # exclusive OR
## [1] TRUE</pre>
```

The availability of two kinds of logical operators can be troublesome for those new to R. Pairs of "equivalent" logical operators behave differently, use similar syntax and use similar symbols! The vectorized operators have single-character names, & and | (similarly to vectorized arithmetic operators like +), while the non-vectorized ones have double-character names, && and ||. There is only one version of the negation operator! that is vectorized. In recent versions of R, an error is triggered when a non-vectorized operator is used with a vector with length > 1, which helps prevent mistakes. In some situations, vectorized logical operators can replace non-vectorized ones, but it is important to use the ones that match the intention of the code, as this enables relevant checks for mistakes. Once the distinction is learnt, using the most appropriate operators also contributes to make code easier to read.

```
c(TRUE, FALSE) & c(TRUE,TRUE) # vectorized AND
## [1] TRUE FALSE
c(TRUE, FALSE) | c(TRUE,TRUE) # vectorized OR
## [1] TRUE TRUE
```

Functions any() and all() take zero or more logical vectors as their arguments, and return a single logical value "summarizing" the logical values in the vectors. Function all() returns TRUE only if all values in the vectors passed as arguments are TRUE, and any() returns TRUE unless all values in the vectors are FALSE.

```
vct2 <- c(TRUE, FALSE, FALSE)
any(vct2)
## [1] TRUE
all(vct2)
## [1] FALSE
any(c(TRUE, FALSE) & c(TRUE,TRUE))
## [1] TRUE
all(c(TRUE, FALSE) & c(TRUE,TRUE))
## [1] FALSE
any(c(TRUE, FALSE) | c(TRUE,TRUE))
## [1] TRUE
all(c(TRUE, FALSE) | c(TRUE,TRUE))
## [1] TRUE</pre>
```

Another important thing to know about logical operators is that they "short-cut" evaluation. If the result is known from the first part of the statement, the rest of the statement is not evaluated. Try to understand what happens when you enter the following commands. Short-cut evaluation is useful, as the first condition can be used as a guard protecting a later condition from being evaluated when it would trigger an error.

```
TRUE || NA
## [1] TRUE
FALSE || NA
## [1] NA
TRUE && NA
## [1] NA
FALSE && NA
## [1] FALSE
TRUE && FALSE && NA
## [1] FALSE
TRUE && TRUE && NA
## [1] NA
```

3.15 Investigate how swapping the order of the operands in the code chunk above affects the values returned, e.g., the first statement becomes NA || TRUE.

When using the vectorized operators on vectors of length greater than one, 'short-cut' evaluation still applies for the result obtained at each index position.

```
c(TRUE, FALSE) & c(TRUE,TRUE) & NA
## [1] NA FALSE
c(TRUE, FALSE) & c(TRUE,TRUE) & c(NA, NA)
## [1] NA FALSE
c(TRUE, FALSE) | c(TRUE,TRUE) | c(NA, NA)
## [1] TRUE TRUE
```

3.16 Based on the description of "recycling" presented on page 31 for numeric operators, explore how "recycling" works with vectorized logical operators. Create logical vectors of different lengths (including length one) and *play* by writing several code statements with operations on them. To get you started, one example is given below. Execute this example, and then create and run your own, making sure that you understand why the values returned are what they are. Sometimes, you will need to devise several examples or test cases to tease out of R an understanding of how a certain feature of the language works, so do not give up early, and make use of your imagination!

```
c(TRUE, FALSE, TRUE, NA) & FALSE
c(TRUE, FALSE, TRUE, NA) | c(TRUE, FALSE)
```

How to test if a vector contains no values other than NA (or NAN) values? A call to is.na() returns a logical vector that we can pass to all(). We can save the intermediate vector temp and pass it as argument to is.na(), or alternatively nest the function calls. The name tmp, for *temporary*, is frequently used for variables whose value is retrieved only once.

```
vct2 <- rep(NA, 5) # toy data
tmp <- is.na(vct2) # tmp for temporary
all(tmp)
## [1] TRUE
all(is.na(vct2)) # nested call
## [1] TRUE</pre>
```

## How to test if a vector contains one or more NA (or NAN) values?

See previous question. We only need to replace all() by any() to obtain the answer.

```
vct2 <- rep(NA, 5)
any(is.na(vct2))
## [1] TRUE</pre>
```

#### 3.6 Comparison operators and operations

Comparison operators return vectors of logical values (see section 3.5 on page 49), with values TRUE or FALSE depending on the outcome.

Equality (==) and inequality (!=) operators are defined not only for numeric values but also for character and most other atomic and many other values. Be aware that operator = is an infrequently used synonym of the assignment operator <- rather than a comparison operator!

```
# be aware that we use two = symbols
"abc" == "ab"
## [1] FALSE
"ABC" == "abc"
## [1] FALSE
"abc" != "ab"
## [1] TRUE
"ABC" != "abc"
## [1] TRUE
```

In the case of numeric values additional comparisons are meaningful and additional operators are defined.

```
1.2 > 1.0

## [1] TRUE

1.2 >= 1.0

## [1] TRUE

1.2 == 1.0

## [1] FALSE

1.2 != 1.0

## [1] TRUE

1.2 <= 1.0

## [1] FALSE

1.2 < 1.0

## [1] FALSE
```

These operators can be used on vectors of any length, returning as a result a logical vector as long as the longest operand. In other words, they behave in the same way as the arithmetic operators described on page 30: their arguments are recycled when needed. Hint: if you do not know what value is stored in numeric vector a, use print(a) after the first code statement below to see its contents.

```
vct3 <- 1:10
vct3 > 5
## [1] FALSE FALSE FALSE FALSE TRUE TRUE TRUE TRUE TRUE
vct3 < 5
## [1] TRUE TRUE TRUE TRUE FALSE FALSE FALSE FALSE FALSE
vct3 == 5
  [1] FALSE FALSE FALSE TRUE FALSE FALSE FALSE FALSE
all(vct3 > 5)
## [1] FALSE
any(vct3 > 5)
## [1] TRUE
vct4 <- vct3 > 5
vct4
## [1] FALSE FALSE FALSE FALSE TRUE TRUE TRUE TRUE TRUE
any(vct4)
## [1] TRUE
all(vct4)
## [1] FALSE
```

Individual comparisons can be useful, but their full role in data analysis and programming is realized when we combine multiple tests using the operations of the Boolean algebra described in section 3.5 on page 49.

For example to test if members of a numeric vector are within a range, in our example, -1 to +1, we can combine the results from two comparisons using the vectorized logical AND operator &, and use parentheses to override the default order of precedence of the operations.

```
vct5 <- -2:3
vct5 >= -1 & vct5 <= 1
## [1] FALSE TRUE TRUE TRUE FALSE FALSE</pre>
```

If we want to find those values outside this same range, we can negate the test.

```
!(vct5 >= -1 & vct5 <= 1)
## [1] TRUE FALSE FALSE TRUE TRUE
```

Or we can combine another two comparisons using the vectorized logical *OR* operator |.

```
vct5 < -1 | vct5 > 1
## [1] TRUE FALSE FALSE FALSE TRUE TRUE
```

In some cases an additional advantage is that logical values require less space in memory for their storage than numeric values.

3.17 Use the statement below as a starting point in exploring how precedence works when logical and arithmetic operators are part of the same statement. *Play* with the example by adding parentheses at different positions and based on the

returned values, work out the default order of operator precedence used for the evaluation of the example given below.

```
vct6 <- 1:10
vct6 > 3 | vct6 + 2 < 3
```

It is important to be aware of the consequences of "short-cut evaluation" (described on page 51). The behavior of many of base-R's functions when NAS are present in their input arguments can be modified. TRUE passed as an argument to parameter na.rm, results in NA values being *removed* from the input **before** the function is applied.

```
vct7 <- c(1:10, NA)
all(vct7 < 20)
## [1] NA
any(vct7 > 20)
## [1] NA
all(vct7 < 20, na.rm=TRUE)
## [1] TRUE
any(vct7 > 20, na.rm=TRUE)
## [1] FALSE
```

In many situations, when writing programs one should avoid testing for equality of floating point numbers ('floats'). This is because of how numbers are stored in computers (see the box on page 35 for an in-depth explanation). Here I show how to gracefully handle rounding errors when using comparison operators. As rounding errors may accumulate, in practice .Machine\$double.eps is frequently too small a value to safely use in tests for "zero.". Whenever possible according to the logic of the calculations, it is best to test for inequalities, for example using  $x \le 1.0$  instead of x == 1.0. If this is not possible, then equality tests should be done by replacing tests like x == 1.0 with abs (x - 1.0) < k, where k is a number larger than eps. Function abs () returns the absolute value, in simpler words, makes all values positive or zero, by changing the sign of negative values, or in mathematical notation |x| = |-x|.

```
sin(pi) == 0 # angle in radians, not degrees!
## [1] FALSE
sin(2 * pi) == 0
## [1] FALSE
abs(sin(pi)) < 1e-15
## [1] TRUE
abs(sin(2 * pi)) < 1e-15
## [1] TRUE
sin(pi)
## [1] 1.224606e-16
sin(2 * pi)
## [1] -2.449213e-16</pre>
```

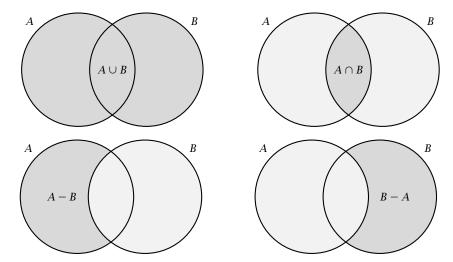


FIGURE 3.1

Boolean algebra. Venn diagrams for algebra of sets operations: union,  $\cup$ , union(); intersection,  $\cap$ , intersect(); difference (asymmetrical), -, setdiff(); equality test setequal(); membership, is.element() and operator %in%

#### 3.7 Sets and set operations

The R language supports set operations on vectors. They can be useful in many different contexts when manipulating and comparing vectors of values. In Bioinformatics it is usual, for example, to make use of character vectors of gene tags. Algebra sets is implemented with functions union(), intersect(), setdiff(), setequal(), is.element() and operator %in% (Figure 3.1). The first three operations return a vector of the same mode as their inputs, and the last three a logical vector. The action of the first three operations is most easily illustrated with Venn diagrams, where the returned value (or result of the operation) is depicted in darker grey.

Set operations applied to vectors with values representing a mundane example, grocery shopping, demonstrate them.

```
fruits <- c("apple", "pear", "orange", "lemon", "tangerine")
bakery <- c("bread", "buns", "cake", "cookies")
dairy <- c("milk", "butter", "cheese")
shopping <- c("bread", "butter", "apple", "cheese", "orange")
intersect(fruits, shopping)
## [1] "apple" "orange"
intersect(bakery, shopping)
## [1] "bread"
intersect(dairy, shopping)
## [1] "butter" "cheese"
"lemon" %in% dairy
## [1] FALSE</pre>
```

```
"lemon" %in% fruits
## [1] TRUE
dairy %in% shopping
## [1] FALSE TRUE TRUE
union(bakery, dairy)
## [1] "bread" "buns" "cake" "cookies" "milk" "butter" "cheese"
setdiff(union(bakery, dairy), shopping) # nested call
## [1] "buns" "cake" "cookies" "milk"
```

Sets describe membership as a binary property, thus when vectors are interpreted as sets, duplicate members are redundant. Duplicate members although accepted as input are always simplified in the returned values.

```
union(c("a", "a", "b"), c("b", "a", "b")) # set operation
## [1] "a" "b"
setequal(c("a", "a", "b"), c("b", "a", "b")) # sets compared
## [1] TRUE
all.equal(c("a", "a", "b"), c("b", "a", "b")) # vectors compared
## [1] "1 string mismatch"
identical(c("a", "a", "b"), c("b", "a", "b")) # vectors compared
## [1] FALSE
```

We construct and save a character vector to use in the next examples.

```
vct1 <- c("a", "b", "c", "b")
```

To test if a given value belongs to a set, we use operator %in% or its function equivalent is.element(). In the algebra of sets notation, this is written  $a \in A$ , where A is a set and a a member. The second statement shows that the %in% operator is vectorized on its left-hand-side (lhs) operand, returning a logical vector.

```
is.element("a", vct1)
## [1] TRUE
"a" %in% vct1
## [1] TRUE
c("a", "a", "z") %in% vct1
## [1] TRUE TRUE FALSE
```

Keep in mind that inclusion, implemented in operator %in%, is an asymmetrical (not reflective) operation among a vector and a set. The right-hand-side (rhs) argument is interpreted as a set, while the left-hand-side (lhs) argument is interpreted as a vector of values to test for membership in the set. In other words, any duplicate member in the lhs operand is retained and tested while the rhs operand is interpreted as a set of unique values. The returned logical vector has the same length as the lhs operand.

```
vct1 %in% "a"
## [1] TRUE FALSE FALSE FALSE
```

The negation of inclusion is  $a \notin A$ , and coded in R by applying the negation operator! to the result of the test done with %in% or function is.element().

```
!is.element("a", vct1)
## [1] FALSE
```

```
!"a" %in% vct1
## [1] FALSE
!c("a", "a", "z") %in% vct1
## [1] FALSE FALSE TRUE
```

Although inclusion is a set operation, it is also very useful for the simplification of if () ... else statements by replacing multiple tests for alternative constant values of the same mode chained by multiple | operators. A useful property of %in% and is.element() is that they never return NA.

Operator %in% is equivalent to function match(), although the additional parameters of match() provide additional flexibility.

In some cases, such as when accepting partial character strings as input, the aim is not an exact match, but a partial match to target character strings. In this case, either charmatch() or pmatch() is the correct tool to use depending on the desired handling of partial, ambiguous and exact matches. Use help() to find the details if you need to use one of them.

3.18 Use operator %in% to write more concisely the following comparisons. Hint: see section 3.5 on page 49 for the difference between | and || operators.

```
vct2 <- c("a", "a", "z")
vct2 == "a" | vct2 == "b" | vct2 == "c" | xvct2 == "d"
```

Convert the logical vectors of length 3 into a vector of length one. Hint: see help for functions all() and any().

With unique() we convert a vector of possibly repeated values into a set of unique values. In the algebra of sets, a certain object belongs or not to a set. Consequently, in a set, multiple copies of the same object or value are meaningless.

```
unique(vct1)
## [1] "a" "b" "c"
```

Function unique() is frequently useful, for example when we want determine the number of distinct values in a vector.

```
length(unique(vct1))
## [1] 3
```

**3.19** Do the values returned by these two statements differ?

```
c("a", "a", "z") %in% vct1
c("a", "a", "z") %in% unique(vct1)
```

Function duplicated() is the counterpart of unique(), returning a logical vector indicating which values in a vector are duplicates of values already present at positions with a lower index.

```
duplicated(vct1)
## [1] FALSE FALSE FALSE TRUE
anyDuplicated(vct1)
## [1] 4
```

The R language includes many functions that simplify tasks related to data analysis. Some are well known like unique(), but others may need to be searched for in the documentation.

3.20 What do you expect to be the difference between the values returned by the three statements in the code chunk below? Before running them, write down your expectations about the value each one will return. Only then run the code. Independently of whether your predictions were correct or not, write down an explanation of what each statement's operation is.

```
union(c("a", "a", "z"), vct1)
c(c("a", "a", "z"), vct1)
c("a", "a", "z", vct1)
```

Are set union and concatenation of vectors equivalent operations? why or why not?

All set algebra examples above use character vectors and character constants. This is just the most frequent use case. Sets operations are valid on vectors of any atomic class, including integer, and computed values can be part of statements. In the second and third statements in the next chunk, we need to use additional parentheses to alter the default order of precedence between arithmetic and set operators.

```
9 %in% 2:4

## [1] FALSE

9 %in% ((2:4) * (2:4))

## [1] TRUE

c(1, 16) %in% ((2:4) * (2:4))

## [1] FALSE TRUE
```

*Empty sets* are an important component of the algebra of sets, in R they are represented as vectors of zero length. These vectors do belong to a class such as numeric or character and must be compatible with other operands in an expression.

```
c("ab", "xy") %in% character()
## [1] FALSE FALSE
character() %in% c("a", "b", "c")
## logical(0)
union("ab", character())
## [1] "ab"
```

Although set operators are defined for numeric vectors, rounding errors in 'floats' can result in unexpected results (see section 3.3 on page 35).

```
c(cos(pi), sin(pi)) %in% c(0, -1)
## [1] TRUE FALSE
c(cos(pi), sin(pi))
## [1] -1.000000e+00 1.224606e-16
```

**3.21** In the algebra of sets notation  $A \subseteq B$ , where A and B are sets, indicates that A is a subset or equal to B. For a true subset, the notation is  $A \subset B$ . The operators with the reverse direction are  $\supseteq$  and  $\supset$ . Implement these four operations in four R statements, and test them on sets (represented by R vectors) with different "overlap" among set members.

## 3.8 The 'mode' and 'class' of objects

Classes are abstractions, they determine the "meaning" and behavior of objects belonging to them. New classes can be defined in user code as well as new methods, i.e., functions or operators tailored to fit them. The *class* is like a "tag" that tells how the value in an object should be interpreted and operated upon.

Variables (names given to objects) have a *class* that depends on the object stored in them. In contrast to some other languages in R assignment to a variable already in use to store an object belonging to a different class is allowed. There is a restriction that all elements in a vector, array or matrix, must be of the same mode (these are called atomic, as they contain homogeneous members). Lists and data frames can be heterogenous (to be described in chapter 4). In practice this means that we can assign an object, such as a vector, with a different class to a name already in use, but we cannot use indexing to assign an object of a different mode to individual members of a vector, matrix or array.

Function class() is used to query the class of an object, and function inherits() is used to test if an object belongs to a specific class or not (including "parent" classes, to be later described).

```
vct1 <- 1:5
class(vct1)
## [1] "integer"
inherits(vct1, "character")
## [1] FALSE
inherits(vct1, "numeric")
## [1] FALSE</pre>
```

Functions with names starting with is. are tests returning a logical value, true, false or NA.

```
is.numeric(vct1) # no distinction of integer or double
## [1] TRUE
is.double(vct1)
## [1] FALSE
is.integer(vct1)
## [1] TRUE
is.logical(vct1)
## [1] FALSE
is.character(vct1)
## [1] FALSE
```

The *mode* of an object is a fundamental property, and limited to those modes defined as part of the R language. In particular, different R objects of a given mode, such as numeric, can belong to different classes. Classes and the dispatch of methods are discussed in section 6.3 on page 176, together with object-oriented programming.

```
mode(c(1, 2, 3)) # no distinction of integer or double
## [1] "numeric"
typeof(c(1, 2, 3))
## [1] "double"
class(c(1, 2, 3))
## [1] "numeric"
mode(c(1L, 2L, 3L)) # no distinction of integer or double
## [1] "numeric"
typeof(c(1L, 2L, 3L))
## [1] "integer"
class(c(1L, 2L, 3L))
## [1] "integer"
mode(factor(c("a", "b", "c"))) # no distinction of integer or double
## [1] "numeric"
typeof(factor(c("a", "b", "c")))
## [1] "integer"
class(factor(c("a", "b", "c")))
## [1] "factor"
mode(c("a", "b", "c"))
## [1] "character"
typeof(c("a", "b", "c"))
## [1] "character"
class(c("a", "b", "c"))
## [1] "character"
mode(c(TRUE, FALSE))
## [1] "logical"
typeof(c(TRUE, FALSE))
## [1] "logical"
class(c(TRUE, FALSE))
## [1] "logical"
```

#### 3.9 'Type' conversions

By type conversion we mean converting a value from one class into a value expressed in a different class. usually the meaning can be retained, at least in part. We can for example convert character strings into numeric values, but this conversion is possible only for character strings conformed by digits, like "100". Most conversions, such as the conversion of character value "100" into numeric value 100 are obvious. Type conversions involving logical values are less intuitive. By convention, functions used to convert objects from one mode or class to a different one have names starting with as. \(^1\).

<sup>&</sup>lt;sup>1</sup>Except for some packages in the 'tidyverse' that use names starting with as\_ instead of as...

```
as.character(102)
## [1] "102"
as.character(TRUE)
## [1] "TRUE"
as.character(3.0e10)
## [1] "3e+10"
as.numeric("203")
## [1] 203
as.logical("TRUE")
## [1] TRUE
as.logical(100)
## [1] TRUE
as.logical(0)
## [1] FALSE
as.logical(-1)
## [1] TRUE
```

Some conversions takes place automatically in expressions involving both numeric and logical values.

```
TRUE + 10

## [1] 11

1 || 0

## [1] TRUE

FALSE | -2:2

## [1] TRUE TRUE FALSE TRUE TRUE
```

3.22 There is flexibility in the conversion from character strings into numeric and logical values. Use the examples below plus your own variations to get an idea of what strings are acceptable and correctly converted and which are not. Do also pay attention at the conversion between numeric and logical values.

```
as.numeric("5E+5")
as.numeric("50e+4")
as.numeric(".12")
as.numeric("0.12")
as.numeric("A")
as.logical("TRUE")
as.logical("THUE")
as.logical("T")
as.logical("t")
as.logical("t")
as.logical("true")
```

3.23 Conversion of fractional numbers into whole numbers can be achieved in different ways, by truncation of the fractional part or rounding it up or down. If we consider both negative and positive numbers, how each of them are handled creates additional possibilities. All these approaches as defined in mathematics, are available through different R functions. These functions, are not conversion functions as they return a numeric value of class double. See page 37. In contrast, as.integer() is a conversion function for type double into type integer, both with mode numeric.

Compare the values returned by trunc() and as.integer() when applied to a floating point number, such as 12.34. Check for the equality of values, and for the *class* and *type* of the returned objects.

Using conversions, the difference between the length of a character vector and the number of characters composing each member "string" within a vector becomes clear.

```
vct1 <- c("1", "2", "3")
length(vct1)
## [1] 3
vct2 <- "123.1"
length(vct2)
## [1] 1
as.numeric(vct1)
## [1] 1 2 3
as.numeric(vct2)
## [1] 123.1
as.integer(vct1)
## [1] 1 2 3
as.integer(vct2)
## [1] 1 2 3</pre>
```

Other functions relevant to the "conversion" of numbers and other values are format(), and sprintf(). This is sometimes informally called "pretty printing". These two functions return character strings, instead of numeric or other values, and are useful for printed output. One could think of these functions as advanced conversion functions returning formatted, and possibly combined and annotated, character strings. However, they are usually not considered normal conversion functions, as they are very rarely used in a way that preserves the original precision of the input values. We show here the use of format() and sprintf() with numeric values, but they can also be used with values of other classes like character, logical, etc.

When using format(), the format used to display numbers is set by passing arguments to several different parameters. As print() calls format() to convert numeric values into character strings, it accepts the same options.

```
vct2 = c(123.4567890, 1.0)
format(vct2) # using defaults
## [1] "123.4568" " 1.0000"
format(123.4567890) # using defaults
## [1] "123.4568"
format(1.0) # using defaults
## [1] "1"
format(vct2, digits = 3, nsmall = 1)
## [1] "123.5" " 1.0"
format(vct2, digits = 3, scientific = TRUE)
## [1] "1.23e+02" "1.00e+00"
```

Function sprintf() is similar to C's function of the same name. The user interface is rather unusual, but very powerful, once one learns the syntax. All the

formatting is specified using a character string as template. In this template, place-holders for data and the formatting instructions are embedded using special codes. These codes start with a percent character. We show in the example below the use of some of these: f is used for numeric values to be formatted according to a "fixed point," while g is used when we set the number of significant digits and e for exponential or *scientific* notation.

```
x = c(123.4567890, 1.0)
sprintf("The numbers are: %4.2f and %.0f", x[1], x[2])
## [1] "The numbers are: 123.46 and 1"
sprintf("The numbers are: %.4g and %.2g", x[1], x[2])
## [1] "The numbers are: 123.5 and 1"
sprintf("The numbers are: %4.2e and %.0e", x[1], x[2])
## [1] "The numbers are: 1.23e+02 and 1e+00"
```

In the template "The numbers are: %4.2f and %.0f", there are two placeholders for numeric values, %4.2f and %.0f, so in addition to the template, we pass two values extracted from the first two positions of vector x. These could have been two different vectors of length one, or even numeric constants. The template itself does not need to be a character constant as in these examples, as a variable can be also passed as argument.

- 3.24 Function format() may be easier to use, in some cases, but sprintf() is more flexible and powerful. Those with experience in the use of the C language will already know about sprintf() and its use of templates for formatting output. Even if you are familiar with C, look up the help pages for both functions, and practice, by trying to create the same formatted output by means of the two functions. Do also play with these functions with other types of data like integer and character.
- We have above described NA as a single value ignoring modes, but in reality NA s come in various flavors. NA\_real\_, NA\_character\_, etc. and NA defaults to an NA of class logical. NA is normally converted on the fly to other modes when needed, so in general NA is all we need to use. The examples below use the extraction operator to demonstrate automatic conversion on assignment. This operator is described in section 3.10 below.

```
vct3 <- c(1, NA)
is.numeric(vct3[2])
## [1] TRUE
is.numeric(NA)
## [1] FALSE
vct4 <- c("abc", NA)
is.character(vct4[2])
## [1] TRUE
is.character(NA)
## [1] FALSE
class(NA)
## [1] "logical"
class(NA_character_)
## [1] "character"</pre>
```

```
vct5 <- NA
c(vct5, 2:3)
## [1] NA 2 3
However, even the statement below works transparently.
vct3[3] <- vct4[2]</pre>
```

### 3.10 Vector manipulation

If you have read earlier sections of this chapter, you already know how to create a vector. If not, see pages 28–33 before continuing.

In this section we are going to see how to extract or retrieve, replace, and move elements such as  $a_2$  from a vector  $a_{i=1...n}$ . Elements are extracted using an index enclosed in single square brackets. The index indicates the position in the vector, starting from one, following the usual mathematical tradition. What in maths notation would be  $a_i$ , in R is represented as a[i] and the whole vector, by excluding the brackets and indexing vector, as a.

We extract the first 10 elements of the vector letters.

```
vct1 <- letters[1:10]</pre>
vct1
    [1] "a" "b" "c" "d" "e" "f" "g" "h" "i" "i"
                 1
                           3
                                4
                                     5
                                                            10 — integer positional indices
                                          6
                                                   8
                               "d"
                                    "e"
                                                   "h"
                                              "g""
      vct1
                                                                   character values
                  a[2]
```

```
vct1[2]
## [1] "b"
```

Four constant vectors are available in base R: letters, LETTERS, month.name and month.abb, of which I used letters in the example above. These vectors are always for English, irrespective of the locale.

```
month.name
## [1] "January" "February" "March" "April" "May" "June"
## [7] "July" "August" "September" "October" "November" "December"
month.name[6]
## [1] "June"
```

In R, indexes always start from one, while in some other programming languages such as C and C++, indexes start from zero. It is important to be aware of this difference, as many computation algorithms are valid only under a given indexing convention.

## **1** How to access the last value in a vector?

```
month.name[length(month.name)]
## [1] "December"
```

It is possible to extract a subset of the elements of a vector in a single operation, using a vector of indexes. The positions of the extracted elements in the result ("returned value") are determined by the ordering of the members of the vector of indexes—easier to demonstrate than to explain.

```
vct1[c(3, 2)]
## [1] "c" "b"
vct1[10:1]
## [1] "j" "i" "h" "g" "f" "e" "d" "c" "b" "a"
```

3.25 The length of the indexing vector is *not* restricted by the length of the indexed vector. However, only numerical indexes that match positions present in the indexed vector can extract values. Those values in the indexing vector pointing to positions that are not present in the indexed vector, result in NAS. This is easier to learn by *playing* with R, than from explanations. Play with R, using the following examples as a starting point.

```
length(a)
vct1[c(3, 3, 3, 3)]
vct1[c(10:1, 1:10)]
vct1[c(1, 11)]
vct1[11]
```

Have you tried some of your own examples? If not yet, do *play* with additional variations of your own before continuing.

Negative indexes have a special meaning; they indicate the positions at which values should be excluded. Be aware that it is *illegal* to mix positive and negative values in the same indexing operation.

```
vct1[-2]
## [1] "a" "c" "d" "e" "f" "g" "h" "i" "j"
vct1[-c(3,2)]
## [1] "a" "d" "e" "f" "g" "h" "i" "j"
vct1[-3:-2]
## [1] "a" "d" "e" "f" "a" "h" "i" "i"
```

3.26 Results from indexing with special values and zero may be surprising. Try to build a rule from the examples below, a rule that will help you remember what to expect next time you are confronted with similar statements using "subscripts" which are special values instead of integers larger or equal to one—this is likely to happen sooner or later as these special values can be returned by different R expressions depending on the value of operands or function arguments, some of them described earlier in this chapter.

```
vct1[ ]
vct1[0]
vct1[numeric(0)]
vct1[NA]
vct1[c(1, NA)]
vct1[NULL]
vct1[c(1, NULL]]
```

Another way of indexing, which is very handy, but not available in most other programming languages, is indexing with a vector of logical values. The logical vector used for indexing is usually of the same length as the vector from which elements are going to be selected. However, this is not a requirement, because if the logical vector of indexes is shorter than the indexed vector, it is "recycled" as discussed in page 31 in relation to other operators.

```
vct1[TRUE]
## [1] "a" "b" "c" "d" "e" "f" "g" "h" "i" "j"
vct1[FALSE]
## character(0)
vct1[c(TRUE, FALSE)]
## [1] "a" "c" "e" "g" "i"
vct1[c(FALSE, TRUE)]
## [1] "b" "d" "f" "h" "j"
vct1 > "c"
## [1] FALSE FALSE FALSE TRUE TRUE TRUE TRUE TRUE TRUE TRUE
vct1[vct1 > "c"]
## [1] "d" "e" "f" "g" "h" "i" "j"
```

Indexing with logical vectors is very frequently used in R because comparison operators are vectorized. Comparison operators, when applied to a vector, return a logical vector, a vector that can be used to extract the elements for which the result of the comparison test was TRUE.

3.27 The examples in this text box demonstrate additional uses of logical vectors: 1) the logical vector returned by a vectorized comparison can be stored in a variable, and the variable used as a "selector" for extracting a subset of values from the same vector, or from a different vector.

```
vct1 <- letters[1:10]
vct2 <- 1:10
selector <- vct1 > "c"
selector
vct1[selector]
vct2[selector]
```

Numerical indexes can be obtained from a logical vector by means of function which().

```
indexes <- which(vct1 > "c")
indexes
vct1[indexes]
vct2[indexes]
```

Make sure to understand the examples above. These constructs are very widely used in R because they allow for concise code that is easy to understand once one

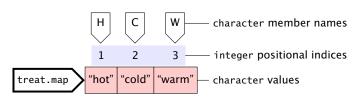
is familiar with the indexing rules. However, if one does not command these rules, many of these terse statements become unintelligible.

In all earlier examples we have used integer valued indices for extraction of elements. In the vectors used as examples above the elements were anonymous or nameless. In R the elements can be assigned names, and these names used in place of numeric indices to extract the named elements. There is one situation where this is very useful: the mapping of values between two representations.

Let's assume we have a long vector encoding treatments using single letter codes and we want to replace these codes with clearer names.

```
treat <- c("H", "C", "H", "W", "C", "H", "H", "W", "W")
```

We can create a named vector to map the single letter codes into some other codes, in this case full words that are easier to understand. Above we used function c() to concatenate several character strings, without assigning any names to them, thus they can extracted from the vector using numeric values for indexing by position. Below, we assign a name to each string. Using operator = we assign the name on the left-hand side (lhs) to the member of the vector on the right-hand-side (rhs).



As treat.map is a named vector, we can use the element names as indices for element extraction.

```
treat.map["H"]
## H
## "hot"
```

The indexing vector can be of a different length than the indexed vector, and the returned value is a new vector of the same length as the indexing vector.

where treat.new is a named vector, from which we will frequently want to remove the names.

```
treat.new <- unname(treat.new)
treat.new
## [1] "hot" "cold" "hot" "warm" "cold" "hot" "hot" "warm" "warm"</pre>
```

It is more common to use named members with lists than with vectors, but in R, in both cases it is possible to use both numeric positional indices and names.

Indexing can be used on either side of an assignment expression. In the chunk below, we use the extraction operator on the left-hand side of the assignments to replace values only at selected positions in the vector. This may look rather esoteric at first sight, but it is just a simple extension of the logic of indexing described above. It works, because the low precedence of the <- operator results in both the left-hand side and the right-hand side being fully evaluated before the assignment takes place. To make the changes to the vectors easier to follow, we use identical vectors with different names for each of these examples.

```
vct2 <- 1:10
vct2
##
   [1] 1 2 3 4 5 6 7 8 9 10
vct2[1] <- 99
vct2
## [1] 99 2 3 4 5 6 7 8
vct2 <- 1:10
vct2[c(2,4)] <- -99 # recycling
vct2
## [1]
         1 - 99
                 3 -99
                                          9 10
vct2 <- 1:10
vct2[c(2,4)] \leftarrow c(-99, 99)
vct2
                                  7
   [1] 1 -99
                 3 99
                              6
                                      8
                                          9 10
vct2 <- 1:10
vct2[TRUE] <- 1 # recycling</pre>
vct2
## [1] 1 1 1 1 1 1 1 1 1 1
vct2 <- 1:10
vct2 <- 1 # no recycling
vct2
## [1] 1
```

We can also use subscripting on both sides of the assignment operator, for example, to swap two elements.

```
vct3 <- letters[1:10]
vct3[1:2] <- vct3[2:1]
vct3
## [1] "b" "a" "c" "d" "e" "f" "a" "h" "i" "i"</pre>
```

3.28 Do play with subscripts to your heart's content, really grasping how they work and how they can be used, will be very useful in anything you do in the future with R. Even the contrived example below follows the same simple rules, just study it bit by bit. Hint: the second statement in the chunk below, modifies a, so, when studying variations of this example you will need to recreate a by executing the first statement, each time you run a variation of the second statement.

```
VCT1 <- letters[1:10]
VCT1[5:1] <- VCT1[c(TRUE, FALSE)]
VCT1</pre>
```

In R, indexing with positional indexes can be done with integer or numeric values. Numeric values can be floats, but for indexing, only integer values are meaningful. Consequently, double values are converted into integer values when used as indexes. The conversion is done invisibly, but it does slow down computations slightly. When working on big data sets, explicitly using integer values can improve performance.

```
vct4 <- LETTERS[1:10]
vct4
## [1] "A" "B" "C" "D" "E" "F" "G" "H" "I" "J"
vct4[1]
## [1] "A"
vct4[1.1]
## [1] "A"
vct4[1.9999] # surprise!!
## [1] "A"
vct4[2]
## [1] "B"</pre>
```

From this experiment, we can learn that if positive indexes are not whole numbers, they are truncated to the next smaller integer.

```
vct4 <- LETTERS[1:10]
vct4
## [1] "A" "B" "C" "D" "E" "F" "G" "H" "I" "J"
vct4[-1]
## [1] "B" "C" "D" "E" "F" "G" "H" "I" "J"
vct4[-1.1]
## [1] "B" "C" "D" "E" "F" "G" "H" "I" "J"
vct4[-1.9999]
## [1] "B" "C" "D" "E" "F" "G" "H" "I" "J"
vct4[-2]
## [1] "A" "C" "D" "E" "F" "G" "H" "I" "J"</pre>
```

From this experiment, we can learn that if negative indexes are not whole numbers, they are truncated to the next larger (less negative) integer. In conclusion, double index values behave as if they where sanitized using function trunc().

This example also shows how one can tease out of R its rules through experimentation.

A frequent operation on vectors is sorting them into an increasing or decreasing order. The most direct approach is to use sort().

```
vct5 <- c(10, 4, 22, 1, 4)
sort(vct5)
## [1] 1 4 4 10 22
sort(vct5, decreasing = TRUE)
## [1] 22 10 4 4 1</pre>
```

An indirect way of sorting a vector, possibly based on a different vector, is to generate with order() a vector of numerical indexes that can be used to achieve the ordering.

**************************************	$a_{1,1}$	$a_{1,2}$	$a_{1,3}$		$a_{1,n}$
	$a_{2,1}$	$a_{2,2}$	$a_{2,3}$		$a_{2,n}$
	$a_{3,1}$	$a_{3,2}$	$a_{3,3}$		$a_{3,n}$
	÷			٠.	
	$a_{m,1}$	$a_{m,2}$	$a_{m,3}$		$a_{m,n}$
	lumns			, ,	

FIGURE 3.2

Diagram of an R matrix showing indexing of members.

```
order(vct5)
## [1] 4 2 5 1 3
vct5[order(vct5)]
## [1] 1 4 4 10 22
vct6 <- c("ab", "aa", "c", "zy", "e")
vct6[order(vct5)]
## [1] "zy" "aa" "e" "ab" "c"</pre>
```

A problem linked to sorting that we may face is counting how many copies of each value are present in a vector. We need to use two functions sort() and rle(). The second of these functions computes *run length* as used in *run length encoding* for which *rle* is an abbreviation. A *run* is a series of consecutive identical values. As the objective is to count the number of copies of each value present, we need first to sort the vector.

```
vct7 <- letters[c(1, 5, 10, 3, 1, 4, 21, 1, 10)]
vct7
## [1] "a" "e" "j" "c" "a" "d" "u" "a" "j"
sort(vct7)
## [1] "a" "a" "a" "c" "d" "e" "j" "j" "u"
rle(sort(vct7))
## Run Length Encoding
## lengths: int [1:6] 3 1 1 1 2 1
## values: chr [1:6] "a" "c" "d" "e" "j" "u"</pre>
```

The second and third statements are only to demonstrate the effect of each step. The last statement uses nested function calls to compute the number of copies of each value in the vector.

### 3.11 Matrices and multidimensional arrays

Matrices have two dimensions, rows and columns, and like vectors all their members share the same mode, and are atomic, i.e., they are homogeneous (Figure 3.2). Most commonly, matrices are used to store numeric, integer or logical values. The number of rows and columns can differ, so matrices can be either square or rectangular in shape, but never ragged.

In R, the first index always denotes rows and the second index always denotes columns. The diagram below depicts a matrix, A, with m rows and n columns and size equal to  $m \times n$  "cells", with individual values denoted by  $a_{i,j}$ . Here we use a simpler representation than that used for vectors on page 28 above, but the same concepts apply.

In R documentation, the individual dimensions of matrices and arrays are frequently called *margins*, numbered in the same order as the indices are given. Thus, in a matrix the first margin corresponds to rows and the second one to columns.

In mathematical notation the same generic matrix is represented as

$$A_{m \times n} = \begin{bmatrix} a_{1,1} & a_{1,2} & \cdots & a_{1,j} & \cdots & a_{1,n} \\ a_{2,1} & a_{2,2} & \cdots & a_{2,j} & \cdots & a_{2,n} \\ \vdots & \vdots & \ddots & \vdots & & \vdots \\ a_{i,1} & a_{i,2} & \cdots & a_{i,j} & \cdots & a_{i,n} \\ \vdots & \vdots & & \vdots & \ddots & \vdots \\ a_{m,1} & a_{m,2} & \cdots & a_{m,j} & \cdots & a_{m,n} \end{bmatrix}$$

where A represents the whole matrix,  $m \times n$  its dimensions, and  $a_{i,j}$  its elements, with i indexing rows and j indexing columns. The lengths of the two dimensions of the matrix are given by m and n, for rows and columns.

Vectors have a single dimension, and, as described on page 28 above, we can query this dimension, their length, with function length(). Matrices have two dimensions, which can be queried individually with ncol() and nrow(), and jointly with dim(). As expected is.matrix() can be used to query the class.

We can create a matrix using the matrix() or as.matrix() constructors. The first argument of matrix() must be a vector. Function as.matrix() is a conversion constructor, with specializations accepting as argument objects belonging to a few other classes.

```
matrix(1:15, ncol = 3)
       [,1] [,2] [,3]
## [1,]
                  11
## [2,]
## [3,]
        5 10
matrix(1:15, nrow = 3)
      [,1] [,2] [,3] [,4] [,5]
## [1,]
        1 4 7
                       10
                            13
## [2,]
          2 5
                   8
                       11
                            14
## [3,]
          3 6
                       12
```

When a matrix is printed in R the row and column indexes are indicated on the left and top margins, in the same way as they would be used to extract whole rows and columns.

Matrices are most useful for storage of numeric values as matrix algebra plays an important role in statistical computations. This notwithstanding, it is possible to create matrices (and arrays) from atomic vectors of other classes such as logical or character. The only difference is the scarcity of meaningful operations other than retrieval of members using two indices.

```
matrix(letters[1:15], nrow = 3)
##     [,1] [,2] [,3] [,4] [,5]
## [1,] "a" "d" "g" "j" "m"
## [2,] "b" "e" "h" "k" "n"
## [3,] "c" "f" "i" "l" "o"
```

When a vector is converted to a matrix, R's default is to allocate the values in the vector to the matrix starting from the leftmost column, and within the column, down from the top. Once the first column is filled, the process continues from the top of the next column, as can be seen above. This order can be changed as you will discover in the playground below.

3.29 Check in the help page for the matrix constructor how to use the byrow parameter to alter the default order in which the elements of the vector are allocated to columns and rows of the new matrix.

```
help(matrix)
```

While you are looking at the help page, also consider the default number of columns and rows.

```
matrix(1:15)
```

And to start getting a sense of how to interpret error and warning messages, run the code below and make sure you understand which problem is being reported. Before executing the statement, analyze it and predict what the returned value will be. Afterwards, compare your prediction, to the value actually returned.

```
matrix(1:15, ncol = 2)
```

Subscripting of matrices and arrays is consistent with that used for vectors; we only need to supply an indexing vector, or leave a blank space, for each dimension. A matrix has two dimensions, so to access an element or group of elements, we use two indices. The first index value selects rows, and the second one, columns.

```
mat1 <- matrix(1:20, ncol = 4)
mat1
##
        [,1] [,2] [,3] [,4]
## [1,]
            1
                 6
                      11
                           16
## [2,]
            2
                 7
                     12
                           17
## [3,]
            3
                 8
                     13
                           18
## [4,]
            4
                 9
                      14
                           19
                10
                      15
                           20
## [5,]
mat1[1, 2]
## [1] 6
mat1[2, 1]
## [1] 2
```

Remind yourself of how indexing of vectors works in R (see section 3.10 on page 64). We will now apply the same rules in two dimensions to extract and replace values. The first or leftmost indexing vector corresponds to rows and the second one to columns, so R uses a rows-first convention for indexing. Missing indexing vectors are interpreted as meaning *extract all rows* and *extract all columns*, respectively.

```
mat1[1, ]
## [1] 1 6 11 16
mat1[ , 1]
## [1] 1 2 3 4 5
mat1[2:3, c(1,3)]
       [,1] [,2]
## [1,]
          2 12
## [2,]
           3 13
mat1[3, 4] < -99
mat1
##
        [,1] [,2] [,3] [,4]
## [1,]
           1
                6
                    11
                         16
## [2,]
                7
           2
                    12
                         17
## [3,]
           3
                8
                    13
                         99
                         19
## [4,]
           4
               9
                    14
         5
                         20
## [5,]
               10
                    15
mat1[4:3, 2:1] <- mat1[3:4, 1:2]
mat1
        [,1] [,2] [,3] [,4]
## [1,]
           1
                6
                    11
                         16
           2
                7
## [2,]
                    12
                         17
                    13
## [3,]
           9
                4
                         99
                3
                         19
## [4,]
           8
                    14
               10
                          20
## [5,]
           5
                    15
```

Vectors are simpler than matrices, and by default when possible the "slice" extracted from a matrix is simplified into a vector by dropping one dimension. By passing drop = FALSE, we can prevent this.

```
is.matrix(mat1[1, ])
## [1] FALSE
is.matrix(mat1[1:2, 1:2])
## [1] TRUE
is.vector(mat1[1, ])
## [1] TRUE
is.vector(mat1[1:2, 1:2])
## [1] FALSE
is.matrix(mat1[1, , drop = FALSE])
## [1] TRUE
is.matrix(mat1[1:2, 1:2, drop = FALSE])
## [1] TRUE
```

Matrices, like vectors, can be assigned names that function as "nicknames" for indices for assignment and extraction. Matrices can have row names and/or column names.

```
colnames(mat1)
## NULL
rownames (mat1)
## NULL
colnames(mat1) <- c("a", "b", "c", "d")</pre>
        a b c d
## [1,] 1 6 11 16
## [2,] 2 7 12 17
## [3,] 9 4 13 99
## [4,] 8 3 14 19
## [5,] 5 10 15 20
mat1[ , c("b", "a")]
         b a
## [1,] 6 1
## [2,] 7 2
## [3,] 4 9
## [4,] 3 8
## [5,] 10 5
colnames(mat1) <- NULL</pre>
mat1
##
        [,1] [,2] [,3] [,4]
## [1,]
           1
                6
                    11
                          16
                7
## [2,]
           2
                          17
                    12
## [3,]
           9
                          99
                4
                    13
## [4,]
           8
                3
                    14
                          19
## [5,]
           5
               10
                    15
                          20
```

1 Matrices can be indexed as vectors, without triggering an error or warning.

```
mat1 <- matrix(1:20, ncol = 4)</pre>
mat1
        [,1] [,2] [,3] [,4]
## [1,]
                6
                     11
           1
                          16
## [2,]
           2
                 7
                     12
                          17
## [3,]
           3
                 8
                     13
                          18
## [4,]
           4
                 9
                     14
                           19
           5
## [5,]
                10
                     15
                           20
dim(mat1)
## [1] 5 4
mat1[10]
## [1] 10
mat1[5, 2]
## [1] 10
```

The next code example demonstrates that indexing as a vector with a single index, always works column-wise even if matrix B was created by assigning vector elements by row.

```
mat2 <- matrix(1:20, ncol = 4, byrow = TRUE)</pre>
mat2
##
        [,1] [,2] [,3] [,4]
## [1,]
                      3
                            4
                      7
                6
                           8
## [2,]
           5
          9
## [3,]
                10
                     11
                          12
## [4,]
          13
                14
                     15
                          16
          17
                18
                     19
                           20
## [5,]
dim(mat2)
## [1] 5 4
mat2[10]
## [1] 18
mat2[5, 2]
## [1] 18
```

In R, a matrix can have a single row, a single column, a single element or no elements. However, in all cases, a matrix will have as *dimensions* attribute an integer vector of length two.

```
vct1 <- 1:6
dim(vct1)
## NULL

one.col.matrix <- matrix(1:6, ncol = 1)
dim(one.col.matrix)
## [1] 6 1

two.col.matrix <- matrix(1:6, ncol = 2)
dim(two.col.matrix)
## [1] 3 2

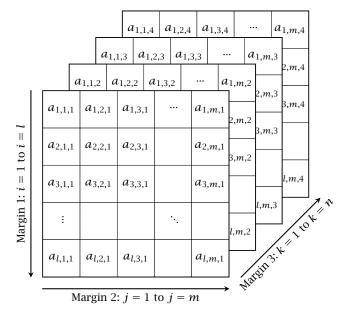
one.elem.matrix <- matrix(1, ncol = 1)
dim(one.elem.matrix)
## [1] 1 1

no.elem.matrix <- matrix(numeric(), ncol = 0)
dim(no.elem.matrix)
## [1] 0 0</pre>
```

Arrays are similar to matrices, but can have one or more dimensions (Figure 3.3). The dimensions of an array can be queried with dim(), similarly as with matrices. Whether an R object is an array can be found out with is.array(). The diagram below depicts an array, A with three dimensions giving a size equal to  $l \times m \times n$ , and individual values denoted by  $a_{i,i,k}$ .

When calling the constructor array(), dimensions are specified with the argument passed to parameter dim.

```
ary1 \leftarrow array(1:27, dim = c(3, 3, 3))
ary1
## , , 1
##
##
        [,1] [,2] [,3]
## [1,]
          1
                 4
                       7
## [2,]
            2
                  5
                       8
## [3,]
                       9
            3
                  6
##
```



**FIGURE 3.3** Diagram of an R array with three dimensions showing indexing of members.

```
, , 2
##
##
##
         [,1] [,2] [,3]
## [1,]
           10
                13
                      16
   [2,]
##
           11
                 14
                      17
##
   [3,]
           12
                 15
                      18
##
##
##
##
         [,1] [,2] [,3]
                      25
## [1,]
           19
                 22
## [2,]
           20
                 23
                      26
                 24
                      27
## [3,]
           21
ary1[2, 2, 2]
## [1] 14
```

In the chunk above, the length of the supplied vector is the product of the dimensions,  $27 = 3 \times 3 \times 3 = 3^3$ . Arrays are printed in slices, with slices across 3rd and higher dimensions printed separately, with their corresponding indexes above each slice and the first two dimensions on the margins of the individual slices, similarly to how matrices are displayed.

3.30 How do you use indexes to extract the second element of the original vector, in each of the following matrices and arrays?

```
VCT2 <- 1:10
MAT1 <- matrix(VCT2, ncol = 2)
MAT2 <- matrix(VCT2, ncol = 2, byrow = TRUE)
MAT3 <- matrix(VCT2, nrow = 2)
MAT4 <- matrix(VCT2, nrow = 2, byrow = TRUE)</pre>
```

```
ARY1 <- array(VCT2, dim = c(5, 2))

ARY2 <- array(VCT2, dim = c(5, 2), dimnames = list(NULL, c("c1", "c2")))

ARY3 <- array(VCT2, dim = c(2, 5))
```

Be aware that vectors and one-dimensional arrays are not the same thing, while two-dimensional arrays are matrices.

- 1. Use the different constructors and query functions to explore this, and its consequences.
- 2. Convert a matrix into a vector using as.vector() and compare the returned values to those in the matrix. Are values extracted by columns or by rows first.

Operators and functions for matrix algebra are available in R as matrices are used in statistical algorithms. I describe below only some of these matrix-specific functions and operators. I also give examples of the use of some of the usual arithmetic operators together with objects of class matrix.

Recycling applies to the usual arithmetic operators when applied to matrices. This is similar to their behavior when all operands are vectors (see page 31).

```
mat3 <- matrix(1:20, ncol = 4)
mat3 + 2
##
         [,1] [,2] [,3] [,4]
## [1,]
            3
                 8
                      13
                           18
## [2,]
            4
                 9
                      14
                            19
## [3,]
            5
                10
                      15
                            20
                            21
## [4,]
            6
                11
                      16
                12
## [5,]
                      17
mat3 * 0:1
         [,1] [,2] [,3] [,4]
## [1,]
            0
                 6
                       0
                           16
## [2,]
            2
                 0
                      12
                            0
## [3,]
            0
                 8
                      0
                            18
                 0
## [4,]
            4
                      14
                            0
## [5,]
            0
                10
                            20
mat3 * 1:0
         [,1] [,2] [,3] [,4]
            1
                 0
                      11
##
   [2,]
            0
                 7
                       0
                           17
## [3,]
            3
                 0
                      13
                            0
## [4,]
            0
                 9
                       0
                           19
## [5,]
                      15
```

3.31 When a matrix and a vector are operands in an arithmetic operation, how the positions of the vector are mapped to positions in the matrix affects the result of the operation. Run the code below to find out. What is the logic behind? matrix(rep(1, 6)) \* 1:6

Function t() transposes a matrix, by swapping columns and rows.

```
[,1] [,2] [,3] [,4]
## [1,]
            1
                 6
                      11
                           16
## [2,]
            2
                 7
                      12
                           17
## [3,]
            3
                 8
                      13
                           18
```

```
## [4,]
                  9
                            19
            4
                      14
## [5,]
            5
                10
                      15
                            20
t(mat3)
##
         [,1] [,2] [,3] [,4] [,5]
## [1,]
            1
                 2
                       3
## [2,]
                 7
                             9
                       8
            6
                                 10
## [3,]
           11
                      13
                                 15
                12
                            14
## [4,]
           16
                17
                      18
                            19
                                  20
```

In the examples above with the usual multiplication operator \*, the operation described is not a matrix product, but instead, the products between individual elements of the matrix and vectors. Operators and functions implementing the operations of matrix algebra are distinct. Matrix algebra gives the rules for operations where both operands are matrices. For example, matrix multiplication is indicated by operator %\*%.

```
mat4 <- matrix(1:16, ncol = 4)
mat4 * mat4
##
        [,1] [,2] [,3] [,4]
## [1,]
           1
                25
                     81 169
## [2,]
               36
                   100
                         196
           4
           9
               49
                   121
                         225
## [3,]
               64
                   144
                         256
## [4,]
          16
mat4 %*% mat4
        [,1] [,2] [,3] [,4]
## [1,]
          90
              202
                         426
                    314
## [2,]
         100
              228
                    356
                         484
## [3,]
         110
               254
                    398
                         542
  [4,]
         120
              280
                    440
                         600
```

Function diag() makes it possible to easily create a diagonal matrix.

```
mat5 <- diag(4)
mat5
##
         [,1] [,2] [,3] [,4]
## [1,]
                 0
                       0
           1
   [2,]
##
            0
                 1
                       0
                            0
## [3,]
            0
                            0
                 0
                       1
            0
                            1
## [4,]
                 0
mat4 %*% mat5
##
         [,1] [,2] [,3] [,4]
## [1,]
          1
                 5
                     9
                           13
## [2,]
            2
                 6
                      10
                           14
## [3,]
                 7
                           15
            3
                      11
## [4,]
                     12
                           16
```

The inverse of a matrix can be found by means of function solve().

Additional operators and functions for matrix algebra like cross-product (crossprod()) and Cholesky root (chol()) are available in base R. Packages, including 'matrixStats', provide additional functions and operators for matrices.

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#### 3.12 Factors

In data analysis and Statistics the distinction between values measured on continuous vs. discrete *scales* is crucial. In a continuous scale, any values are in theory possible. In a discrete scale, the observations are values from a few categories.

In contrast to other statistical software in which a variable is set as continuous or discrete when defining a model to be fitted or when setting up a test, in R this distinction is based on whether the explanatory variable is numeric (continuous) or a factor (discrete). This approach makes sense because in most cases considering an explanatory variable as categorical or not, depends on the quantity stored and/or the design of the experiment or survey. In other words, being categorical is a property of the data. The order of the levels in an unordered factor does not affect simple calculations or the values plotted, but as we will see in chapters 7 and 9, it can affect the contrasts used by some tests of significant, and the arrangement or positions of the levels along axes and keys in plots.

In an R factor, values indicate discrete unordered categories, most frequently the treatments in an experiment, or categories in a survey. Factor can be created either from numerical or character vectors. The different possible values are called *levels*. Factors created with factor() are always unordered or categorical. R also supports ordered factors, created with function ordered() with identical user interface. The distinction, however, only affects how they are interpreted in statistical tests as discussed in chapter 7.

When using factor() or ordered() we create a factor from a vector, but this vector can be created on-the-fly and anonymous as shown in this example. When the vector is numeric and no labels are supplied, level labels are character strings matching the numbers. The default ordering of the levels is alphanumerical.

```
factor(x = c(1, 2, 2, 1, 2, 1, 1))
## [1] 1 2 2 1 2 1 1
## Levels: 1 2

ordered(x = c(1, 2, 2, 1, 2, 1, 1))
## [1] 1 2 2 1 2 1 1
## Levels: 1 < 2
factor(x = c(1, 2, 2, 1, 2, 1, 1), ordered = TRUE)
## [1] 1 2 2 1 2 1 1
## Levels: 1 < 2</pre>
```

When the pattern of levels is regular, it is possible to use function gl(), generate levels, to construct a factor. Nowadays, it is usual to read data into R from files in which the treatment codes are already available as character strings or numeric values, however, when we need to create a factor within R, gl() can save some typing. In this case instead of passing a vector as argument, we pass a recipe to create it: n is the number of levels, and k the number of contiguous repeats (called "replicates" in R documentation) and length the length of the factor to be created.

```
gl(n = 2, k = 5, labels = c("A", "B"))
## [1] A A A A A B B B B B
## Levels: A B
gl(n = 2, k = 1, length = 10, labels = c("A", "B"))
## [1] A B A B A B A B A B
## Levels: A B
```

It is always preferable to use meaningful labels for levels, even if R does not require it. Here the vector is stored in a variable named my.vector. In a real data analysis situation in most cases the vector would have been read from a file on disk and would be longer.

```
vct1 <- c("treated", "treated", "control", "control", "control", "treated")
factor(vct1)
## [1] treated treated control control treated
## Levels: control treated</pre>
```

The ordering of levels is established at the time a factor is created, and by default is alphabetical. This default ordering of levels is frequently not the one needed. We can pass an argument to parameter levels of function factor() to set a different ordering of the levels.

```
factor(x = vct1, levels = c("treated", "control"))
## [1] treated treated control control control treated
## Levels: treated control
```

The labels ("names") of the levels can be set when calling factor(). Two vectors are passed as arguments to parameters levels and labels with levels and matching labels in the same position. The argument passed to levels determines the order of the levels based on their old names or values, and the argument passed to labels gives new names to the levels.

```
factor(x = c("a", "a", "b", "b", "b", "a"), levels = c("a", "b"), la-
bels = c("treated", "control"))
## [1] treated treated control control treated
## Levels: treated control
```

The argument passed to labels can be a named vector that maps new labels onto the values as stored in the vector passed as argument to parameter x (see named vectors and mapping on page 67).

```
factor(x = c("a", "a", "b", "b", "b", "a"), labels = c(a = "treated", b = "con-
trol"))
## [1] treated treated control control treated
## Levels: treated control
```

In the examples above we passed a numeric vector or a character vector as an argument for parameter x of function factor(). It is also possible to pass a factor as an argument to parameter x. This makes it possible to modify the ordering of levels or replace the labels in a factor.

```
fct1 <- factor(x = vct1)
fct1
## [1] treated treated control control control treated
## Levels: control treated
factor(x = fct1, levels = c("treated", "control"))
## [1] treated treated control control control treated
## Levels: treated control</pre>
```

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**Merging factor levels.** We use factor() as shown below, setting the same label for the levels we want to merge.

3.32 Edit the code in the chunk above to use only a named vector for labels instead of separate vectors passed to levels and labels.

We can use indexing on factors in the same way as with vectors. In the next example, we use a test returning a logical vector to extract all "controls." We use function <code>levels()</code> to look at the levels of the factors, as with vectors, <code>lengtgh()</code> to query the number of values stored.

```
fct1
## [1] treated treated control control treated
## Levels: control treated
levels(fct1)
## [1] "control" "treated"
length(fct1)
## [1] 6
fct1.control <- fct1[fct1 == "control"]
fct1.control
## [1] control control control
## Levels: control treated
levels(fct1.control) # same as in my.factor
## [1] "control" "treated"
length(fct1.control) # shorter than my.factor
## [1] 3</pre>
```

# **3** How to drop unused levels in a factor?

It can be seen above that subsetting does not drop unused factor levels. Constructor function factor() can be used to explicitly drop the unused factor levels.

```
fct1.control <- factor(fct1.control)
levels(fct1.control) # the unused level was dropped
## [1] "control"</pre>
```

## **3** How to convert a factor into a vector with matching values?

This operation is not obvious, specially when the factor was created from a numeric vector.

```
vct3 <- rep(3:5, 4)
vct3
## [1] 3 4 5 3 4 5 3 4 5 3 4 5
fct3 <- factor(vct3)
fct3
## [1] 3 4 5 3 4 5 3 4 5 3 4 5
## Levels: 3 4 5
as.numeric(fct3)
## [1] 1 2 3 1 2 3 1 2 3 1 2 3
as.numeric(as.character(fct3))
## [1] 3 4 5 3 4 5 3 4 5 3 4 5</pre>
```

Why is a double conversion needed? Internally, factor values are are stored as running integers starting from one, each distinct integer value corresponding to a level. These underlying integer values are returned by as.numeric() when applied to a factor. The labels of the factor levels are always stored as character strings, even when these characters are digits. In contrast to as.numeric(), as.character() returns the character labels of the levels for each of the values stored in the factor. If these character strings represent numbers, they can be converted, in a second step, using as.numeric() into the original numeric values. Use of class and mode is described on section 3.8 on page 59, and str() on page 91.

```
class(fct3)
## [1] "factor"
mode(fct3)
## [1] "numeric"
str(fct3)
## Factor w/ 3 levels "3","4","5": 1 2 3 1 2 3 1 2 3 1 ...
```

- 3.33 Create a factor with levels labeled with words. Create another factor with the levels labeled with the same words, but ordered differently. After this convert both factors to numeric vectors using as.numeric(). Explain why the two numeric vectors differ or not from each other.
- Safely reordering and renaming factor levels. The simplest approach is to use factor() and its levels parameter as shown on page 80. In these more advanced examples we use levels() to retrieve the names of the levels from the factor itself to protect from possible bugs due to typing mistakes, or for changes in the naming conventions used.

Reverse previous order using rev().

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```
<- factor(c("treated",</pre>
                                   "treated",
                                                  "control".
                                                                "control",
                                                                             "con-
trol", "treated"))
levels(fct4)
## [1] "control" "treated"
fct4 <- factor(fct4, levels = rev(levels(fct4)))</pre>
levels(fct4)
## [1] "treated" "control"
   Sort in decreasing order, i.e., opposite to default.
fct5 <- factor(fct4,
               levels = sort(levels(fct4), decreasing = TRUE))
levels(fct5)
## [1] "treated" "control"
   Alter ordering using subscripting; especially useful with three or more levels.
fct6 <- factor(fct4, levels = levels(fct4)[c(2, 1)])</pre>
levels(fct6)
## [1] "control" "treated"
```

Reordering the levels of a factor based on summary quantities from data stored in a numeric vector is very useful, especially when plotting. Function reorder() can be used in this case. It defaults to using mean() for summaries, but other suitable summary functions, such as median() can be supplied in its place.

```
fct7 <- gl(2, 5, labels = c("A", "B"))
vct4 <- c(5.6, 7.3, 3.1, 8.7, 6.9, 2.4, 4.5, 2.1, 1.4, 2.0)
fct7
## [1] A A A A A B B B B B
## Levels: A B
fct7ord <- reorder(fct7, vct4)
levels(fct7ord)
## [1] "B" "A"
fct7rev <- reorder(fct7, -vct4) # a simple trick: change sign
levels(fct7rev)
## [1] "A" "B"</pre>
```

In the last statement, using the unary negation operator, which is vectorized, allows us to easily reverse the ordering of the levels, while still using the default function, mean(), to summarize the data.

**3.34 Reordering factor values.** It is possible to arrange the values stored in a factor either alphabetically according to the labels of the levels or according to the order of the levels. (The use of rep() is explained on page 30.)

```
# gl() keeps order of levels
FCT1 <- gl(4, 3, labels = c("A", "F", "B", "Z"))
FCT1
as.integer(FCT1)
# factor() orders levels alphabetically
FCT2 <- factor(rep(c("A", "F", "B", "Z"), times = rep(3, times = 4))) # nested calls
FCT2
as.integer(FCT2)
levels(FCT2)[as.integer(FCT2)]</pre>
```

We see above that the integer values by which levels in a factor are stored,

are equivalent to indices or "subscripts" referencing the vector of labels. Function sort() operates on the values' underlying integers and sorts according to the order of the levels while order() operates on the values' labels and returns a vector of indices that arrange the values alphabetically.

```
sort(FCT2)
FCT2[order(FCT2)]
FCT2[order(as.integer(FCT2))]
```

Run the examples in the chunk above and work out why the results differ.

Factors encode levels as integer values in a vector. In many cases, statistical computations, require the same information to be encoded as binary values using multiple *dummy variables*. Factors are much friendlier for the user to manage. They are converted into the equivalent dummy variables when a model formula is translated into a *model matrix*. This is handled transparently by most functions implementing fitting of statistical models to data (see sections 7.8 and 7.13 on pages 197 and 224).

### 3.13 Further reading

For further reading on the aspects of R discussed in the current chapter, I suggest the book *The Art of R Programming: A Tour of Statistical Software Design* (Matloff 2011).

# Base R: "Collective Nouns"

The information that is available to the computer consists of a selected set of *data* about the real world, namely, that set which is considered relevant to the problem at hand, that set from which it is believed that the desired results can be derived. The data represent an abstraction of reality...

Niklaus Wirth Algorithms + Data Structures = Programs, 1976

## 4.1 Aims of this chapter

Data-set organization and storage is one of the keys to efficient data analysis. How to keep together all the information that belongs together, say all measurements from an experiment and corresponding metadata such as treatments applied and/or dates. The title "collective nouns" is based on the idea that a data set is a collection of data objects.

In this chapter you will familiarize with how data sets are usually managed in R. I use both abstract examples to emphasize the general properties of data sets and the R classes available for their storage and a few more specific examples to exemplify their use in a more concrete way. While in chapter 3 the focus was on atomic data types and objects, like vectors, useful for the storage of collections of values of a given type, like numbers, in the present chapter the focus is on the storage within a single object of heterogeneous data, such as a combination of factors, and character and numeric vectors. Broadly speaking, heterogeneous *data containers*.

As in the previous chapter, I use diagrams to describe the structure of objects.

#### 4.2 Data from surveys and experiments

The data we plot, summarize and analyze in R, in most cases originate from measurements done as part of experiments or surveys. Data collected mechanically from user interactions with web sites or by crawling through internet content originate from a statistical perspective from surveys. The value of any data comes from knowing their origin, say treatments applied to plants, or country from where web site users connect, sometimes several properties are of interest to describe the origin of the data and in other cases observations consist in the measurement of multiple properties on each subject under study. Consequently, all software designed for data analysis implements ways of dealing with data sets as a whole both during storage and when passing them as arguments to functions. A data set is a usually heterogeneous collection of data with related information.

In R, lists are the most flexible type of objects useful for storing whole data sets. In most cases we do not need this much flexibility, so rectangular collections of observations are most frequently stored in a variation upon lists called data frames. These objects can have as their members the vectors and factors we described in chapter3.

Any R object can have attributes, allowing objects to carry along additional bits of information. Some like comments are part of R and aimed at storage of ancillary information or metadata by users. Other attributes are used internally by R and finally users can store arbitrary ancillary data using attributes created *ad hoc*.

#### 4.3 Lists

In R, objects of class list are in several respects similar the vectors described in chapter 3 but differently to vectors, the members they contain can be heterogeneous, i.e., different members of the same list can belong to different classes. In addition, while the member elements of a vector must be *atomic* values like numbers or character strings, any R object can be a list member including other lists.

In R, the members of a list can be considered as following a sequence, and accessible through numerical indexes, the same as the members of vectors. Members of a list as well as members of a vector can be named, and retrieved (indexed) through their names. In practice, named lists are more frequently used than named vectors. Lists are created using function list() similarly as c() is used for vectors.

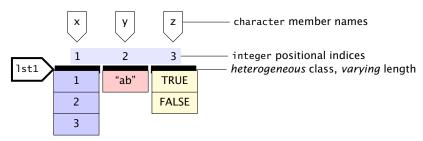
- In R lists can have as members not only objects storing data on observations and categories, but also function definitions, model formulas, unevaluated expressions, matrices, arrays, and objects of user defined classes.
- List and list-like objects are widely used in R because they make it possible to keep, for example, the data, instructions for operations and results from operations together in a single R object that can saved, copied, etc. as a unit. This

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avoids the proliferation of multiple disconnected objects with their interrelations being encoded only by their names, or even worse in separate notes or even in a person'd memory, all approaches that are error prone. Model fit functions described in chapter 7 are good examples of this approach. Objects used to store the instructions to build plots with multiple layers as described in chapter 9 are also good examples.

Our first list has as its members three different vectors, each one belonging to a different class: numeric, character and logical. The three vectors also differ in their length: 6, 1, and 2, respectively.

```
lst1 <- list(x = 1:3, y = "ab", z = c(TRUE, FALSE))
str(lst1)
## List of 3
## $ x: int [1:3] 1 2 3
## $ y: chr "ab"
## $ z: logi [1:2] TRUE FALSE
names(lst1)
## [1] "x" "y" "z"</pre>
```



With lists it is best to use informative names for indexing, as their members are heterogenous usually containing loosely related/connected data. Names make code easier to understand and mistakes more visible. Using names also makes code more robust to future changes in the position of list members in lists created upstream of our own R code. Below, we use both positional indices and names to highlight the similarities between lists and vectors.

Lists can behave as vectors with heterogeneous elements as members, as we will describe next. Lists can also be nested, so tree-like structures are also possible (see section 4.3.2 on page 91).

## **8** How to create an empty list?

In the same way as numeric() by default creates a numeric vector of length zero, list() by default creates a list object with no members.

```
list()
## list()
```

#### 4.3.1 Member extraction, deletion and insertion

In section 3.10 on page 64 we saw that the extraction operator [ ] applied to a vector, returns a vector, longer or shorter, possibly of length one, or even length

zero. Similarly, applying operator [ ] to a list returns a list, possibly of different length: lst1["x"] or lst[1] return a list containing only one member, the numeric vector stored at the first position of lst1. In the last statement in the chunk below, lst1[c(1, 3)] returns a list of length two as expected.

```
lst1["x"]
## $x
## [1] 1 2 3
lst1[1]
## $x
## [1] 1 2 3
lst1[c(1, 3)]
## $x
## [1] 1 2 3
##
## $z
## [1] TRUE FALSE
```

As with vectors negative positional indices remove members instead of extracting them. See page 90 for a safer approach to deletion of list members.

```
lst1[-1]
## $y
## [1] "ab"
##
## $z
## [1] TRUE FALSE
lst1[c(-1, -3)]
## $y
## [1] "ab"
```

Using operator [[ ]] (double square brackets) for indexing a list extracts the element stored in the list, in its original mode. In the example below, lst1[["x"]] and lst1[[1]] return a numeric vector. We might say that extraction operator [[ ]] reaches "deeper" into the list than operator [ ]. Operator \$, used in the second statement below, provides a shorthand notation, equivalent to using [[ ]] with a constant character value as argument.

```
lst1$x
## [1] 1 2 3
lst1[["x"]]
## [1] 1 2 3
lst1[[1]]
## [1] 1 2 3
```

- The default behavior also differs in that only \$ does partial matching of the member name (recognizes incomplete names), which makes dangerous its use in scripts or package code.
- We mentioned above that indexing by name can be done either with double square brackets, [[]], or with \$. Operators [] and [[]] work like normal R functions, accepting as arguments passed to them both constant values and variables for indexing. In contrast, \$ mainly intended for use when typing at the console, accepts only bare member names on its *rhs*. With [[]] the name of the variable or

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column is given as a character string, enclosed in quotation marks, or as a variable with mode character. A number as a positional index is also accepted.

```
lst1 <- list(abcd = 123, xyzw = 789)
lst1[[1]]
## [1] 123
lst1[["abcd"]]
## [1] 123
vct1 <- "abcd"
lst1[[vct1]]
## [1] 123</pre>
```

When using \$, the name is entered as a constant, without quotation marks, and cannot be a variable or a number.

```
lst1$abcd
## [1] 123
lst1$ab
## [1] 123
lst1$a
## [1] 123
```

Both in the case of lists and data frames (see section 4.4 on page 94), when using double square brackets, by default an exact match is required between the name in the object and the name used for indexing. In contrast, with \$, an unambiguous partial match is silently accepted. For interactive use, partial matching is helpful in reducing typing. However, in scripts, and especially R code in packages, it is best to avoid the use of \$ as partial matching to a wrong variable present at a later time, e.g., when someone else revises the script, can lead to very difficult-to-diagnose errors.

In addition, as \$ is implemented by first attempting a match to the name and then calling [[ ]], using \$ for indexing can result in slightly slower performance compared to using [[ ]]. It is possible to set R option warnPartialMatchDollar so that partial matching triggers a warning when using \$ to extract a member, which can be very useful when debugging.

```
is.vector(lst1[1])
## [1] TRUE
is.list(lst1[1])
## [1] TRUE
is.vector(lst1[[1]])
## [1] TRUE
is.list(lst1[[1]])
## [1] FALSE
```

The two extraction operators can be used together as shown below, with lst1[[1]] extracting the vector from lst1 and [3] extracting the member at position 3 of the vector.

```
lst1[[1]][3]
## [1] NA
```

Extraction operators can be used on the *lhs* as well as on the *rhs* of an assign-

ment, and lists can be empty, i.e, be of length zero. The example below makes use of this to build a list step by step.

```
1st2 <- list()
lst2[["x"]] <- 1:3</pre>
lst2[["y"]] <- "ab"</pre>
1st2[["z"]] <- c(TRUE, FALSE)</pre>
```

4.1 Compare 1st2 to 1st1, used for the examples above. Then run the code below and compare them again. Try to understand why 1st2 has changed as it did. Pay also attention to possible changes to the members' names.

```
1st2[["y"]] <- 1st2[["x"]]</pre>
```

Lists, as usually defined in languages like C, are based on pointers to memory locations, with pointers stored at each node. These pointers chain or link the different member nodes (this allows, for example, sorting of lists in place by modifying the pointers). In such implementations, indexing by position is not possible, or at least requires "walking" down the list, node by node. R does not implement pointers to "addresses", or locations, in memory. In R, list members can be accessed through positional indexes or member names, similarly to vectors. Of course, insertions and deletions in the middle of a list, shift the position of members and change which member is pointed at by indexes for positions past the modified location. The names, in contrast remain valid.

```
list(a = 1, b = 2, c = 3)[-2]
## $a
## [1] 1
##
## $c
## [1] 3
```

Three frequent operations on lists are concatenation, insertions and deletions. The same functions as with vectors are used: functions c() for concatenation and append() to append and insert lists. Lists can be combined only with other lists, otherwise the use is similar as with vectors (see pages 28-29).

```
lst3 <- append(lst1, list(yy = 1:10, zz = letters[5:1]), after = 2)</pre>
1st3
## $abcd
## [1] 123
##
## $xyzw
## [1] 789
##
## $yy
   [1] 1 2 3 4 5 6 7 8 9 10
##
##
## $zz
## [1] "e" "d" "c" "b" "a"
   To delete a member from a list we assign NULL to it.
```

```
1st1$y <- NULL
1st1
## $abcd
## [1] 123
```

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```
##
## $xyzw
## [1] 789
```

To investigate the members contained in a list, function str() (*structure*), used above, is convenient, especially when lists have many members. Structure formats lists more compactly than print() applied directly to a list.

```
print(lst1)
## $abcd
## [1] 123
##
## $xyzw
## [1] 789
str(lst1)
## List of 2
## $ abcd: num 123
## $ xyzw: num 789
```

#### 4.3.2 Nested lists

Lists can be nested, i.e., lists of lists can be constructed to an arbitrary depth. In the example below 1st4 and 1st5 are members of 1st6, i.e., 1st4 and 1st5 are nested within 1st6.

```
lst4 <- list("a", "aa", 10)
lst5 <- list("b", TRUE)
lst6 <- list(A = lst4, B = lst5) # nested
str(lst6)

## List of 2
## $ A:List of 3
## ..$ : chr "a"
## ..$ : chr "aa"
## ..$ : num 10
## $ B:List of 2
## ..$ : chr "b"
## ..$ : logi TRUE</pre>
```

A nested list can alternatively be constructed within a single statement in which several member lists are created. Here we combine the first three statements in the earlier chunk into a single one.

```
lst7 <- list(A = list("a", "aa", 10), B = list("b", TRUE))
str(lst7)

## List of 2

## $ A:List of 3

## ..$ : chr "a"

## ..$ : chr "aa"

## ..$ : num 10

## $ B:List of 2

## ..$ : chr "b"

## ..$ : logi TRUE</pre>
```

A list can contain a combination of list and vector members.

```
C = c(1, 3, 9),
             D = 4321)
str(1st8)
## List of 4
  $ A:List of 3
     ..$ : chr "a"
     ..$ : chr "aa"
##
     ..$ : num 10
   $ B:List of 2
##
     ..$ : chr "b"
##
##
     ..$: logi TRUE
    $ C: num [1:3] 1 3 9
##
   $ D: num 4321
```

The logic behind extraction of members of nested lists using indexing is the same as for simple lists, but applied recursively—e.g., 1st7[[2]] extracts the second member of the outermost list, which is another list. As, this is a list, its members can be extracted using again the extraction operator: 1st7[[2]][[1]]. It is important to remember that these concatenated extraction operations are written so that the leftmost operator is applied to the outermost list.

The example above uses the [[ ]] operator, but the left to right precedence also applies to concatenated calls to [ ] and to calls combining both operators.

4.2 What do you expect each of the statements below to return? *Before running the code*, predict what value and of which mode each statement will return. You may use implicit or explicit calls to print(), or calls to str() to visualize the structure of the different objects.

```
LST9 <- list(A = list("a", "aa", "aaa"), B = list("b", "bb"))
# str(LST9)
LST9[2:1]
LST9[1]
LST9[[1]][2]
LST9[[1]][[2]]
LST9[2]
LST9[2][[1]]
```

When dealing with deep lists, it is sometimes useful to limit the number of levels of nesting returned by str() by means of a numeric argument passed to parameter max.levels.

```
str(lst8, max.level = 1)
## List of 4
## $ A:List of 3
## $ B:List of 2
## $ C: num [1:3] 1 3 9
## $ D: num 4321
```

Sometimes we need to flatten a list, or a nested structure of lists within lists. Function unlist() is what should be normally used in such cases.

The list 1st10 is a nested system of lists, but all the "terminal" members are character strings. In other words, terminal nodes are all of the same mode, allowing the list to be "flattened" into a character vector.

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```
lst10 <- list(A = list("a", "aa", "aaa"), B = list("b", "bb"))</pre>
vct1 <- unlist(lst10)</pre>
vct1
     Α1
          A2
                А3
                        в1
                              В2
                      "b" "bb"
   "a" "aa" "aaa"
##
is.list(lst10)
## [1] TRUE
is.list(vct1)
## [1] FALSE
mode(lst10)
## [1] "list"
mode(vct1)
## [1] "character"
names(lst10)
## [1] "A" "B"
names(vct1)
## [1] "A1" "A2" "A3" "B1" "B2"
```

The returned value is a vector with named member elements. We use function str() to figure out how this vector relates to the original list. The names, always of mode character, are based on the names of list elements when available, while characters depicting positions as numbers are used for anonymous nodes. We can access the members of the vector either through numeric indexes or names.

```
str(vct1)
## Named chr [1:5] "a" "aa" "aaa" "b" "bb"
## - attr(*, "names")= chr [1:5] "A1" "A2" "A3" "B1" ...
vct1[2]
## A2
## "aa"
vct1["A2"]
## A2
## "aa"
```

4.3 Function unlist() has two additional parameters, with default argument values, which we did not modify in the example above. These parameters are recursive and use.names, both of them expecting a logical value as an argument. Modify the statement c.vec <- unlist(c.list), by passing FALSE as an argument to these two parameters, in turn, and in each case, study the value returned and how it differs with respect to the one obtained above.

Function unname() can be used to remove names safely—i.e., without risk of altering the mode or class of the object.

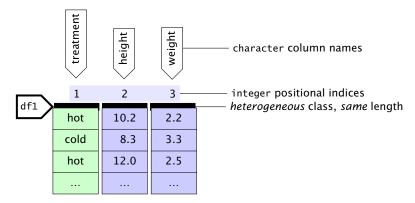
```
unname(vct1)
## [1] "a" "aa" "aaa" "b" "bb"
unname(lst10)
## [[1]]
## [[1]][[1]]
## [1] "a"
##
## [[1]][[2]]
## [1] "aa"
##
```

```
## [[1]][[3]]
## [1] "aaa"
##
##
##
[[2]]
## [[2]][[1]]
## [1] "b"
##
## [[2]][[2]]
## [1] "bb"
```

#### 4.4 Data frames

Data frames are a special type of list, in which all members have the same length, giving origin to a matrix-like object, in which columns can belong to different classes. Most commonly the member "columns" are vectors or factors, but they can also be matrices with the same number of rows as the enclosing data frame, or lists with the same number of members as rows in the enclosing data frame.

Data frames are central to most data manipulation and analysis procedures in R. They are commonly used to store observations, with numeric columns holding data for continuous variables and factor columns data for categorical variables. Binary variables can be stored in logical columns. Text data can be stored in character columns. Date and time can be stored in columns of specific classes, such as POSIXct. In the diagram below, column treatment is a factor with two levels encoding two conditions, hot and cold. Columns height and weight are numeric vectors containing measurements.



Data frames are created with constructor function data.frame() with a syntax similar to that used for lists.

```
## 1
                 10.2
                         2.2
           hot
## 2
                  8.3
                          3.3
          cold
## 3
           hot
                 12.0
                          2.5
## 4
          cold
                  9.0
                          2.8
## 5
           hot
                 11.2
                          2.4
## 6
          cold
                  8.7
                          3.0
colnames (df1)
## [1] "treatment" "height"
                                "weight"
rownames (df1)
## [1] "1" "2" "3" "4" "5" "6"
str(df1)
## 'data.frame': 6 obs. of 3 variables:
   $ treatment: Factor w/ 2 levels "cold","hot": 2 1 2 1 2 1
    $ height : num 10.2 8.3 12 9 11.2 8.7
              : num 2.2 3.3 2.5 2.8 2.4 3
## $ weight
class(df1)
## [1] "data.frame"
mode(df1)
## [1] "list"
is.data.frame(df1)
## [1] TRUE
is.list(df1)
## [1] TRUE
```

We can see above that when printed each row of a data.frame is preceded by a row name. Row names are character strings, just like column names. The data.frame() constructor adds by default row names representing running numbers. Default row names are rarely of much use, except to track insertions and deletions of rows during debugging.

4.4 As the expectation is that all member variables (or "columns") have equal length, if vectors of different lengths are supplied as arguments, the shorter vector(s) is/are recycled, possibly several times, until the required full length is reached, as shown below for treatment.

Are df1 crated above and df2 created here equal?

With function class() we can query the class of an R object (see section 3.8 on page 59). As we saw in the previous chunk, list and data.frame objects belong to two different classes. However, their mode is the same. Consequently, data frames inherit the methods and characteristics of lists, as long as they have not been hidden by new ones defined for data frames (for an explanation of *methods*, see section 6.3 on page 176).

Extraction of individual member variables or "columns" can be done like in a list with operators [[ ]] and \$ (see call out in 88).

```
df1$height
## [1] 10.2 8.3 12.0 9.0 11.2 8.7
df1[["height"]]
## [1] 10.2 8.3 12.0 9.0 11.2 8.7
```

```
df1[[2]]
## [1] 10.2 8.3 12.0 9.0 11.2 8.7
class(df1[["height"]])
## [1] "numeric"
```

In the same way as with lists, we can add member variables to data frames. Recycling takes place if needed.

```
df1$x2 <- 6:1
df1[["x3"]] <- "b"
str(df1)
## 'data.frame': 6 obs. of 5 variables:
## $ treatment: Factor w/ 2 levels "cold","hot": 2 1 2 1 2 1
## $ height : num 10.2 8.3 12 9 11.2 8.7
## $ weight : num 2.2 3.3 2.5 2.8 2.4 3
## $ x2 : int 6 5 4 3 2 1
## $ x3 : chr "b" "b" "b" "b" ...</pre>
```

4.5 We have added two columns to the data frame, and in the case of column x3 recycling took place. This is where lists and data frames differ substantially in their behavior. In a data frame, although class and mode can be different for different member variables (columns), they are required to be vectors or factors of the same length (or a matrix with the same number of rows, or a list with the same number of members). In the case of lists, there is no such requirement, and recycling never takes place when adding a member. Compare the values returned below for LST1, to those in the example above for df1.

```
LST1 <- list(x = 1:6, y = "a", z = c(TRUE, FALSE))

str(LST1)

## List of 3

## $ x: int [1:6] 1 2 3 4 5 6

## $ y: chr "a"

## $ z: logi [1:2] TRUE FALSE

LST1$x2 <- 6:1

LST1$x3 <- "b"

str(LST1)

## List of 5

## $ x: int [1:6] 1 2 3 4 5 6

## $ y: chr "a"

## $ z: logi [1:2] TRUE FALSE

## $ x2: int [1:6] 6 5 4 3 2 1

## $ x3: chr "b"
```

## **19** How to make a list of data frames?

We create a list of data frames in the same way as we create a nested list of lists, or in fact of a list of any other R objects. See page section 4.3.2 on page 91.

```
list(df1, df2)
## [[1]]
    treatment height weight x2 x3
## 1
          hot
               10.2
                         2.2 6 b
## 2
          cold
                8.3
                         3.3 5 b
                12.0
## 3
          hot
                         2.5 4 b
          cold
                 9.0
                         2.8 3 b
## 5
          hot
                11.2
                         2.4 2 b
## 6
          cold
                 8.7
                         3.0 1 b
##
## [[2]]
##
     treatment height weight
## 1
               10.2
          hot
## 2
                 8.3
                         3.3
          cold
## 3
          hot
                12.0
                         2.5
## 4
          cold
                 9.0
                         2.8
          hot
                11.2
                         2.4
## 6
          cold
```

# **?** How to create an empty data frame?

In the same way as numeric() by default creates a numeric vector of length zero, data.frame() by default creates a data.frame with zero rows and no columns.

```
data.frame()
## data frame with 0 columns and 0 rows
```

## **?** How to add new column to a data frame (to the front and end)?

In the same way as me can assign a new member to a list using the extraction operator [[ ]], we can add a new column to a data frame (see page 89). In this case, if the column name does not already exist, the assigned vector or factor is appended as the last column (no recycling applied to short vectors or factors unless of length one).

To add a column at the front, we can use function cbind() (column bind).

Being two dimensional and rectangular in shape, data frames, in relation to indexing and dimensions behave similarly to a matrix. They have two margins, rows and columns, and two indices identify the location of a member "cell". We provide some examples here, but please consult section 3.10 on page 64 and section 3.11 on page 71 for additional details.

Matrix-like notation allows simultaneous extraction from multiple columns, which is not possible with lists. The value returned is in most cases a "smaller" data frame as in this example.

```
df1[2:3, 1:2]
    treatment height
## 2
         cold
                 8.3
## 3
          hot
                12.0
# first column, df1[[1]] preferred
df1[ , 1]
## [1] hot cold hot cold hot cold
## Levels: cold hot
# first column, df1[["x"]] or df1$x preferred
df1[ , "treatment"]
## [1] hot cold hot cold hot cold
## Levels: cold hot
# first row
df1[1, ]
##
    treatment height weight x2 x3
                        2.2 6 b
## 1
          hot
               10.2
# first two rows of the third and fourth columns
df1[1:2, c(FALSE, FALSE, TRUE, TRUE, FALSE)]
    weight x2
       2.2 6
## 1
## 2
       3.3
            5
# the rows for which comparison is true
df1[df1$treatment == "hot" , ]
    treatment height weight x2 x3
## 1
          hot
                10.2
                         2.2 6 b
## 3
           hot
                12.0
                         2.5 4 b
                         2.4 2 b
## 5
          hot
                11.2
# the heights > 8
df1[df1$height > 8, "height"]
## [1] 10.2 8.3 12.0 9.0 11.2 8.7
```

As explained earlier for vectors (see section 3.10 on page 64), indexing can be present both on the right-hand side and left-hand side of an assignment, allowing the replacement individual values as well as rectangular chunks.

The next few examples do assignments to "cells" of df1, either to one whole column, or individual values. The last statement in the chunk below copies a number from one location to another by using indexing of the same data frame both on the right side and left side of the assignment.

```
df1[1, 2] <- 99
df1
##
    treatment height weight x2 x3
## 1
               99.0
                        2.2 6 b
         hot
## 2
         cold
                8.3
                        3.3 5
                               h
## 3
          hot
                12.0
                        2.5 4
                               h
## 4
         cold
                9.0
                        2.8
                            3
                               b
## 5
          hot
                11.2
                        2.4
                            2
                               b
                        3.0 1
## 6
         cold
                 8.7
```

```
df1[ , 2] <- -99
df1
##
     treatment height weight x2 x3
## 1
           hot
                  -99
                         2.2 6 b
                  -99
## 2
                         3.3 5 b
          cold
## 3
                  -99
                         2.5 4 b
           hot
## 4
          cold
                  -99
                         2.8 3 b
## 5
           hot
                  _99
                         2.4 2 b
                  -99
                         3.0
                              1 b
## 6
          cold
df1[["height"]] <- c(10, 12)
df1
##
     treatment height weight x2 x3
## 1
           hot
                   10
                         2.2
## 2
          cold
                   12
                         3.3
                              5
                                 b
                         2.5
## 3
           hot
                   10
                              4
                                 b
## 4
          cold
                   12
                         2.8
                              3
                                 b
## 5
          hot
                   10
                         2.4
                              2
                                 b
          cold
                   12
                         3.0
                              1
## 6
                                 b
df1[1, 2] <- df1[6, 3]
df1
##
     treatment height weight x2 x3
## 1
           hot
                    3
                         2.2 6
## 2
          cold
                   12
                         3.3 5 b
                   10
                         2.5 4 b
## 3
           hot
## 4
          cold
                   12
                         2.8 3 b
## 5
           hot
                   10
                         2.4 2 b
                   12
                         3.0 1 b
## 6
          cold
df1[3:6, 2] <- df1[6, 3]
df1
##
     treatment height weight x2 x3
## 1
           hot
                    3
                         2.2
                              6
## 2
          cold
                   12
                         3.3
                              5
                                 b
                         2.5
## 3
           hot
                    3
                              4
                                 b
                    3
                         2.8
                              3
## 4
          cold
                                 b
                              2
## 5
           hot
                    3
                         2.4
                                 b
## 6
          cold
                    3
                         3.0
                              1
                                 b
```

Similarly as with matrices, if we extract a single column from a data frame using matrix-like indexing, it is by default simplified into a vector or factor, i.e., the column-dimension is dropped. By passing drop = FALSE, we can prevent this. Contrary to matrices, rows are not simplified in the case of data frames.

```
is.data.frame(df1[1, ])
## [1] TRUE
is.data.frame(df1[ , 2])
## [1] FALSE
is.data.frame(df1[ , "treatment"])
## [1] FALSE
is.vector(df1[1:2, 2:3])
## [1] TRUE
is.vector(df1[ , 2])
## [1] TRUE
is.factor(df1[ , "treatment"])
## [1] TRUE
is.vector(df1[1:2, 2:3])
```

In contrast to matrices and data frames, the extraction operator [ ] of tibbles—defined in package 'tibble'— never simplifies returned one-column tibbles into vectors (see section 8.4.2 on page 245 for details on the differences between data frames and tibbles).

4.6 Usually data frames are created from lists or by passing individual vectors and factors to the constructors. It is also possible to construct data frames starting from matrices, other data frames and named vectors and combinations of them. In these cases additional nuances become important. We give only some examples here, as the details are well described in help(data.frame).

We use a named numeric vector, and a factor. The names are moved from the vector to the rows of the data frame! Consult help(data.frame) for an explanation.

```
vct1 \leftarrow c(one = 1, two = 2, three = 3, four = 4)
fct1 <- as.factor(c(1, 2, 3, 2))
df1 <- data.frame(fct1, vct1)</pre>
df1
          fct1 vct1
                  1
## one
             1
                   2
## two
             2
## three
             3
                  3
## four
df1$my.vector
## NULL
```

If we protect the vector with R's identity function I() the names are not removed from the vector as can be seen by extracting the column from the data frame.

```
df2 <- data.frame(fct1, I(vct1))</pre>
df2
##
          fct1 vct1
## one
             1
                   1
             2
                   2
## two
                   3
## three
             3
## four
df2$my.vector
## NULL
```

If we start with a matrix instead of a vector, the matrix is by default split into separate columns in the data frame. If the matrix has no column names, new ones are created.

If we protect the matrix with function I(), it is not split, and the whole matrix becomes a column in the data frame.

```
df5 <- data.frame(fct1, I(mat1))</pre>
df5
##
     fct1 mat1.1 mat1.2 mat1.3
## 1
                1
                        5
         2
                2
                               10
## 2
                         6
         3
                3
                        7
## 3
                               11
         2
## 4
                4
                        8
                               12
df5$my.matrix
## NULL
```

If we start with a list, each member with a suitable number of elements, each member becomes a column in the data frame. In the case of a too short one, recycling is applied.

```
lst1 <- list(a = 4:1, b = letters[4:1], c = "n", d = "z")
df6<- data.frame(fct1, lst1)
df6

## fct1 a b c d
## 1     1 4 d n z
## 2     2 3 c n z
## 3     3 2 b n z
## 4     2 1 a n z</pre>
```

The behaviour is quite different if we protect the list with I(): then the list is added in whole as a variable or column in the data frame. In this case the length or number of members in the list itself must match the number of rows in the data frame, while the length of the individual members of the list can vary. This is similar to the default behaviour of tibbles, but R data frames require explicit use of I() (see chapter 8 on page 241 for details about package 'tibble').

```
df7<- data.frame(fct1, I(lst1))</pre>
df7
##
     fct1
                  1st1
## a
         1 4, 3, 2, 1
## b
         2 d, c, b, a
## c
         3
                     n
         2
## d
                     Ζ
df7$my.list
## NULL
```

What is this exercise about? Do check the documentation carefully and think of uses where the flexibility gained by use of function I() to protect arguments passed to the data.frame() constructor can be useful. In addition, write code to extract individual members of embedded matrices and lists using indexing in a single R statement in each case. Finally test if the behavior is the same when assigning new member variables (or "columns") to an existing data frame.

#### 4.4.1 Sub-setting data frames

When the names of data frames are long, complex conditions become awkward to write using indexing—i.e., subscripts. In such cases subset() is handy because evaluation is done in the "environment" of the data frame, i.e., the names of the columns are recognized if entered directly when writing the condition. Function subset() "filters" rows, usually corresponding to observations or experimental

units. The condition is computed for each row, and if it returns TRUE, the row is included in the returned data frame, and excluded if FALSE.

We create a data frame with six rows and three columns. For column y, we rely on R automatically extending "a" by repeating it six times, while for column z, we rely on R automatically extending c(TRUE, FALSE) by repeating it three times.

4.7 What is the behavior of subset() when the condition is NA? Find the answer by writing code to test this, for a case where tests for different rows return NA, TRUE and FALSE.

When calling functions that return a vector, data frame, or other structure, the extraction operators [ ], [[ ]], or \$ can be appended to the rightmost parenthesis of the function call, in the same way as to the name of a variable holding the same data

- 4.8 When do extraction operators applied to data frames return a vector or factor, and when do they return a data frame? Please, experiment with your own code examples to work out the answer.
- In the case of subset() we can select columns directly as shown below, while for most other functions, extraction using operators [ ], [[ ]] or \$ is needed.

```
subset(df8, x > 3, select = 2)
##  y
## 4 a
## 5 a
## 6 a
subset(df8, x > 3, select = x)
##  x
## 4 4
## 5 5
## 6 6
```

```
subset(df8, x > 3, select = "x")
##     x
## 4 4
## 5 5
## 6 6
```

None of the examples in the last four code chunks alters the original data frame df8. We can store the returned value using a new name if we want to preserve df8 unchanged, or we can assign the result to df8, deleting in the process, the previously stored value.

In the examples above, the names in the expression passed as the second argument to subset() were searched within df8 and found. However, if not found in the data frame, objects with matching names are searched for in the global environment (as variables outwith the data frame, visible from the user's workspace). There being no variable A in the data frame df8, vector A from the environment is silently used in the chunk below resulting in a returned data frame with no rows as A > 3 returns FALSE.

```
A <- 1
subset(df8, A > 3)
## [1] x y z
## <0 rows> (or 0-length row.names)
```

This also applies to the expression passed as argument to parameter select, here shown as a way of selecting columns based on names stored in a character vector.

The use of subset() is convenient, but more prone to bugs compared to directly using the extraction operator [ ]. This same "cost" to achieving convenience applies to functions like attach() and with() described below. The longer time that a script is expected to be used, adapted and reused, the more careful we should be when using any of these functions. An alternative way of avoiding excessive verbosity is to keep the names of data frames short.

A frequently used way of deleting a column by name from a data frame is to assign NULL to it—i.e., in the same way as members are usually deleted from lists. This approach modifies df9 in place, rather than returning a modified copy of df9.

```
df9 <- df8
head(df9)
## x y z
## 1 1 a TRUE
## 2 2 a FALSE
## 3 3 a TRUE
## 4 4 a FALSE
```

```
## 5 5 a TRUE
## 6 6 a FALSE

df9[["y"]] <- NULL
head(df9)

## x z
## 1 1 TRUE
## 2 2 FALSE
## 3 3 TRUE
## 4 4 FALSE
## 5 5 TRUE
## 6 6 FALSE
```

Alternatively, we can use negative indexing to remove columns from a copy of a data frame. In this example we remove a single column. As base R does not support negative indexing by name with the extraction operator, we need to find the numerical index of the column to delete. (See the examples above using subset() with bare names to delete columns.)

Instead of using the equality test, we can use the operator %in% or function grep1() to create a logical vector useful to delete or select multiple columns in a single statement.

4.9 In the previous code chunk we deleted the last column of the data frame df8, but using the extraction operator, we modified only the returned copy of df8, leaving df8 unchanged. Thus we reuse it here for a surprising trick. You should first untangle how it changes the positions of columns and rows, and afterwards think how and why indexing with the extraction operator [ ] on both sides of the assignment operator <- can be useful when working with data.

```
df8[1:6, c(1,3)] \leftarrow df8[6:1, c(3,1)]
df8
```

Although in this last example we used numeric indexes to make it more interesting, in practice, especially in scripts or other code that will be reused, do use column or member names instead of positional indexes whenever possible. This makes code much more reliable, as changes elsewhere in the script could alter the order of columns and *invalidate* numerical indexes. In addition, using meaningful names makes programmers' intentions easier to understand.

## 4.4.2 Summarizing and splitting data frames

Function summary() can be used to obtain a summary from objects of most R classes, including data frames. It is also possible to use sapply(), lapply() or vapply() to apply any suitable function to data by columns (see section 5.8 on page 154 for a description of these functions and their use).

```
summary(df8)
##
##
         :1.00
                  Length:6
                                      Mode :logical
   1st Qu.:2.25
                  Class :character
                                      FALSE:3
  Median :3.50
                  Mode :character
                                      TRUE:3
##
  Mean
          :3.50
##
   3rd Qu.:4.75
          :6.00
##
   Max.
```

R function split() makes it possible to split a data frame into a list of data frames, based on the levels of a factor, even if the rows are not ordered according to factor levels.

We create a data frame with six rows and three columns. In the case of column z, we rely on R to automatically extend c("a", "b") by repeating it three times so as to fill the six rows.

```
df10 \leftarrow data.frame(x1 = 1:6, x2 = c(1, 5, 4, 2, 6, 3), z = c("a", "b"))
split(df10, df10$z)
## $a
##
     x1 x2 z
## 1 1 1 a
## 3 3
        4 a
## 5
     5
        6 a
##
## $b
   x1 x2 z
##
## 2 2 5 b
         2 b
## 4 4
## 6 6 3 b
```

The same operation can be specified using a one-sided formula ~z to indicate the grouping.

Function unsplit() can be used to reverse splitting done by split().

split() is sometimes used in combination with apply functions (see section 5.8 on page 154) to compute group or treatment summaries. However, in most cases it is simpler to use aggregate() for computing such summaries.

Related to splitting a data frame is the calculation of summaries based on a subset of cases, or more commonly summaries for all observations but after grouping them based on the values in a column or the levels of a factor.

## **1** How to summarize one variable from a data frame by group?

To summarize a single variable by group we can use aggregate().

```
aggregate(x = iris$Petal.Length, by = list(iris$Species), FUN = mean)
## Group.1 x
## 1 setosa 1.462
## 2 versicolor 4.260
## 3 virginica 5.552
```

## **?** How to summarize numeric variables from a data frame by group?

To summarize variables we can use aggregate() (see section 8.7.2 on page 259 for an alternative approach using package 'dplyr').

```
aggregate(x = iris[ , sapply(iris, is.numeric)], by = list(iris$Species), FUN = mean)
        Group.1 Sepal.Length Sepal.Width Petal.Length Petal.Width
         setosa
                       5.006
                                    3.428
                                                 1.462
                                                              0.246
                       5.936
                                    2.770
                                                  4.260
## 2 versicolor
                                                              1.326
                       6.588
                                    2.974
## 3 virginica
                                                  5.552
```

For these data as the only non-numeric variable is **species** we could have also used formula notation as shown below.

There is also a formula-based aggregate() method (or "variant") available (R *formulas* are described in depth in section 7.13 on page 224). In aggregate(), the left hand side (*lhs*) of the formula indicates the variable to summarize and the right hand side (*rhs*) the factor used to split the data before summarizing them.

```
aggregate(x1 ~ z, FUN = mean, data = df10)
##  z x1
## 1 a 3
## 2 b 4
```

We can summarize more than one column at a time.

If all the columns not used for grouping are valid input to the function passed as argument to fun the formula can be simplified using . with meaning "all columns except those on the *rhs* of the formula".

Function aggregate() can be also used to aggregate time series data based on time intervals (see help(aggregate)).

#### 4.4.3 Re-arranging columns and rows

As with members of vectors and lists, to change the position of columns or row in a data frame we use the extraction operator and indexing by name or position. In a matrix-like object, such as data frames the first index corresponds to rows and the second to columns.

The most direct way of changing the order of columns and/or rows in data

frames (as for matrices and arrays) is to use subscripting. Once we know the original position and target position we can use column names or positions as indexes on the right-hand side, listing all columns to be retained, even those remaining at their original position.

When using the extraction operator [ ] on both the left-hand-side and right-hand-side with a numeric vector as argument to swap two columns, the vectors or factors are swapped, while the names of the columns are not! To retain the correspondence between column naming and column contents after swapping or rearranging the columns *using numeric indices*, we need to separately move the names of the columns. This may seem counter intuitive, unless we think in terms of positions being named rather than the contents of the columns being linked to the names.

```
df11 <- data.frame(A = 1:10, B = 3, C = c("A", "B"))
head(df11, 2)
##
    АВС
## 1 1 3 A
## 2 2 3 B
df11[ , 1:2] <- df11[ , 2:1]
head(df11, 2)
    АВС
## 1 3 1 A
## 2 3 2 B
colnames(df11)[1:2] <- colnames(df11)[2:1]</pre>
head(df11, 2)
##
    BAC
## 1 3 1 A
## 2 3 2 B
```

Taking into account that order() returns the indexes needed to sort a vector (see page 69), we can use order() to generate the indexes needed to sort the rows of a data frame. In this case, the argument to order() is usually a column of the data frame being arranged. However, any vector of suitable length, including the result of applying a function to one or more columns, can be passed as an argument to order(). Function order() is not useful for sorting columns of data frames *based* on data from the columns as it requires a vector across columns as input, which is possible only when all columns are of the same class. (In the case of matrix and array this approach can be applied to any of their dimensions as all their elements homogenously belong to one class.)

## How to order columns or rows in a data frame?

We use column names or numeric indexes with the extraction operator [ ] only on the *rhs* of the assignment. For example, to arrange the columns of data set iris in decreasing alphabetical order, we use sort() as shown, or order() (see page 69).

```
sorted_cols_iris <- iris[ , sort(colnames(iris), decreasing = TRUE)]</pre>
head(sorted_cols_iris, 6)
     Species Sepal. Width Sepal. Length Petal. Width Petal. Length
      setosa
                      3.5
                                     5.1
                                     4.9
                      3.0
                                                  0.2
      setosa
                                                                1.4
                                     4.7
                                                                1.3
      setosa
                      3.2
      setosa
                      3.1
                                     4.6
                                                  0.2
                                                                1.5
## 5
      setosa
                      3.6
                                     5.0
                                                  0.2
                                                                1.4
      setosa
                      3.9
                                     5.4
                                                  0.4
                                                                1.7
```

Similarly we use values in a column as argument to order() to obtain the numeric indices to sort rows.

```
sorted_rows_iris <- iris[order(iris$Petal.Length), ]</pre>
head(sorted_rows_iris, 6)
      Sepal.Length Sepal.width Petal.Length Petal.width Species
## 23
               4.6
                            3.6
                                          1.0
## 14
               4.3
                            3.0
                                          1.1
                                                       0.1
               5.8
                            4.0
## 15
                                          1.2
                                                       0.2
                            3.2
               5.0
                                          1.2
                                                       0.2
## 3
                4.7
                            3.2
                                          1.3
                                                       0.2
                                                             setosa
## 17
                             3.9
                5.4
                                          1.3
                                                       0.4
                                                             setosa
```

4.10 Create a new data frame containing three numeric columns with three different haphazard sequences of values and a factor with two levels. Call these columns A, B, C and F. 1) Sort the rows of the data frame so that the values in A are in decreasing order. 2) Sort the rows of the data frame according to increasing values of the sum of A and B without adding a new column to the data frame or storing the vector of sums in a variable. In other words, do the sorting based on sums calculated on-the-fly. 1) Sort the rows by level of factor F, and 2) by level of factor F and by values in B within each factor level. Hint: revisit the exercise on page 83 were the use of order() on factors is described.

#### 4.4.4 Re-encoding or adding variables

It is common that some variables need to be added to an existing data frame based on existing variables, either as a computed value or based on mapping for example treatments to sample codes already in a data frame. In the second case, named vectors can be used to replace values in a variable or to add a variable to a data frame.

Mapping is possible because the length of the value returned by the extraction operator [ ] is given by the length of the indexing vector (see section 3.10 on page 64). Although we show toy-like examples, this approach is most useful with data frames containing many rows.

If the existing variable is a character vector or factor, we need to create a named vector with the new values as data and the existing values as names.

```
df12 <-
 data.frame(genotype = rep(c("WT", "mutant1", "mutant2"), 2),
            value = c(1.5, 3.2, 4.5, 8.2, 7.4, 6.2))
mutant <- c(WT = FALSE, mutant1 = TRUE, mutant2 = TRUE)</pre>
df12$mutant <- mutant[df12$genotype]</pre>
##
    genotype value mutant
## 1
          WT 1.5 FALSE
## 2 mutant1
              3.2
                     TRUE
## 3 mutant2
               4.5
                     TRUF
## 4
         WT
               8.2 FALSE
## 5 mutant1
               7.4
                     TRUF
## 6 mutant2
                6.2
                      TRUE
```

If the existing variable is an integer vector, we can use a vector without names, being careful that the positions in the *mapping* vector match the values of the existing variable

```
df13 <- data.frame(individual = rep(1:3, 2),</pre>
                    value = c(1.5, 3.2, 4.5, 8.2, 7.4, 6.2))
genotype <- c("WT", "mutant1", "mutant2")</pre>
df13$genotype <- genotype[df13$individual]
df13
     individual value genotype
##
## 1
              1
                  1.5
                             WT
## 2
              2
                  3.2 mutant1
## 3
              3
                  4.5 mutant2
## 4
              1
                  8.2
                             WT
## 5
              2
                  7.4
                       mutant1
## 6
              3
                  6.2 mutant2
```

4.11 Add a variable named genotype to the data frame below so that for individual 4 its value is "wT", for individual 1 its value is "mutant1", and for individual 2 its value is "mutant2".

```
DF1 <- data.frame(individual = rep(c(2, 4, 1), 2),
value = c(1.5, 3.2, 4.5, 8.2, 7.4, 6.2))
```

## 4.4.5 Operating within data frames

In the case of computing new values from existing variables named vectors are of limited use. Instead, variables in a data frame can be added or modified with R functions transform(), with() and within(). These functions can be thought as convenience functions as the same computations can be done using the extraction operators to access individual variables, in the lhs, rhs or both lhs and rhs (see section 3.10 on page 64).

In the case of with() only one, possibly compound code statement is affected and this statement is passed as an argument. As before, we need to fully specify the left-hand side of the assignment. The value returned is the one returned by the statement passed as an argument, in the case of compound statements, the value returned by the last contained simple code statement to be executed. Consequently, if the intent is to modify the container, assignment to an individual member variable (column in this case) is required.

In this example, column A of df14 takes precedence, and the returned value is the expected one.

```
df14 <- data.frame(A = 1:10, B = 3)
df14$C <- with(df14, (A + B) / A) # add column
head(df14, 2)
## A B C
## 1 1 3 4.0
## 2 2 3 2.5</pre>
```

In the case of within(), assignments in the argument to its second parameter affect the object returned, which is a copy of the container (In this case, a whole data frame), which still needs to be saved through assignment. Here the intention is to modify it, so we assign it back to the same name, but it could have been assigned to a different name so as not to overwrite the original data frame.

```
df14$C <- NULL
df15 <- within(df14, C <- (A + B) / A) # midified copy
head(df15, 2)
## A B C
## 1 1 3 4.0
## 2 2 3 2.5</pre>
```

In the example above, using within() makes little difference compared to using with() with respect to the amount of typing or clarity, but with multiple member variables being operated upon, as shown below, within() has an advantage resulting in more concise and easier to understand code.

Repeatedly pre-pending the name of a *container* such as a list or data frame to the name of each member variable being accessed can make R code verbose and difficult to understand. Functions attach() and its matching detach() allow us to change where R first looks for the names of objects we include in a code statement. When using a long name for a data frame, entering a simple calculation can easily result in a difficult to read statement. Here even with a very short name, the difference is noticeable.

```
df14$C <- (df14$A + df14$B) / df14$A
df14$D <- df14$A * df14$B
df14$D <- df14$A / df14$B + 1
head(df14, 2)
## A B C D
## 1 1 3 4.0 1.333333
## 2 2 3 2.5 1.666667</pre>
```

Using attach() we can alter where R looks up names and consequently simplify the statement. With detach() we can restore the original state. It is important to remember that here we can only simplify the right-hand side of the assignment, while the "destination" of the result of the computation still needs to be fully specified on the left-hand side of the assignment operator. We include below only one statement between attach() and detach() but multiple statements are allowed. Furthermore, if variables with the same name as the columns exist in the search path, these will take precedence, something that can result in bugs or crashes, or as seen below, a message warns that variable A from the global environment will be used instead of column A of the attached df17. The returned value is, of course, not the desired one.

```
df17 <- data.frame(A = 1:10, B = 3)</pre>
## [1] 1
attach(df17)
## The following object is masked _by_ .GlobalEnv:
##
## [1] 1
detach(df17)
## [1] 1
attach(df17)
## The following object is masked _by_ .GlobalEnv:
##
##
df17$C <- (A + B) / A
detach(df17)
head(df17, 2)
    АВС
## 1 1 3 4
## 2 2 3 4
```

Use of attach() and detach(), which work as a pair of ON and OFF switches, can result in an undesired after-effect on name lookup if the script terminates after attach() is executed but before detach() is called, as the attached object is not detached. In contrast, with() and within(), being self-contained, guarantee that cleanup takes place. Consequently, the usual recommendation is to give preference to the use of with() and within() over attach() and detach().

# 4.5 Reshaping and editing data frames

As mentioned above, in most cases in R data rows represent measurement events or observations possibly on multiple response variables and factors describing groupings, i.e., a "long" shape. However, when measurements are repeated in time, columns rather frequently represent observations of the same response variable at

different times, i.e., a "wide" shape. Other cases exist where reshaping is needed. Function reshape() can convert wide data frames into long data frames and vice versa. See section 8.6 on page 254 on package 'tidyr' for an alternative approach to reshaping data with a friendlier user interface.

We start by creating a data frame of hypothetical data measured on two occasions. With these data, for example if we wish to compute growth of each subject, by computing the difference in weight and in height between the two times, one approach is to reshape the data frame into a wider shape and subsequently subtract the columns.

```
# artifical data
df1 \leftarrow data.frame(id = rep(1:4, rep(2,4)),
                   Time = factor(rep(c("Before", "After"), 4)),
                   Weight = rnorm(n = 4, mean = c(20.1, 30.8)),
                  Height = rnorm(n = 4, mean = c(9.5, 14.2)))
df1
##
     id
          Time
                 Weight
                            Height
## 1
     1 Before 20.46903 10.292563
         After 30.93381 14.512298
      1
      2 Before 18.05201 9.444587
      2
         After 31.83868 15.391775
      3 Before 20.46903 10.292563
         After 30.93381 14.512298
      3
      4 Before 18.05201 9.444587
     4 After 31.83868 15.391775
# make it wider
df2 <- reshape(df1, timevar = "Time", idvar = "id", direction = "wide")</pre>
df2
##
     id Weight.Before Height.Before Weight.After Height.After
## 1 1
             20.46903
                           10.292563
                                         30.93381
                                                       14.51230
## 3
     2
             18.05201
                            9.444587
                                         31.83868
                                                       15.39178
## 5
                           10.292563
             20.46903
                                         30.93381
                                                       14.51230
                            9.444587
             18.05201
                                         31.83868
                                                       15.39178
# possible further calculation
within(df2,
        Height.growth <- Height.After - Height.Before
        Weight.growth <- Weight.After - Weight.Before
       })
##
     id Weight.Before Height.Before Weight.After Height.After Weight.growth
## 1
     1
             20.46903
                           10.292563
                                         30.93381
                                                       14.51230
                                                                      10.46478
##
  3
             18.05201
                            9.444587
                                          31.83868
                                                       15.39178
                                                                      13.78667
## 5
             20.46903
                           10.292563
                                          30.93381
                                                       14.51230
                                                                      10.46478
##
             18.05201
                            9.444587
                                          31.83868
                                                       15.39178
                                                                      13.78667
##
     Height.growth
## 1
          4.219736
## 3
          5.947188
## 5
          4.219736
##
  7
          5.947188
```

Alternatively, we may want to convert df1 into a longer shape, with a single column with measurements, and a new column indicating whether the measured variable was height or weight. For this operation to succeed, we need to add a column with a unique value for each row in df1, and one easy way is to copy row names into a column. The names of the parameters of function reshape() are meaningful

only when dealing with time. Thus, reading the code below becomes rather difficult. It is also to note that the user is responsible of passing the values to times in the correct order.

```
df1$ID <- rownames(df1) # unique ID for each row
# make it longer
reshape(df1,
        idvar = "ID",
        timevar = "Quantity"
        times = c("Weight", "Height"),
        v.names = "Value"
        direction = "long"
        varying = c("Weight", "Height"))
##
            id
                 Time ID Quantity
                                      Value
## 1.Weight 1 Before 1
                           Weight 20.469030
                           Weight 30.933814
## 2.Weight
                      2
            1 After
                      3
## 3.Weight
            2 Before
                           Weight 18.052008
## 4.Weight
            2 After
                           Weight 31.838682
            3 Before
## 5.Weight
                       5
                           Weight 20.469030
## 6.Weight
            3 After
                       6
                           Weight 30.933814
            4 Before
## 7.Weight
                           Weight 18.052008
            4 After
## 8.Weight
                           Weight 31.838682
## 1.Height
            1 Before
                           Height 10.292563
                       1
## 2.Height
             1 After
                           Height 14.512298
## 3.Height
             2 Before
                           Height 9.444587
## 4.Height
             2 After
                           Height 15.391775
             3 Before
## 5.Height
                       5
                           Height 10.292563
## 6.Height
             3 After
                       6
                           Height 14.512298
            4 Before
                       7
## 7.Height
                           Height 9.444587
## 8.Height
            4 After
                      8
                           Height 15.391775
```

To edit a data frame programmatically, one can use the approaches already discussed, using the extraction operators [ ] or [[ ]] on the *lhs* of <- to replace member elements. This in combination with functions like gsub() makes it possible to "edit" the contents of data frames.

Methods View(), edit() and fix() can be used interactively to display and edit R objects. When using R from within IDEs like RStudio, calling these functions with a data frame as argument opens in most cases the IDE's own worksheet-like data editors, and for other types of objects a text editor pane. Output is not included for this chunk, as the use of these functions requires user interaction. Please, run these examples in R and in an IDE like RStudio.

```
View(cars)
edit(cars)
```

These functions can be used at the R console also when R is used on its own, but the editors activated are different ones. In any case, the use of scripts has made the interactive use of R at the console less frequent and the need to edit R objects previously saved in the user's current workspace nearly disappear. View(), edit() and fix() are unusual in that their definitions are dependent on system variables that at least when using R on its own, can be modified by the user.

## 4.6 Attributes of R objects

R objects can have attributes. Attributes are named *slots* normally used to store ancillary data such as object properties functioning as additional fields where to store additional information in any R object. There are no restrictions on the class of what is assigned to an attribute. They can be used to store metadata accompanying the data stored in an object, which is important for reproducible research and data sharing. They can be set and read by user code and they are also used internally by R among other things to store the class an object belongs to, column and row names in data frames and matrices and the labels of levels in factors. Although most R objects have attributes, they are rarely displayed explicitly when an object is printed, while the structure of objects as displayed by function str() includes them.

Although we rarely need to set or extract values stored in attributes explicitly, many of the features of R that we take for granted are implemented using attributes: columns names in data frames are stored in an attribute. Matrices are vectors with additional attributes.

```
df1 \leftarrow data.frame(x = 1:6, y = c("a", "b"), z = c(TRUE, FALSE, NA))
df1
##
     х у
## 1 1 a TRUE
## 2 2 b FALSE
## 3 3 a
## 4 4 b TRUE
## 5 5 a FALSE
## 6 6 b
attributes (df1)
## $names
## [1] "x" "y" "z"
##
## $class
## [1] "data.frame"
## $row.names
## [1] 1 2 3 4 5 6
str(df1)
## 'data.frame': 6 obs. of 3 variables:
  $ x: int 1 2 3 4 5 6
   $ y: chr "a" "b" "a" "b" ...
   $ z: logi TRUE FALSE NA TRUE FALSE NA
```

Attribute "comment" is meant to be set by users to store a character string—e.g., to store metadata as text together with data. As comments are frequently used, R has functions for accessing and setting comments.

```
comment(df1)
## NULL
comment(df1) <- "this is stored as a comment"
comment(df1)
## [1] "this is stored as a comment"</pre>
```

Functions like names(), dim() or levels() return values retrieved from attributes stored in R objects, whereas names()<-, dim()<- or levels()<- set (or unset with NULL) the value of the respective attributes. Dedicated query and set functions do not exist for all attributes. Functions attr(), attr()<- and attributes() can be used with any attribute. With attr() we query, and with attr()<- we set individual attributes by name. With attributes() we retrieve all attributes of an object as a named list. In addition, method str() displays all components and structure of R objects including their attributes.

Continuing with the previous example, we can retrieve and set the value stored in the "comment" attribute using these functions. In the second statement we delete the value stored in the attribute by assigning NULL to it.

```
attr(df1, "comment")
## [1] "this is stored as a comment"
attr(df1, "comment") <- NULL
attr(df1, "comment")
## NULL
comment(df1) # same as previous line
## NULL</pre>
```

The "names" attribute of df1 was set by the data.frame() constructor when it was created above. In the next example, in the first statement we retrieve the names, and implicitly print them. In the second statement, read from right to left, we retrieve the names, convert them to upper case and save them back to the same attribute.

```
names(df1)
## [1] "x" "y" "z"
colnames(df1) # same as names()
## [1] "x" "y" "z"
colnames(df1) <- toupper(colnames(df1))
colnames(df1)
## [1] "X" "Y" "Z"
attr(df1, "names") # same as previous line
## [1] "X" "Y" "Z"</pre>
```

4.12 In general, R objects do not have by default names assigned to members. As seen on page 67 we can give names to vector members during construction with a call to c() or we can assign names (set attribute names) with function names()<- to existing vectors. Lists behave almost the same as vectors, although members of nested objects can also be named. Data frames have attributes names and row.names, that can be accessed with functions names() or colnames(), and function rownames(), respectively. The attributes can be set with functions names()<- or colnames()<-, and rownames()<-. The data.frame() constructor sets (column) names and row names by default. The matrix() constructor by default does not set dimnames or names attributes. When names are assigned to a matrix with names()<-, the matrix behaves like a vector, and the names are assigned to individual members. Functions dimnames()<-, colnames()<- and rownames()<- are used to assign names to columns and rows. The matching functions dimnames(), colnames() and rownames() are used to access these values.

When no names have been set, names(), colnames(), rownames(), and dimnames() return NULL. In contrast, labels(), intended to be used for printing, returns made-up names based on positions.

Run the examples below and write similar examples for list and data.frame. For matrix, write an additional statement that uses dimnames()<- to set row and column names simultaneously.

```
VCT1 <- 5:10
names(VCT1)
labels(VCT1)
names(VCT1) <- letters[5:10]
names(vct1)
labels(VCT1)

MAT1 <- matrix(1:10, ncol = 2)
dimnames(MAT1)
labels(MAT1)
colnames(MAT1) <- c("a", "b")
colnames(MAT1)
dimnames(MAT1)
labels(MAT1)
labels(MAT1)</pre>
```

We can add a new attribute, under our own control, as long as its name does not clash with those of existing attributes.

```
attr(df1, "my.attribute") <- "this is stored in my attribute"
attributes(df1)
## $names
## [1] "X" "Y" "Z"
##
## $class
## [1] "data.frame"
##
## $row.names
## [1] 1 2 3 4 5 6
##
## $my.attribute
## [1] "this is stored in my attribute"</pre>
```

The attributes used internally by R can be directly modified by user code. In most cases this is unnecessary as R provides pairs of functions to query and set the relevant attributes. This is true for the attributes dim, names and levels. In the example below we read the attributes from a matrix.

```
mat1 <- matrix(1:10, ncol = 2)
attributes(mat1)
## $dim
## [1] 5 2
dim(mat1)
## [1] 5 2
dimnames(mat1)
## NULL</pre>
```

```
labels(mat1)
## [1] "1" "2" "3" "4" "5"
## [[2]]
## [1] "1" "2"
mat1
        [,1] [,2]
##
##
  \lceil 1, \rceil
           1
   [2,]
           3
##
           4
                 9
attr(mat1, "dim")
## [1] 5 2
attr(mat1, "dim") <- c(2, 5)</pre>
mat1
        [,1] [,2] [,3] [,4] [,5]
## [1,]
           1
                 3
                      5
                            7
## [2,]
attr(mat1, "dim") <- NULL</pre>
is.vector(mat1 )
## [1] TRUE
mat1
    [1] 1 2 3 4 5 6 7 8 9 10
```

In this case we could have used dim() instead of attr().

There is no restriction to the creation, setting, resetting and reading of attributes, but not all functions and operators that can be used to modify objects will preserve non-standard attributes. This can be a problem when using some R packages, such as the 'tidyverse'. So, using private attributes is a double-edged sword that usually is worthwhile considering only when designing a new class together with the corresponding methods for it. A good example of extensive use of class-specific attributes are the values returned by model fitting functions like lm() (see section 7.9 on page 198).

# 4.7 Saving and loading data

## 4.7.1 Data sets in R and packages

To be able to present more meaningful examples, we need some real data. Here we use cars, one of the many data sets included in base R. Function data() is used to load data objects that are included in R or contained in packages (whether a call to data() is needed or not depends on how the package where the data is defined was configured). It is also possible to import data saved in files with *foreign* formats, defined by other software or commonly used for data exchange.

Package 'foreign', included in the R distribution, as well as contributed packages make available functions capable of reading and decoding various foreign formats. How to read or import "foreign" data is discussed in R documentation in *R Data Import/Export*, and in this book, in chapter 10 on page 367. It is also good to keep in mind that in R, URLs (Uniform Resource Locators) are accepted as arguments to the file or path parameter of many functions (see section 10.12 on page 397).

In the next example we load data available in R package 'datasets' as R objects by calling function data(). The loaded R object cars is a data frame. (Package 'datasets' is part of the R distribution and always available).

```
data(cars)
```

#### **4.7.2** .rda files

By default, at the end of a session, the current workspace containing the results of one's work is saved into a file called .RData. In addition to saving the whole workspace, it is possible to save one or more R objects present in the workspace to disk using the same file format (with file name tag .rda or .Rda). One or more objects, belonging to any mode or class can be saved into a single file using function save(). Reading the file restores all the saved objects into the current workspace with their original names. These files are portable across most R versions—i.e., old formats can be read and written by newer versions of R, although the newer, default format may be not readable with earlier R versions. Whether compression is used, and whether the "binary" data is encoded into ASCII characters, allowing maximum portability at the expense of increased size can be controlled by passing suitable arguments to save().

We create a data frame object and then save it to a file. The file name used can be any valid one in the operating system, however to ensure compatibility with multiple operating systems, it is good to use only ASCII characters. Although not enforced, using the name tag .rda or .Rda is recommended.

We delete the data frame object and confirm that it is no longer present in the workspace (see page ?? for details about remove() and objects()).

```
remove(df1)
objects(pattern = "df1")
## character(0)
```

We read the file we earlier saved to restore the object.

```
load(file = "df1.rda")
objects(pattern = "df1")
## [1] "df1"
```

```
df1
## x y
## 1 1 5
## 2 2 4
## 3 3 3
## 4 4 2
## 5 5 1
```

The default format used is binary and compressed, which results in smaller files.

4.13 In the example above, only one object was saved, but one can simply give the bare names of additional objects as arguments separated by commas ahead of file. Just try saving more than one data frame to the same file. Then the data frames plus a few vectors. After creating each file, clear the workspace and then restore from the file the objects you saved.

Sometimes it is easier to supply the names of the objects to be saved as a vector of character strings passed as an argument to parameter list (in spite of the name the argument passed must be a vector, not a list). One use case is saving a group of objects based on their names. In this case one can use ls() to obtain a vector of character strings with the names of objects matching a simple pattern or a complex *regular expression* (see section 3.4 on page 46). The example below uses this approach in two steps, first saving in variable objects a character vector with the names of the objects matching a pattern, and then using this saved vector as an argument to parameter list in the call to save().

```
dfs <- ls(pattern = "*.df")
save(list = dfs, file = "my-dfs.rda")</pre>
```

The two statements above can be combined into a single statement by nesting the function calls.

```
save(list = ls(pattern = "*.df"), file = "my-dfs.rda")
```

**4.14** Practice using different patterns with objects(). You do not need to save the objects to a file. Just have a look at the list of object names returned.

As a coda, I show how to clean up by deleting the two files we created. Function file.remove() can be used to delete files stored in the operating system file system, usually on a hard disk drive or a solid state drive, as long as the user has enough rights. No confirmation is requested, so care not to delete valuable files is required. Function unlink(), is not an exact equivalent, as it can also delete folders and supports recursion through nested folders. The name *unlink* is borrowed from that of the equivalent function in Unix and Linux.

```
file.remove(c("my-dfs.rda", "df1.rda"))
## [1] TRUE TRUE
```

#### **4.7.3** .rds files

The RDS format can be used to save individual objects instead of multiple objects (usually using file name tag .rds). They are read and saved with functions readRDS() and saveRDS(), respectively. The value returned by a call to readRDS() is

the object read from the file on disk. When RDS files are read, different from when RDA files are loaded, assigning the object read to a name is frequently the first step. This name can be any valid R name. Of course, it is also possible to use the object returned by readRDS() as an argument to a function by nesting the function calls.

```
saveRDS(df1, "df1.rds")
```

If we read the file at the R console, by default the read R object will be printed at the console.

If we assign the read object to a different name, it is possible to check if the object read is identical to the one saved.

```
df2 <- readRDS("df1.rds")
identical(df1, df2)
## [1] TRUE

As above, we clean up by deleting the file.
file.remove("df1.rds")</pre>
```

## 4.7.4 dput()

## [1] TRUE

In general the use of .rda and .rds files is preferred. Function dput() is sometimes used to share data as part of a code chunk at StackOverflow, mostly as a convenient way of converting a data frame or list into plain text that can be pasted into the code chunk listing to reconstruct the object. If no argument is passed to parameter file, the result of deparsing an object is printed at the R console.

```
dput(df1)
## structure(list(x = 1:5, y = 5:1), class = "data.frame", row.names = c(NA,
## -5L))
```

There exists a companion function dget() to recreate the object.

Output to, and input from, text-based file formats as well as to and from various binary formats *foreign* to R is described in chapter 10 on page 367.

## 4.8 Plotting

In most cases the most effective way of obtaining and overview of a data set is by plotting it using multiple approaches. The base-R generic method plot() can be used to plot different data. It is a generic method that has specializations suitable

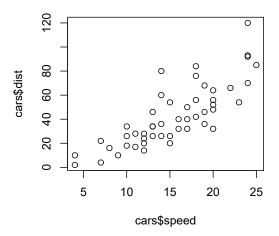
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for different kinds of objects (see section 6.3 on page 176 for a brief introduction to objects, classes and methods). In this section we only very briefly demonstrate the use of the most common base-R graphics functions. They are well described in the book *R Graphics* (Murrell 2019). We will not describe the Lattice (based on S's Trellis) approach to plotting (Sarkar 2008). Instead we describe in detail the use of the *layered grammar of graphics* and plotting with package 'ggplot2' in chapter 9 on page 265.

#### 4.8.1 Plotting data

It is possible to pass two variables (here columns from a data frame) directly as arguments to the x and y parameters of plot().

```
plot(x = cars$speed, y = cars$dist)
```



We can also use with() or attach() as described in section 4.4.5 on page 109. (Same plot as above, not shown.)

```
with(cars, plot(x = speed, y = dist))
```

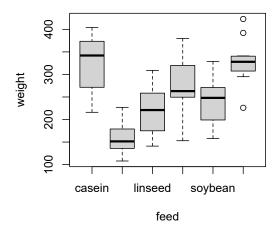
However, it is best to use a *formula* to specify the variables to be plotted on the x and y axes, passing additionally as an argument to parameter data a data frame containing these variables. The formula dist  $\sim$  speed, is read as dist explained by speed—i.e., dist is mapped to the y-axis as the dependent variable and speed to the x-axis as the independent variable. The names used in the formula, are looked up as columns in the data, frame argument passed to data, thus similarly as when using with(). As described in section 7.8 on page 197 the same syntax is used to describe models to be fitted to observations. (Same plot as above, not shown.)

```
plot(dist ~ speed, data = cars)
```

Within R there exist different specializations, or "flavors," of method plot() that become active depending on the class of the variables passed as arguments: passing two numerical variables results in a scatter plot as seen above. In contrast passing one factor and one numeric variable to plot() results in a box-and-

whiskers plot being produced. To exemplify this we need to use a different data set, here chickwts as cars does not contain any factors. Use help("chickwts") to learn more about this data set, also included in R.

plot(weight ~ feed, data = chickwts)



## 4.8.2 Graphical output

Graphical output, such as produced by plot(), is rendered by means of *graphical output devices*. When R is used interactively, a software device is opened automatically to output the graphical output to a physical device, usually the computer screen. The name of the R software device used may depend on the operating system (e.g., MS-Windows or Linux), or on the IDE (e.g., RStudio).

In R, software graphical devices not necessarily generate output on a physical device like a printer, as several of these devices translate the plotting commands into a file format and save it to disk. Several different graphical devices are available in R and they differ in the kind of output they produce: raster or bitmap files (e.g., TIFF, PNG and JPEG formats), vector graphics files (e.g., SVG, EPS and PDF), or output to a physical device like the screen of a computer. Additional devices are available through contributed R packages.

RStudio makes it possible to export plots into graphic files through a menubased interface in the *Plots* viewer tab. This interface uses some of the R devices that are available at the console and through scripts. For the sake of reproducibility, it is preferable to include the R commands used to export plots in the scripts used for data analysis.

Devices follow the paradigm of ON and OFF switches, opening and closing a destination for print(), plot() and related functions. Some devices producing a file as output, save their output one plot at a time to single-page graphic files while others write the file only when the device is closed, possibly as a multi-page file.

When opening a device the user supplies additional information. For the PDF and SVG devices that produce output in a vector-graphics format, width and height

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of the output are specified in *inches*. A default file name is used unless we pass a character string as an argument to parameter file.

```
pdf(file = "output/my-file.pdf", width = 6, height = 5, onefile = TRUE)
plot(dist ~ speed, data = cars)
plot(weight ~ feed, data = chickwts)
dev.off()
## cairo_pdf
## 2
```

Raster devices return bitmaps and width and height are specified in most cases in *pixels*.

```
png(file = "output/my-file.png", width = 600, height = 500)
plot(weight ~ feed, data = chickwts)
dev.off()
## cairo_pdf
## 2
```

The approach of direct output to a software device is used in base R by plot() and its companions text(), lines(), and points(). plot() outputs a graphs onto the other three functions can add to. The addition of plot components, as shown below, is done directly to the output device, i.e., when output is to the computer screen the partial plot is visible at each step.

```
png(file = "output/my-file.png", width = 600, height = 500)
plot(dist ~ speed, data = cars)
text(x = 10, y = 110, labels = "some texts to be added")
dev.off()
## cairo_pdf
## 2
```

This is not the only approach available in R for building complex plotys. As we will see in chapter 9 on page 265, an alternative approach is to build a *plot object* as a list of member components, that can be saved as any other R object. This object is later rendered as a whole on a graphical device by calling print() once.

# 4.9 Further reading

For further reading on the aspects of R discussed in the current chapter, I suggest the book *The Art of R Programming: A Tour of Statistical Software Design* (Matloff 2011), with emphasis on the R language and programming. An in depth description of plotting and graphic devices in R is available in the book *R Graphics* (Murrell 2019).

# Base R: "Paragraphs" and "Essays"

An R script is simply a text file containing (almost) the same commands that you would enter on the command line of R.

Jim Lemon Kickstarting R

## 5.1 Aims of this chapter

For those who have mainly used graphical user interfaces, understanding why and when scripts can help in communicating a certain data analysis protocol can be revelatory. As soon as a data analysis stops being trivial, describing the steps followed through a system of menus and dialogue boxes becomes extremely tedious.

Moreover, graphical user interfaces tend to be difficult to extend or improve in a way that keeps step-by-step instructions valid across program versions and operating systems.

Many times, exactly the same sequence of commands needs to be applied to different data sets, and scripts make both implementation and validation of such a requirement easy.

In this chapter, I will walk you through the use of R scripts, starting from an extremely simple script.

# 5.2 Writing scripts

In R language, the closest match to a natural language essay is a script. A script is built from multiple interconnected code statements needed to complete a given task. Simple statements, equivalent to sentences, can be combined into compound statements, equivalent to natural language paragraphs. Frequently, we combine simple sequences of statements into a sequence of actions necessary to complete

a task. The sequence is not necessarily linear, as branching and repetition are also available.

Scripts can vary from simple scripts containing only a few code statements, to complex scripts containing hundreds of code statements. In the rest of the present section I discuss how to write readable and reliable scripts and how to use them.

## 5.2.1 What is a script?

A *script* is a text file that contains (almost) the same commands that you would type at the R console prompt. A true script is not, for example, an MS-Word file where you have pasted or typed some R commands.

When typing commands/statements at the R console, we "feed" one line of text at a time. When we end the line by typing the enter key, the line of text is interpreted and evaluated. We then type the next line of text, which gets in turn interpreted and evaluated, and so on. In a script we write nearly the same text in an editor and save multiple lines containing commands into a text file. Interpretation takes place only later, when we *source* the file as a whole into R.

A script file has the following characteristics.

- The script is a plain text file, i.e., a file containing bytes that represent alphanumeric characters in a standardized character set like UTF8 or ASCII.
- The text in the file contains valid R statements (including comments) and nothing else.
- Comments start at a # and end at the end of the line.
- The R statements are in the file in the order that they must be executed, and respecting the line continuation rules of R.
- R scripts customarily have file names ending in .r or .R.

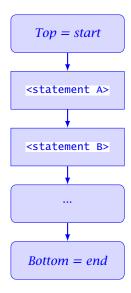
The statements in the text file, are read, interpreted and evaluated sequentially, from the start to the end of the file, as represented in the diagram (Figure 5.1).

As we will see later in the chapter, code statements can be combined into larger statements and evaluated conditionally and/or repeatedly, which allows us to control the realised sequence of evaluated statements.

In addition to being valid it is important that scripts are also understandable to humans, consequently a clear writing style and consistent adherence to it are important.

It is good practice to write scripts so that they are self-contained. To make a script self-contained, one must include code to load the packages used, load or import data from files, perform the data analysis and display and/or save the results of the analysis. Such scripts can be used to apply the same analysis algorithm to other data by reading data from a different file and/or to reproduce the same analysis at a later time using the same data. Such scripts document all steps used for the analysis.

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#### FIGURE 5.1

Diagram of script showing sequentially evaluated code statements; ··· represent additional statements in the script.

## 5.2.2 How do we use a script?

A script can be "sourced" using function source(). If a text file called my.first.script.rcontains the text

```
# this is my first R script
print(3 + 4)
  it can be sourced by typing at R console
source("my.first.script.r")
## [1] 7
```

Execution of the statements in the file makes R display [1] 7 at the console as, below the command we typed in. The commands themselves are not shown (by default the sourced file is not *echoed* to the console) and the results of computations are not printed unless one includes explicit print() commands in the script.

Scripts can be run both by sourcing them into an open R session, or at the operating system command prompt (see section 2.3 on page 12). In RStudio, the script in the currently active editor tab can be sourced using the "source" button. The drop-down menu of this button has three entries: "Source", quietly to the R console, "Source with echo" showing the code as it is run, and "Source as local job", using a new instance of R in the background. In the last case, the R console remains free for other uses while the script is running.

When a script is *sourced*, the output can be saved to a text file instead of being shown in the console. It is also easy to call R with the R script file as an argument directly at the operating system shell or command-interpreter prompt—and obviously also from shell scripts. The next two chunks show commands entered at the OS shell command prompt rather than at the R command prompt.

#### RScript my.first.script.r

You can open an operating system's *shell* from the Tools menu in RStudio, to run this command. The output will be printed to the shell console. If you would like to save the output to a file, use output redirection using the operating system's syntax.

#### RScript my.first.script.r > my.output.txt

While developing or debugging a script, one usually wants to run (or *execute*) one or a few statements at a time. This can be done in RStudio using the "run" button after either positioning the cursor in the line to be executed, or selecting the text to be run (the selected text can be part of a line, a whole line, or a group of lines, as long as it is syntactically valid). The key-shortcut Ctrl-Enter is equivalent to pressing the "run" button.

#### 5.2.3 How to write a script

As with any type of writing, different approaches may be preferred by different R users. In general, the approach used, or mix of approaches, will also depend on how confident one is that the statements will work as expected—one already knows the best approach vs. one is exploring different alternatives.

Three approaches are listed below. They all can result in equally good code, but as work in progress they differ. In the first approach, the script as whole is likely to contain bugs before fully tested. In the middle approach, only the most recently added statements are likely to contain bugs. In the last one the script contains at all times only valid R code, even if incomplete. The third approach also has the advantage that code remains in the R console *History* and can be retrieved with a delay, e.g., after comparison against an alternative statement.

**If one is very familiar with similar problems** One would just create a new text file and write the whole thing in the editor, and then test it. This is rather unusual.

**If one is moderately familiar with the problem** One would write the script as above, but testing it, step by step, as one is writing it, i.e., running parts of the script as one adds them. This is the approach I use most frequently.

If one is mostly playing around Then if one is using RStudio, one can type statements at the console prompt. As you should know by now, everything you run at the console is saved to the "History." In RStudio, the History is displayed in its own pane, and in this pane one can select any previous statement(s) and by clicking on a single icon, copy and paste them to either the R console prompt, or the cursor position in the editor pane. In this way one can build a script by copying and pasting from the history to the script file, the bits that have worked as you wanted.

5.1 By now you should be familiar enough with R to be able to write your own script.

1. Create a new R script (in RStudio, from the File menu, leftmost "+" icon, or by typing "Ctrl + Shift + N").

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- 2. Save the file as my.second.script.r.
- 3. Use the editor pane in RStudio to type some R commands and comments.
- 4. Run individual commands.
- 5. *Source* the whole file.

## 5.2.4 The need to be understandable to people

It is not enough for program code to be understood by a computer and that it returns the correct answer. Both large programs and small scripts have to be readable to humans, and the intention of the code understandable. In most cases R code will be maintained, reused and modified over time. In many cases it serves to document a given computation and to make it possible to reproduce it.

When one writes a script, it is either because one wants to document what has been done or because one plans to use it again in the future. In the first case other persons will read it and in the second case one rarely remembers all the details. Thus, spending time and effort on the writing style paying special attention to following recommendations is important.

- Avoid the unusual. People using a certain programming language tend to use some implicit or explicit rules of style—style includes *indentation* of statements, *capitalization* of variable and function names. As a minimum try to be consistent with yourself.
- Use meaningful names for variables, and any other object. What is meaningful depends on the context. Depending on common use, a single letter may be more meaningful than a long word. However self-explanatory names are usually better: e.g., using n.rows and n.cols is much clearer than using n1 and n2 when dealing with a matrix of data. Probably number.of.rows and number.of.columns would make the script verbose, and take longer to type without gaining anything in return. Sometimes, short textual explanations in comments (ignored by R) are needed to achieve readability for humans.
- How to make the words visible in names: traditionally in R one would use dots to separate the words and use only lower case. Some years ago, it became possible to use underscores. The use of underscores is quite common nowadays because it is "safer", as in some situations a dot may have a special meaning. Names like Numcols, using "camel case", are only infrequently used in R programming but is common in other languages like Pascal.

The *Tidyverse style guide* for writing R code (https://style.tidyverse.org/) provides more detailed "rules". However, more important than strictly following a published guideline is to be consistent in the style one, a team of programmers or data analysts, or even members of an organization use. In the current book, I have not followed this guide in all respects, instead following in some cases the style used in R documentation. However, I have attempted to be consistent.

5.2 Here is an example of bad style in a script. Edit the code in the chunk below so that it becomes easier to read.

```
a <- 2 # height
b <- 4 # length
C <-
    a *
b
C -> variable
    print(
"area: ", variable
```

The points discussed above already help a lot. However, one can go further in achieving the goal of human readability by interspersing explanations and code "chunks" and using all the facilities of typesetting, even of formatted maths formulas and equations, within the listing of the script. Furthermore, by including the results of the calculations and the code itself in a typeset report built automatically one ensures that they match each other. This greatly contributes to data analysis reproducibility, which is becoming a widespread requirement both in academia and in industry.

This approach is called literate programming and was first proposed by Knuth (1984) through his WEB system. In the case of R programming, the first support of literate programming was in 'Sweave', which has been superseded by 'knitr' (Xie 2013). This package supports the use of Markdown or ETEX (Lamport 1994) as the markup language for the textual contents and also formats and applies syntax highlighting to code. Rmarkdown is an extension to Markdown that makes it easier to include R code in documents (see http://rmarkdown.rstudio.com/). It is the basis of R packages that support typesetting large and complex documents ('bookdown'), web sites ('blogdown'), package vignettes ('pkgdown') and slides for presentations (Xie 2016; Xie et al. 2018). Quarto, which provides an enhanced version of R markdown, is implemented in R package 'quarto' together with the quarto program as a separate executable. The use of 'knitr' and 'quarto' is very well integrated into the RStudio IDE. The generation of typeset reports is outside the scope of the book, but it is an important skill to learn. It is well described in the books and web sites cited.

## 5.2.5 Debugging scripts

The use of the word *bug* to describe a problem in computer hardware and software started in 1946 when a real bug, more precisely a moth, got between the contacts of a relay in an electromechanical computer causing it to malfunction and Grace Hooper described the first computer *bug*. The use of the term bug in engineering predates the use in computer science, and consequently, the first use of bug in computing caught on easily.

A suitable quotation from a letter written by Thomas Alva Edison 1878 (as given by Hughes 2004):

It has been just so in all of my inventions. The first step is an intuition, and comes with a burst, then difficulties arise-this thing gives out and [it is] then that "Bugs"-as such little faults and difficulties are called-show themselves and

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months of intense watching, study and labor are requisite before commercial success or failure is certainly reached.

The quoted paragraph above makes clear that only very exceptionally does any new design fully succeed. The same applies to R scripts as well as any other non-trivial piece of computer code. From this it logically follows that testing and debugging are fundamental steps in the development of R scripts and packages. Debugging, as an activity, is outside the scope of this book. However, clear programming style and good documentation are indispensable for efficient testing and reuse.

Even for scripts used for analyzing a single data set, we need to be confident that the algorithms and their implementation are valid, and able to return correct results. This is true both for scientific reports, expert reports and any data analysis related to assessment of compliance with legislation or regulations. Of course, even in cases when we are not required to demonstrate validity, say for decision making purely internal to a private organization, we will still want to avoid costly mistakes.

The first step in producing reliable computer code is to accept that any code that we write needs to be tested and, if possible, validated. Another important step is to make sure that input is validated within the script and a suitable error produced for bad input (including valid input values falling outside the range that can be reliably handled by the script).

If during testing, or during normal use, a wrong value is returned by a calculation, or no value (e.g., the script crashes or triggers a fatal error), debugging consists in finding the cause of the problem. The cause can be either a mistake in the implementation of an algorithm, as well as in the algorithm itself. However, many apparent *bugs* are caused by bad or missing handling of special cases like invalid input values, rounding errors, division by zero, etc., in which a program crashes instead of elegantly issuing a helpful error message.

Diagnosing the source of bugs is, in most cases, like detective work. One uses hunches based on common sense and experience to try to locate the lines of code causing the problem. One follows different *leads* until the case is solved. In most cases, at the very bottom we rely on some sort of divide-and-conquer strategy. For example, we may check the value returned by intermediate calculations until we locate the earliest code statement producing a wrong value. Another common case is when some input values trigger a bug. In such cases it is frequently best to start by testing if different "cases" of input lead to errors/crashes or not. Boundary input values are usually the telltale ones: e.g., for numbers, zero, negative and positive values, very large values, very small values, missing values (NA), vectors of length zero (numeric()), etc.

Error messages When debugging, keep in mind that in some cases a single bug can lead to a whole cascade of error messages. Do also keep in mind that typing mistakes, originating when code is entered through the keyboard, can wreak havock in a script: usually there is little correspondence between the number of error messages and the seriousness of the bug triggering them. When several errors are triggered, start by reading the error message printed first, as later errors can be an indirect consequence of earlier ones.

There are special tools, called debuggers, available, and they help enormously. Debuggers allow one to step through the code, executing one statement at a time, allowing inspection of the objects present in the R environment. It is even possible to execute additional statements at the R console, e.g., to modify the value of a variable, while execution is paused. An R debugger is available within RStudio and also through the R console.

When writing your first scripts, you will manage perfectly well, and learn more by running the script one line at a time, and when needed temporarily inserting print() statements to "look" at how the value of variables changes at each step. A debugger allows a lot more control, as one can "step in" and "step out" of function definitions, and set and unset break points where execution will stop. However, using a debugger is not as simple as using print().

If you get stuck trying to find the cause of a bug, do extend your search both to the most trivial of possible causes, and later on to the least likely ones (such as a bug in a package installed from CRAN or R itself). Of course, when suspecting a bug in code you have not written, it is wise to very carefully read the documentation, as the "bug" may be just a misunderstanding of what a certain piece of code is expected to do. Also keep in mind that as discussed on page 6, you will be able to find online already-answered questions to many of your likely problems and doubts. For example, searching with Google for the text of an error message is usually well rewarded. Most important to remember is that bugs do pop up frequently in newly written code, and occasionally in old code. Nobody is immune to them: not the code you write, packages you use or R itself.

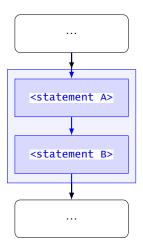
# 5.3 Compound statements

Individual statements can be grouped into *compound statements* by enclosing them in curly braces (Figure 5.2). Conceptually is like putting these statements into a box that allows us to operate with them as an anonymous whole.

```
print("...")
## [1] "..."
{
    print("A")
    print("B")
}
## [1] "A"
## [1] "B"
print("...")
## [1] "..."
```

The grouping of the two middle statements above is of no consequence, as it does not alter sequential evaluation. In the example above only side effects are of interest. In the example below, the value returned by a compound statement is that returned by the last statement evaluated within it. Individual statements can

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#### FIGURE 5.2

Diagram of a compound code statement is a grouping of statements that in some contexts behaves as a single statement. In the diagram, statements A and B have been grouped into a compound statement.

be separated by an end-of-line as above, or by a semicolon (;) as shown below, for two statements, each of them implementing an arithmetic operation.

```
{1 + 2; 3 + 4}
## [1] 7
```

The example above demonstrates that only the value returned by the compound statement as a whole is displayed automatically at the R console, i.e., the implicit call to print() is applied to the compound statement. Thus, even though both statements were evaluated, we only see the result returned by the second one.

**5.3** Nesting is also possible. Before running the compound statement below try to predict the value it will return, and then run the code and compare your prediction to the value returned.

```
\{1 + 2; \{a < -3 + 4; a + 1\}\}
```

Grouping is of little use by itself. It becomes useful together with control-ofexecution constructs, when defining functions, and similar cases where we need to treat a group of code statements as if they were a single statement. We will see several examples of the use of compound statements in the current chapter and in chapter 6 on page 169.

#### 5.4 Function calls

We will describe functions in detail and how to create new ones in chapter 6. We have already been using functions since chapter 3. Functions are structurally R statements, in most cases, compound statements, using formal parameters as

placeholders. When one calls a function one passes arguments for the different parameters (or placeholder names) and the (compound) statement conforming the *body* of the function is evaluated after "replacing" the placeholders by the values passed as arguments.

In the first example we have two statements. The first one computes log(100) by calling function log10() with 100 as argument and stores the returned value in variable a. In the second statement we pass variable a as argument to print() and as a side effect the value 2 is displayed.

```
a <- log10(100)
print(a)
## [1] 2
```

Function calls can be nested. The example above can be rewritten as.

```
print(log10(100))
## [1] 2
```

The difference is that we avoid the explicit creation of a variable. Whether this is an advantage or not depends on whether we use variable a in later statements or not.

Statements with more levels of nesting than shown above become very difficult to read, so alternative notations can help.

# 5.5 Data pipes

Pipes have been at the core of shell scripting in Unix since early stages of its design (Kernigham and Plauger 1981) as well as in Linux distributions. Within an OS, pipes are chains of small programs or "tools" that carry out a single well-defined task (e.g., ed, gsub, grep, more, etc.). Data such as text is described as flowing from a source into a sink through a series of steps at which a specific transformations take place. In Unix and Linux shells like sh or bash, sinks and sources are files, but in Unix and Linux files are an abstraction that includes all devices and connections for input or output, including physical ones such as terminals and printers.

```
stdin | grep("abc") | more
```

How can *pipes* exist within a single R script? When chaining functions into a pipe, data is passed between them through temporary R objects stored in memory, which are created and destroyed automatically. Conceptually there is little difference between Unix shell pipes and pipes in R scripts, but the implementations are different.

What do pipes achieve in R scripts? They relieve us from the responsibility of creating and deleting the temporary objects and of enforcing the sequential execution of the different steps. Pipes usually improve readability of scripts by allowing more concise code.

Since year 2021, starting from version 4.1.0, R includes a native pipe operator (|>) as part of the language. Subsequently, the placeholder (\_) was implemented in version 4.2.0 and its functionality expanded in version 4.3.0. Another two im-

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plementations of pipes, that have been available as R extensions for some years in packages 'magrittr' and 'wrapr', are described in chapter 8 on page 241.

I describe R's pipe syntax based on R 4.3.0. I start by showing the same operations coded using nested function calls, using explicit saving of intermediate values in temporary objects, and using the pipe operator.

Nested function calls are concise, but difficult to read when the depth of nesting increases.

```
sum(sqrt(1:10))
## [1] 22.46828
```

Saving intermediate results explicitly results in clear but verbose code.

```
data.in <- 1:10
data.tmp <- sqrt(data.in)
sum(data.tmp)
## [1] 22.46828
rm(data.tmp) # clean up!</pre>
```

A pipe using operator |> makes the data flow clear and keeps the code concise.

```
1:10 |> sqrt() |> sum()
## [1] 22.46828
```

We can assign the result of the computation to a variable, most elegantly using the -> operator on the *rhs* of the pipe.

```
1:10 |> sqrt() |> sum() -> my_rhs.var
my_rhs.var
## [1] 22.46828
```

We can also use the <- operator on the *lhs* of the pipe, i.e., for assignments a pipe behaves as a compound statement.

```
my_lhs.var <- 1:10 |> sqrt() |> sum()
my_lhs.var
## [1] 22.46828
```

Formally, the  $\mid$ > operator from base R takes two operands, just like operator + does. The value returned by the *lhs* (left-hand side) operand, which can be any R expression, is passed as argument to the function-call operand on *rhs* (right-hand side). The called function must accept at least one argument. This default syntax that implicitly passes the argument by position to the first parameter of the function would limit which functions could be used in a pipe construct. However, it is also possible to pass the piped argument explicitly by name to any parameter of the function on the *rhs* using an underscore (\_) as placeholder.

```
1:10 |> sqrt(x = _) |> sum(x = _)
## [1] 22.46828
```

The placeholder can be also used with extraction operators.

```
1:10 |> sqrt(x = _) |> _[2:8] |> sum(x = _) ## [1] 15.306
```

Base R functions like subset() have a signature that is natural for use in pipes by implicitly passing the piped value as argument to its first formal parameter, while others like assign() do not. For example, when calling function assign() to

save a value using a name available as a character string we would like to pass the piped value as argument to parameter value which is not the first. In such cases we can use \_ as a placeholder and pass it by name.

```
obj.name <- "data.out"
1:10 |> sqrt() |> sum() |> assign(x = obj.name, value = _)
```

Alternatively, we can define a wrapper function, with the desired order for the formal parameters. This approach can be worthwhile when the same function is called repeatedly within a script.

```
value_assign <- function(value, x, ...) {
  assign(x = x, value = value, ...)
}
obj.name <- "data.out"
1:10 |> sqrt() |> sum() |> value_assign(obj.name)
```

In general whenever we use temporary variables to store values that are passed as arguments only once, we can nest or chain the statements making the saving of intermediate results into a temporary variable implicit instead of explicit. Examples of some useful idioms follow.

Addition of computed variables to a data frame using within() (see section 4.4.5 on page 109) and selecting rows with subset() (see section 4.4.1 on page ??) are combined in our first simple example. For clarity, we use the \_ placeholder to indicate the value returned by the preceding function in the pipe.

```
data.frame(x = 1:10, y = rnorm(10)) >
  within(data = _,
          {
            x4 \leftarrow x\Lambda4
            is.large \leftarrow x^4 > 1000
         }) |>
  subset(x = _, is.large)
##
                     y is.large
## 6
       6 - 0.70310950
                           TRUE
                                  1296
## 7
       7 -0.97664248
                            TRUE
                                  2401
       8 0.01088894
## 8
                            TRUE
                                  4096
       9 -1.93480912
                                  6561
## 9
                            TRUE
## 10 10 -0.83861693
                           TRUE 10000
```

5.4 Without using the \_ placeholder and a more compact layout, the code above becomes. Compare the code below to that above to work out how I simplified the code.

```
data.frame(x = 1:10, y = rnorm(10)) |>
  within({x4 <- x^4; is.large <- x^4 > 1000}) |>
  subset(is.large)
```

Subset can be also used to select variables or columns from data frames and matrices.

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```
##
               y is.large
                              x4
## 6
       0.4556332
                     TRUE
                           1296
## 7
       0.8521401
                     TRUE
                            2401
       1.1870304
                     TRUE
                           4096
## 9
      -0.7253693
                     TRUE 6561
## 10 0.3915134
                     TRUE 10000
data.frame(x = 1:10, y = rnorm(10)) \mid >
  within(data = _,
           χ4 <- χΛ4
           is.large \leftarrow x^4 > 1000
         }) |>
  subset(x = \_, select = c(y, x4))
##
                У
## 1
     -0.31734540
                      1
## 2 -0.26275409
                     16
## 3
      0.03800997
                     81
## 4 -1.01047728
                    256
## 5
     -1.40768778
                    625
## 6
     -0.53467718
                   1296
## 7
     -0.99826591
                   2401
## 8
     -0.94664346
                   4096
## 9
      1.85068752
                  6561
## 10 1.79449701 10000
data.frame(group = factor(rep(c("T1", "T2", "Ct1"), each = 4)),
           y = rnorm(12) |>
  subset(x = _, group %in% c("T1", "T2")) |>
  aggregate(data = _, y ~ group, mean)
   aroup
                    V
## 1
        T1 0.2282816
## 2
        T2 - 0.7547058
```

The extraction operators are accepted on the *rhs* of a pipe only starting from R 4.3.0. With these versions \_[["y"]], as shown below, as well as its equivalent \_\$y can be used. Function getElement() used as getElement("y"), being a normal function, can be used in situations where operators are not accepted, like on the *rhs* of |> in older versions of R.

Additional functions designed to be used in pipes are available through packages as described in chapter 8.

5.5 In the last three examples, in which function calls is the explicit use of the placeholder needed, and in which ones is it optional? Hint: edit the code, removing the parameter name, =, and \_, and test whether the edited code works and returns the same value as before.

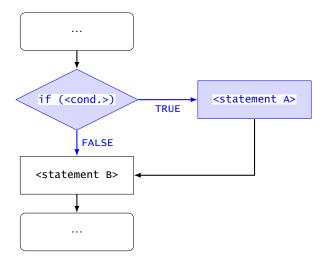


FIGURE 5.3 Flowchart for if construct.

## 5.6 Conditional evaluation

By default R statements in a script are evaluated (or executed) in the sequence they appear in the script *listing* or text. We give the name *control of execution constructs* to those special statements that allow us to alter this default sequence, by either skipping or repeatedly evaluating individual statements. The statements whose evaluation is controlled can be either simple or compound. Some of the control of execution flow statements, function like *ON-OFF switches* for program statements. Others allow statements to be executed repeatedly while or until a condition is met, or until all members of a list or a vector are processed.

These *control of execution constructs* can be also used at the R console, but it is usually awkward to do so as they can extend over several lines of text. In simple scripts, the *flow of execution* can be fixed and linear from the first to the last statement in the script. However, *control of execution constructs* are a crucial part of most useful scripts. As we will see next, a compound statement can include multiple simple or nested compound statements. R has two types of *if* statements, non-vectorized and vectorized.

#### 5.6.1 Non-vectorized if, else and switch

The if construct "decides," depending on a logical value, whether the next code statement is executed (if TRUE) or skipped (if FALSE) (Figure 5.3). The flow chart shows how if works: <statement A> is either evaluated or skipped depending on the value of <condition>, while <statement B> is always evaluated.

The usefulness of *if* statements stems from the possibility of computing the logical value used as <condition> with comparison operators (see section 3.6 on page 52) and logical operators (see section 3.5 on page 49).

We start with toy examples demonstrating how *if* statements work. Later we will see examples closer to real use cases. Here if controls the evaluation or not of the simple statement print("Hello!").

We use the name *flag* for a logical variable set manually, preferably near the top of the script. Real flags were used in railways to indicate to trains whether to stop or continue at stations and which route to follow at junctions. Use of logical flags in scripts is most useful when switching between two behaviors that depend on multiple separate statements.

```
flag <- TRUE
if (flag) print("Hello!")
## [1] "Hello!"</pre>
```

5.6 Play with the code above by changing the value assigned to variable flag, FALSE, NA, and logical(0).

In the example above we use variable flag as the *condition*.

Nothing in the R language prevents this condition from being a logical constant. Explain why if (FALSE) in the syntactically-correct statement below is of no practical use.

```
if (FALSE) print("Hello!")
```

Conditional execution is much more useful than what could be expected from the previous examples, because the statement whose execution is being controlled can be a compound statement of almost any length or complexity. A very simple example follows, with a compound statement containing two statements, each one, a call to function print() with a different argument.

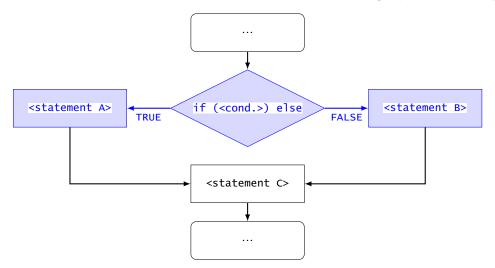
```
printing <- TRUE
if (printing) {
    print("A")
    print("B")
}
## [1] "A"
## [1] "B"</pre>
```

The condition passed as an argument to if, enclosed in parentheses, can be anything yielding a logical vector of length one. As this condition is *not* vectorized, a longer vector will trigger an R warning or error depending on R's version.

The if ... else ... construct "decides," depending on a logical value, which of two code statements is executed (Figure 5.4). The flow chart shows how it works: either <statement A> or <statement B> is evaluated and the other skipped depending on the value of <condition>, while <statement C> is always evaluated.

```
a <- 10
if (a < 0) print("'a' is negative") else print("'a' is not negative")
## [1] "'a' is not negative"
print("This is always printed")
## [1] "This is always printed"</pre>
```

As can be seen above, the statement immediately following if is executed if the condition returns TRUE and that following else is executed if the condition



**FIGURE 5.4** Flowchart for if ...else construct.

returns FALSE. Statements after the conditionally executed if and else statements are always executed, independently of the value returned by the condition.

5.7 Play with the code in the chunk above by assigning different numeric vectors to a.

Do you still remember the rules about continuation lines?

```
# 1
a <- 1
if (a < 0) print("'a' is negative") else print("'a' is not negative")
## [1] "'a' is not negative"</pre>
```

Why does the statement below (not evaluated here) trigger an error while the one above does not?

```
# 2 (not evaluated here)
if (a < 0) print("'a' is negative")
else print("'a' is not negative")</pre>
```

How do the continuation line rules apply when we add curly braces as shown below.

```
# 1
a <- 1
if (a < 0) {
    print("'a' is negative")
} else {
    print("'a' is not negative")
}
## [1] "'a' is not negative"</pre>
```

In the example above, we enclosed a single statement between each pair of curly braces, but as these braces create compound statements, multiple statements could have been enclosed between each pair.

5.8 Play with the use of conditional execution, with both simple and compound statements, and also think how to combine if and else to select among more than two options.

In R, the value returned by any compound statement is the value returned by the last simple statement executed within the compound one. This means that we can assign the value returned by an if and else statement to a variable. This style is less frequently used, but occasionally can result in easier-to-understand scripts.

```
a <- 1
my.message <-
   if (a < 0) "'a' is negative" else "'a' is not negative"
print(my.message)
## [1] "'a' is not negative"</pre>
```

If the condition statement returns a value of a class other than logical, R will attempt to convert it into a logical. This is sometimes used instead of a comparison to zero, as the conversion from integer yields TRUE for all integers except zero. The code below illustrates a rather frequently used idiom for checking if there is something available to display.

```
message <- "abc"
if (length(message)) print(message)
## [1] "abc"</pre>
```

5.9 Study the conversion rules between numeric and logical values, run each of the statements below, and explain the output based on how type conversions are interpreted, remembering the difference between *floating-point numbers* as implemented in computers and *real numbers* ( $\mathbb{R}$ ) as defined in mathematics (see page 27).

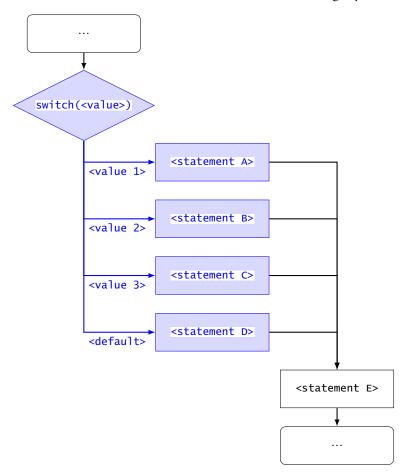
```
if (0) print("hello")
if (-1) print("hello")
if (0.01) print("hello")
if (1e-300) print("hello")
if (1e-323) print("hello")
if (1e-324) print("hello")
if (1e-500) print("hello")
if (as.logical("true")) print("hello")
if (as.logical(as.numeric("1"))) print("hello")
if (as.logical("1")) print("hello")
if ("1") print("hello")
```

Hint: if you need to refresh your understanding of the type conversion rules, see section 3.9 on page 60.

In addition to if and if ... else, there is in R a switch statement (Figure 5.5). It can be used to select among *cases*, or several alternative statements, based on an expression evaluating to a numeric or a character value of length equal to one.

A switch statement returns a value, just like if, the value returned by the switch statement is the value returned by one of the statements. Each of the alternative statements is called a *case*. The value passed as argument to switch functions as an index selecting one of them.

In the first example we use a character variable as the condition, named cases, and a final unlabelled case as default in case of no match. In real use, a computed



**FIGURE 5.5** Flowchart for a switch construct.

value or user input would be used in place of my.object. As with the logical argument to if, the character string value passed as argument must be a vector of length one.

Multiple condition values can share the same statement.

```
0
)
b
## [1] 0.5
```

5.10 Do play with the use of the switch statement. Look at the documentation for switch() using help(switch) and study the examples at the end of the help page. Explore what happens if you set my.object <- "ten", my.object <- "three", my.object <- NA\_character\_ or my.object <- character(). Then remove the , 0 as default value, and repeat.

When the expression used as a condition returns a value that is not a character, it will be interpreted as an integer index. In this case no names are used for the cases, and the last one is always interpreted as the default.

- 5.11 Continue playing with the use of the switch statement. Explore what happens if you set my.number <- 10, my.number <- 3, my.number <- NA or my.object <- numeric(). Then remove the , 0 as default value, and repeat.
- The statements for the cases in a switch() statement can be compound statements as in the case of if, and they can even be used for a side effect. For example the example above can edited to print a message when the default value is returned.

The switch statement can substitute for chained if ... else statements when all the conditions can be described by constant values or distinct values returned by the same test. The advantage is more concise and readable code. The equivalent of the first switch example above when written using if ... else becomes longer. Given how terse code using switch is, those not yet familiar with its use may find the more verbose style used below easier to understand. On the other hand, with numerous cases a switch statement is easier to read and understand.

```
my.object <- "two"
if (my.object == "one") {
   b <- 1
} else if (my.object == "two") {
   b <- 1 / 2
} else if (my.object == "four") {
   b <- 1 / 4
} else {
   b <- 0
}
b
## [1] 0.5</pre>
```

5.12 Consider another alternative approach, the use of a named vector to map values. In most of the examples above the code for the cases is a constant value or an operation among constant values. Implement one of this examples using a named vector instead of a switch statement.

### 5.6.2 Vectorized ifelse()

Vectorized *ifelse* is a peculiarity of the R language, but very useful for writing concise code that may execute faster than logically equivalent but not vectorized code. Vectorized conditional execution is coded by means of *function* ifelse() (written as a single word). This function takes three arguments: a logical vector usually the result of a test (parameter test), an expression to use for TRUE cases (parameter yes), and an expression to use for FALSE cases (parameter no). At each index position along the vectors, the value included in the returned vector is taken from yes if the corresponding member of the test logical vector is TRUE and from no if the corresponding member of test is FALSE. All three arguments can be any R statement returning the required vectors.

The flow chart for ifelse() is similar to that for if ... else shown on page 138 but applied in parallel to the individual members of vectors; e.g. the condition expression is evaluated at index position 1 controls which value will be present in the returned vector at index position 1, and so on.

It is customary to pass arguments to ifelse by position. We give a first example with named arguments to clarify the use of the function.

```
my.test <- c(TRUE, FALSE, TRUE, TRUE)
ifelse(test = my.test, yes = 1, no = -1)
## [1] 1 -1 1 1</pre>
```

In practice, the most common idiom is to have as an argument passed to test, the result of a comparison calculated on the fly. In the first example we compute the absolute values for a vector, equivalent to that returned by R function abs().

```
nums <- -3:+3
ifelse(nums < 0, -nums, nums)
## [1] 3 2 1 0 1 2 3</pre>
```

In the case of ifelse(), the length of the returned value is determined by the length of the logical vector passed as an argument to its first formal parameter (named test)! A frequent mistake is to use a condition that returns a logical vec-

tor of length one, expecting that it will be recycled because arguments passed to the other formal parameters (named yes and no) are longer. However, no recycling will take place, resulting in a returned value of length one, with the remaining elements of the vectors passed to yes and no being discarded. Do try this by yourself, using logical vectors of different lengths. You can start with the examples below, making sure you understand why the returned values are what they are.

```
ifelse(TRUE, 1:5, -5:-1)
## [1] 1
ifelse(FALSE, 1:5, -5:-1)
## [1] -5
ifelse(c(TRUE, FALSE), 1:5, -5:-1)
## [1] 1 -4
ifelse(c(FALSE, TRUE), 1:5, -5:-1)
## [1] -5 2
ifelse(c(FALSE, TRUE), 1:5, 0)
## [1] 0 2
```

5.13 Some additional examples to play with, with a few surprises. Study the examples below until you understand why returned values are what they are. In addition, create your own examples to test other possible cases. In other words, play with the code until you fully understand how ifelse() statements work.

```
a <- 1:10
ifelse(a > 5, 1, -1)
ifelse(a > 5, a + 1, a - 1)
ifelse(any(a > 5), a + 1, a - 1) # tricky
ifelse(logical(0), a + 1, a - 1) # even more tricky
ifelse(NA, a + 1, a - 1) # as expected
```

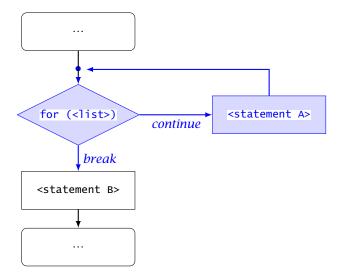
Hint: if you need to refresh your understanding of logical values and Boolean algebra see section 3.5 on page 49.

**5.14** Write, using ifelse(), a single statement to combine numbers from the two vectors **a** and **b** into a result vector **d**, based on whether the corresponding value in vector **c** is the character "a" or "b". Then print vector **d** to make the result visible.

```
a <- -10:-1
b <- +1:10
c <- c(rep("a", 5), rep("b", 5))
```

If you do not understand how the three vectors are built, or you cannot guess the values they contain by reading the code, print them, and play with the arguments, until you understand what each parameter does. Also use help(rep) and/or help(ifelse) to access the documentation.

**5.15** Continuing from the playground above, test the behaviour of ifelse() with NA, NULL and logical() passed as arguments to test. Also test the behaviour when only some members of a logical vector are not available (NA).



**FIGURE 5.6** Flowchart for a for iteration loop.

## 5.7 Iteration

We give the name *iteration* to the process of repetitive execution of a program statement—e.g., *computed by iteration*. We use the same word, *iteration*, to name each one of these repetitions of the execution of a statement—e.g., *the second iteration*.

Iteration constructs make it possible to "decide" at run time the number of iterations, i.e., when execution breaks out of the loop and continues at the next statement in the script. Iteration can be used to apply the same computations to the different members of a vector or list (this section), but also to apply different functions to members of a vector, matrix, list or data frame (section 5.10 on page 160).

In R three types of iteration loops are available: for, while and repeat constructs. They differ in the origin of the values they iterate over, and in the type of test used to terminate iteration. When the same algorithm can be implemented with more than one of these constructs, using the least flexible of them usually results in easier to understand code.

In R, explicit loops as described in this section can in some cases be replaced by calls to *apply* functions (see section 5.8 on page 154) or with vectorized functions and operators (see page 30). The choice among these approaches affects readability and performance (see section 5.11 on page 162).

#### 5.7.1 for loops

The most frequently used type of loop is a for loop. These loops work in R by "walking through" a list or vector of values to act upon (Figure 5.6). Within a

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loop these values are available, sequentially, one at a time through a variable that functions as a placeholder. The implicit test for the end of the vector or list takes place at the top of the construct before the loop statement is evaluated. The flow chart has the shape of a *loop* as the execution can be directed to an earlier position in the sequence of statements, allowing the same section of code to be evaluated multiple times, each time with a new value assigned to the placeholder variable.

In the diagram above the argument to for() is shown as <list> but it can also be a vector of any mode. Objects of most classes derived from list or from an atomic vector can also fulfil the same role. The extraction operation with a numeric index must be supported by objects of the class passed as argument.

Similarly to if constructs, only one statement is controlled by for, however this statement can be a compound statement enclosed in braces { } (see pages 132 and 138).

```
b <- 0 # variable needs to set to a valid numeric value!
for (a in 1:5) b <- b + a
b
## [1] 15</pre>
```

Here the statement b <- b + a is executed five times, with placeholder variable a sequentially taking each of the values, 1, 2, 3, 4, and 5, in anonymous vector 1:5. The name used as placeholder has to fulfil the same requirements as an ordinary R variable name. The list or vector following in can contain any valid R objects, as long as the code statements in the loop body can handle them.

In a for() loop construct, even when it is a variable, the vector or list passed as argument cannot be modified by the code statement within the for loop.

A loop can be "unrolled" into a linear sequence of statements. Let's work through the for loop above.

```
b < -0
# start of loop
# first iteration
a < -1
b < -b + a
# second iteration
a < -2
b \leftarrow b + a
# third iteration
a < -3
b \leftarrow b + a
# fourth iteration
a < -4
b \leftarrow b + a
# fifth iteration
a <- 5
b \leftarrow b + a
# end of loop
## [1] 15
```

The operation implemented in this example is a very frequent one, the sum of a vector, so base R provides a function optimized for efficiently computing it.

```
sum(1:5)
## [1] 15
```

It is important to note that a list or vector of length zero is a valid argument to for(), that triggers no error, but skips the statements in the loop body.

```
b <- 0
for (a in numeric()) b <- b + a
print(b)
## [1] 0</pre>
```

By printing at each iteration variable b, the partial results at each iteration can be observed. Brackets are needed to form a compound statement from the two simple statements so that print(b) is also executed at each iteration.

```
a <- c(1, 4, 3, 6, 8)
for(x in a) {
  b <- x*2
  print(b)
  }
## [1] 2
## [1] 8
## [1] 6
## [1] 12
## [1] 16</pre>
```

The iteration constructs for, while, and repeat always silently return NULL, which is a different behaviour than that of if.

```
b <- for(x in a) x*2
x
## [1] 8
b
## NULL</pre>
```

Thus as shown in earlier examples of for loops, computed values need to be assigned to one or more variables within the loop so that they are not lost.

While in the examples above the code directly walked through the values in the vector, and alternative approach is to walk through a sequence of indices using the extraction operator [ ] to access the values in vectors or lists. This approach makes it possible to walk through more than one list or vector. In the example below, elements of vectors a and b are accessed concurrently, a providing the input and b used to store the corresponding computed value.

```
b <- numeric() # an empty vector
for(i in seq(along.with = a)) {
   b[i] <- a[i]^2
}
b
## [1] 1 16 9 36 64</pre>
```

5.16 Adding calls to print() makes visible the values taken by variables i, a, and b at each iteration. Try to understand where these values come from at each iteration, by playing with the code and modifying it.

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```
b <- numeric() # an empty vector
for(i in seq(along.with = a)) {
  b[i] <- a[i]^2
  print(i)
  print(a)
  print(b)
}</pre>
```

The same approach of adding calls to print() can be used for debugging any code that does not return the expected results.

Above I used seq(along.with = a) to build a numeric vector containing a sequence of the same length as vector a. Using this *idiom* ensures that a vector, in this example a, with length zero will be handled correctly, with numeric(0) assigned to b.

 $\square$  5.17 Run the examples below and explain why the two approaches are equivalent only when the length of a is one or more. Find the answer by assigning to A, vectors of different lengths, including zero (using A <- numeric(0)).

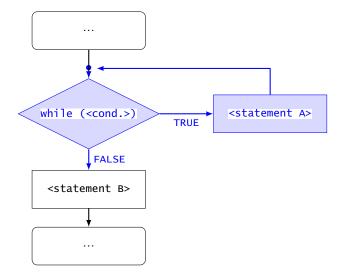
```
# assign a numeric vector to variable A
B <- numeric(length(A))
for(i in seq(along.with = A)) {
   B[i] <- A[i]^2
}
B
C <- numeric(length(A))
for(i in 1:length(A)) {
   C[i] <- A[i]^2
}
C</pre>
```

Using seq() as above creates a sequence of numbers in i, that includes all members of a in the "walk-trough". There is no requirement in the R for this, and including only some of the valid indexes, or including them in arbitrary order is possible if needed, however this is rarely the case.

Vectorization usually results in the simplest and fastest code, as shown below (see section 5.11 on 162). However, not all for loops can be replaced by vectorized statements.

```
b <- a^2
b
## [1] 1 16 9 36 64
```

for loops as described above, in the absence of errors, have statically predictable behavior. The compound statement in the loop will be executed once for each member of the vector or list. Special cases may require the alteration of the normal flow of execution in the loop. Two cases are easy to deal with, one is stopping iteration early with a call to break(), and another is jumping ahead to the next iteration with a call to next(). The example below shows the use of these two functions: we ignore negative values contained in a, and exit or break out of the loop when the accumulated sum b exceeds 100.



**FIGURE 5.7** Flowchart for a while iteration loop.

```
b <- 0
a <- -10:100
idxs <- seq_along(a)
for(i in idxs) {
   if (a[i] < 0) next()
   b <- b + a[i]
   if (b > 100) break()
}
b
## [1] 105
i
## [1] 25
a[i]
## [1] 14
```

Hint: if you find the code in the example above difficult to understand, insert print() statements and run it again inspecting how the values of a, b, idxs and i behave within the loop.

In for loops the use of break() and next() should be reserved for exceptional conditions. When the for construct is not flexible enough for the computations being implemented, using a while or a repeat loop is preferable.

### 5.7.2 while loops

while loops are more flexible than for loops (Figure 5.7). Instead of walking through a list or vector, iteration is controlled by a logical condition of length one, just like in if. Differently to if, the controlled statement is executed repeatedly as long as the condition remains TRUE.

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```
a <- 2
while (a < 50) {
    print(a)
    a <- a^2
}
## [1] 2
## [1] 16
print(a)
## [1] 256</pre>
```

To ensure that a while loop is exited instead of circling for ever, the condition, a < 50 in the example above, must depend on a value that is modified by the controlled statement, like a in this case.

**5.18** Make sure that you understand why the final value of **a** is larger than 50.

The statements above can be simplified, by nesting the assignment inside a call to print.

```
a <- 2
print(a)
while (a < 50) print(a <- a^2)</pre>
```

In R, statements like c <- 1:5 return *invisibly* (with no implicit call to print()) the value assigned. This makes possible *chained* assignments to several variables within a single statement like in the example below, as well as using an assignment statement as an argument to a function or operator.

```
a <- b <- c <- 1:5
```

**5.19** Explain why a second print(a) has been added before while(). Hint: experiment if necessary.

As with for loops we can use an index variable in a while loop to walk through vectors and lists. The difference is that we have to update the index values explicitly in our own code. As example below is the code example for for from page 148 rewritten using while.

```
a <- c(1, 4, 3, 6, 8)
b <- numeric() # an empty vector
i <- 1
while(i <= length(a)) {
   b[i] <- a[i]^2
   print(b)
   i <- i + 1
}
## [1] 1 16
## [1] 1 16
## [1] 1 16 9 36
## [1] 1 16 9 36 64
b
## [1] 1 16 9 36 64</pre>
```

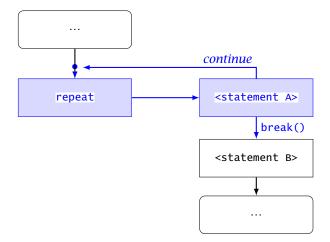


FIGURE 5.8

Flowchart for a repeat iteration loop.

while loops as described above will terminate when the condition tested is FALSE. In cases that require stopping iteration based on an additional test condition within the compound statement, we can call break() in the body of an if or else statement within the while statement. As in the case of for loops, it is good to use break() only for exceptional conditions.

### 5.7.3 repeat loops

The repeat construct is the most flexible as iteration only stops with a call to break(). One or more calls to break() can be located anywhere within the compound statement that forms the body of the loop (Figure 5.8).

```
a <- 2
repeat{
   print(a)
   if (a > 50) break()
   a <- a^2
}
## [1] 2
## [1] 4
## [1] 16
## [1] 256</pre>
```

5.20 Try to explain why the example above returns the values it does. Use the approach of adding print() statements, as described on page 148.

When repeat loop constructs contain more than one call to break(), each within a different if or else statement, indentation and/or comments can be used to highlight in the listing this infrequent use case.

**5.21** Explain why a repeat construct is equivalent to a while construct with the test condition set equal to logical constant TRUE.

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## 5.7.4 Nesting of loops

All the execution-flow control statements seen above can be nested, as syntactically they are themselves statements. I show an example with two for loops used to walk through rows and columns of a matrix constructed as follows.

```
A <- matrix(1:50, nrow = 10)
##
           [,1] [,2] [,3] [,4] [,5]
##
     [1,]
                         21
                               31
                   11
##
     [2,]
              2
                   12
                         22
                               32
                                      42
##
              3
                   13
                         23
                                33
                                      43
##
     [4,]
              4
                   14
                         24
                                34
                                      44
                   15
                          25
##
     [5,]
              5
                                35
                                      45
##
     [6,]
              6
                   16
                         26
                                36
                                      46
                   17
                         27
                                37
##
     [7,]
                                      47
##
    [8,]
              8
                   18
                         28
                                38
                                      48
##
    [9,]
              9
                   19
                         29
                                39
                                      49
## [10,]
             10
                   20
                         30
```

The nested loops below compute the sum for each row of the matrix. In the example below, the value of i changes for each iteration of the outer loop. The value of j changes for each iteration of the inner loop, and the inner loop is run in full for each iteration of the outer loop. The inner loop index j changes fastest.

```
row.sum <- numeric()
for (i in 1:nrow(A)) {
   row.sum[i] <- 0
   for (j in 1:ncol(A))
      row.sum[i] <- row.sum[i] + A[i, j]
}
print(row.sum)
## [1] 105 110 115 120 125 130 135 140 145 150</pre>
```

The nested loops above work correctly with any two-dimensional matrix with at least one column and one row, but *crash* with an empty matrix (matrix() or matrix(numeric())). Thus it is good practice to enclose the for loop in an if statement as protection. For the example above a suitable logical condition is !is.null(dim(A)) && !any(dim(A) == 0.

5.22 1) Modify the code in last chunk above so that it sums the values only in the first three columns of A, and 2) modify the same code so that it sums the values only in the last three rows of A.

Does the code you wrote work as expected when the number of rows in A is different from 10? and, also if the number of columns in A is different from 5? What would happen if A had fewer than three columns? Try to think first what to expect based on the code you wrote. Then create matrices of different sizes and test your code. After that, if necessary, try to improve the code, so that wrong results are never returned.

# 5.8 *Apply* functions

Apply functions apply a function passed as an argument to parameter fun or equivalent, to elements in a collection of R objects passed as an argument to parameter x or equivalent. Collections to which fun is to be applied can be vectors, lists, data frames, matrices or arrays. As long as the operations to be applied are independent—i.e., the results from one iteration are not used in another iteration—apply functions can replace for, while or repeat loops.

Conceptually, for, while and repeat loops are interpreted as controlling sequential evaluation of program statements. In contrast, R's *apply* functions are, conceptually, thought as evaluating a function in parallel for each of the different members of their input. So, while in loops the results of earlier iterations through a loop can be stored in variables and used in subsequent iterations, this is not possible in the case of *apply* functions.

The different *apply* functions in base R differ in the class of the values they accept for their x parameter, the class of the object they return and/or the class of the value returned by the applied function. lapply() and sapply() expect a vector or list as an argument passed through x. lapply() returns a list or an array; and vapply() always *simplifies* its returned value into a vector, while sapply() does the simplification according to the argument passed to its simplify parameter. All these *apply* functions can be used to apply an R function that returns a value of the same or a different class as its argument. In the case of apply() and lapply() not even the length of the values returned for each member of the collection passed as an argument, needs to be consistent. Function apply() is used to apply a function to the elements along one dimension of an object that has two or more *dimensions* returning an array or a list or a vector depending on the size, and consistency in length and class among the values returned by the applied function.

## 5.8.1 Applying functions to vectors, lists and data frames

Here I exemplify the use of lapply(), sapply() and vapply(). In the chunks below they are used to apply function log() to each member of a numeric vector. This is a function defined in R itself, but user-defined functions and functions imported from packages can be applied identically. How to define packages and define new functions are the subject of chapter 6 (on page 169).

The individual member objects in the list or vector passed as argument to parameter x of *apply* functions are passed as a positional argument to the first formal parameter of the applied function, i.e., only some R functions can be passed as argument to FUN.

```
set.seed(123456) # so that vct1 does not change
vct1 <- runif(6) # A short vector as input to keep output short
str(vct1)
## num [1:6] 0.798 0.754 0.391 0.342 0.361 ...</pre>
```

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```
z <- lapply(X = vct1, FUN = log)
str(z)
## List of 6
## $ : num -0.226
## $ : num -0.283
## $ : num -0.938
## $ : num -1.07
## $ : num -1.02
## $ : num -1.62</pre>
```

The code above calls log() once with each of the six members of vct1 as argument and collects the returned values into a list, hence the lin lapply().

```
z <- sapply(X = vct1, FUN = log)
str(z)
## num [1:6] -0.226 -0.283 -0.938 -1.074 -1.018 ...</pre>
```

The code above calls log() as in the previous example but collects the returned values into a vector, i.e., by default it *simplifies* the list into a vector or matrix when possible, hence the s in sapply(). Simplification can be skipped, in this case returning a list as lapply() above (not shown).

```
z <- sapply(X = vct1, FUN = log, simplify = FALSE)
str(z)</pre>
```

vapply() always returns a vector (no example shown), hence the v in its name.
The computed results are the same using lapply(), sapply() or vapply(), but the
class and structure of the objects returned can differ, as well as how numbers are
printed.

Function log() has a second parameter named base that can be passed and argument to override the default base (*e*) used to compute natural logarithms. Additional arguments like this can be passed by name, using the name of the parameter in the function passed as argument to FUN, in this case base.

```
z <- sapply(X = vct1, FUN = log, base = 10)
str(z)
## num [1:6] -0.0981 -0.1229 -0.4075 -0.4665 -0.4421 ...</pre>
```

Anonymous functions can be defined (see section 6.2 on page 169) and directly passed as argument to FUN without the need of separately assigning them to a name.

```
z <- sapply(X = vct1, FUN = function(x) {log10(x + 1)})
str(z)
## num [1:6] 0.255 0.244 0.143 0.128 0.134 ...</pre>
```

As explained in section 4.4 on page 94, class data.frame is derived from class list. The columns in a data frame are equivalent to members of a list, and functions can thus be applied to columns. The data frame cars from package 'datasets' contains data for speed and for stopping distance for cars stored in two columns or member variables, named speed and dist. The members of the returned numeric vector, containing the computed means, are named accordingly.

```
sapply(X = cars, FUN = mean)
## speed dist
## 15.40 42.98
```

Here is a possible way of obtaining means and standard deviations of member vectors. The argument passed to fun.value provides a template for the type of the returned value and its organization into rows and columns. Notice that the rows in the output are now named according to the names in fun.value.

A function that returns a numeric vector of length 2 containing mean and standard deviation can be defined by calling existing functions (see section 6.2 on page 169).

```
mean_and_sd <-
function(x, na.rm = FALSE) {
    c(mean = mean(x, na.rm = na.rm), sd = sd(x, na.rm = na.rm))
}</pre>
```

and vapply() used to apply it to each member vector of the list. The argument passed to FUN.VALUE serves as a template indicating the values returned by function mean\_and\_sd().

- 5.23 Apply function mean\_and\_sd() defined above to the data frame cars from 'datasets'. The aim is to obtain the mean and standard deviation for each numeric column.
- 5.24 Obtain the summary of dataset airquality with function summary(), but in addition, write code with an *apply* function to count the number of non-missing values in each column. Hint: using sum() on a logical vector returns the count of TRUE values as TRUE, and FALSE are transparently converted into numeric 1 and 0, respectively, when logical values are used in arithmetic expressions.

In the examples above the *apply* functions were used to "reduce' the data by applying summary functions. In the next code chunk <code>lapply()</code> is used to construct the <code>list</code> of five vectors <code>lsl</code> using a vector of five numbers as argument passed to parameter x. As above, additional *named* arguments are relayed to each call of <code>rnorm()</code>.

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In addition to functions returning pseudo-random draws from different probability distributions, constructors for objects of various classes can be used similarly.

## 5.8.2 Applying functions to matrices and arrays

Matrices and arrays have two or more dimensions, and contrary to data frames, they are not a special kind of one-dimensional lists. In R the dimensions of a matrix, rows and columns, over which a function is applied are called *margins* (see section 3.11, and Figure 3.2 on page 70). The argument passed to parameter MARGIN determines *over* which margin the function will be applied. Arrays can have many dimensions (see Figure 3.3 on page 76), and consequently more margins. In the case of arrays with more than two dimensions, it is possible and can be useful to apply functions over multiple margins at once.

The individual *slices* of the matrix or array passed as argument to parameter x of *apply* functions are passed as a positional argument to the first formal parameter of the applied function, i.e., only some R functions can be passed as argument to FUN.

Matrix mat1 constructed here will be used in examples. Adding names helps with understanding both here and when using matrices in real data analysis situations.

```
mat1 <- matrix(rnorm(6, mean = 10, sd = 1), ncol = 2)
mat1 <- round(mat1, digits = 1)
dimnames(mat1) <- # add row and column names
   list(paste("row", 1:nrow(mat1)), paste("col", 1:ncol(mat1)))
mat1
## col 1 col 2
## row 1 10.1 11.7
## row 2 9.3 10.6
## row 3 10.9 9.2</pre>
```

Column (or row) means of matrices can be easily computed with apply(). However, in contrast to when using other *apply* functions, an argument must be passed to parameter MARGIN.

```
apply(mat1, MARGIN = 2, FUN = mean)
## col 1 col 2
## 10.1 10.5
```

5.25 Edit the example above so that it computes row means instead of column means

**5.26** As described above, we can pass arguments by name to the applied function. Can you guess why parameter names of *apply* functions are fully in uppercase, something very unusual for R coding style?

If the function applied returns a value of the same length as its input, then the dimensions of the value returned by apply() are the same as those of its input. Using the identity function I() that returns its argument unchanged, facilitates the comparison of output against input.

```
z <- apply(X = mat1, MARGIN = 2, FUN = I)
dim(z)</pre>
```

```
## [1] 3 2

## col 1 col 2

## row 1 10.1 11.7

## row 2 9.3 10.6

## row 3 10.9 9.2
```

Passing Margin = 1 as below instead of Margin = 2 as above, rows and columns are transposed in the returned value!.

```
z <- apply(X = mat1, MARGIN = 1, FUN = I)
dim(z)
## [1] 2 3
z
## row 1 row 2 row 3
## col 1 10.1 9.3 10.9
## col 2 11.7 10.6 9.2</pre>
```

The next, more realistic example, applies function summary() that returns a value usually shorter than its input, but longer than one. Both for column summaries (MARGIN = 2) and row summaries (MARGIN = 1), a matrix is returned. Each columns, a numeric vector in this example, contains the vector returned by a call to summary(). Column and row names from mat1 are preserved, as well as the names in the value returned by summary().

```
z \leftarrow apply(x = mat1, MARGIN = 2, FUN = summary)
##
           col 1 col 2
## Min.
             9.3 9.20
             9.7 9.90
## 1st Qu.
           10.1 10.60
## Median
            10.1 10.50
## Mean
## 3rd Qu. 10.5 11.15
            10.9 11.70
## Max.
z \leftarrow apply(X = mat1, MARGIN = 1, FUN = summary)
Ζ
##
           row 1 row 2
                          row 3
                  9.300
                          9.200
## Min.
            10.1
## 1st Qu.
            10.5
                  9.625 9.625
## Median
            10.9 9.950 10.050
            10.9 9.950 10.050
## Mean
## 3rd Ou. 11.3 10.275 10.475
## Max.
            11.7 10.600 10.900
```

In all examples above, we have used ordinary functions. Binary operators in R are functions with two formal parameters which can be called using infix notation in expressions—i.e., a + b. By back-quoting their names they can be called using the same syntax as for ordinary functions, and consequently also passed to the FUN parameter of apply functions. A toy example, equivalent to the vectorized operation vct1 + 5 follows. By enclosing operator + in back ticks (`) and passing by name a constant to its second formal parameter (e2 = 5) operator + behaves like an ordinary function. See section 6.2.3 on page 175).

```
set.seed(123456) # so that vct1 does not change
vct1 <- runif(10)</pre>
```

**TABLE 5.1** 

R functions that can substitute for iteration loops. They accept vectors as argument, except for rowsums(), colsums(), rowMeans(), and colMeans() which accept matrix objects as argument. Only functions that return a value with the same dimensions as the argument passed as input are vectorized in the sense used in this book.

Function	Computation	Returned class, length
sum()	$\sum_{i=1}^n x_i$	numeric, 1
rowSums()	$\sum_{j=1}^{l} x_i$	numeric, $n$
colSums()	$\sum_{i=1}^{n} x_j$	numeric, $l$
mean()	$\sum_{i=1}^{n} x_i$	numeric, $1$
rowMeans()	$\sum_{j=1}^{l} x_i/l$	numeric, $n$
colMeans()	$\sum_{i=1}^{n} x_j/n$	numeric, $\emph{l}$
prod()	$\prod_{i=1}^n x_i$	numeric, $1$
cumsum()	$\sum_{i=1}^{1} x_i, \cdots \sum_{i=1}^{j} x_i, \cdots \sum_{i=1}^{n} x_i$	numeric, $n_{ m out}=n_{ m in}$
cumprod()	$\prod_{i=1}^1 x_i, \cdots \prod_{i=1}^j x_i, \cdots \prod_{i=1}^n x_i$	numeric, $n_{ m out}=n_{ m in}$
cummax()	cumulative maximum	numeric, $n_{ m out}=n_{ m in}$
cummin()	cumulative minimum	numeric, $n_{ m out}=n_{ m in}$
runmed()	running median	numeric, $n_{ m out}=n_{ m in}$
diff()	$x_2-x_1, \cdots x_i-x_{i-1}, \cdots x_n-x_{n-1}$	numeric, $n_{ m out}=n_{ m in}-1$
<pre>diffinv()</pre>	inverse of diff	numeric, $n_{ m out}=n_{ m in}+1$
factorial()	x!	numeric, $n_{ m out}=n_{ m in}$
rle()	run-length encoding	rle, $n_{ m out} < n_{ m in}$
inverse.rle()	run-length decoding	vector, $n_{\text{out}} > n_{\text{in}}$

```
z <- sapply(X = vct1, FUN = `+`, e2 = 5)
str(z)
## num [1:10] 5.8 5.75 5.39 5.34 5.36 ...</pre>
```

# 5.9 Functions that replace loops

R provides several functions that can be used to avoid writing iterative loops. The most frequently used are taken for granted: mean(), var() (variance), sd() (standard deviation), max(), and min(). Replacing code implementing an iterative algorithm by a single function call simplifies the script's code and can make it easier to understand. These functions are written in C and compiled, so even when iterative algorithms are used, they are fast (see section 5.11 on page 162). Table 5.1 lists several functions from base R that implement iterative algorithms. All these functions take a vector of arbitrary length as their first argument, except for inverse.rle().

 $\blacksquare$  5.27 Build a numeric vector such as x <- c(1, 9, 6, 4, 3) and pass it as argument to the functions in Table 5.1. Do the corresponding computations manually for the functions your find most relevant, trying to understand what values they calculate.

# 5.10 The multiple faces of loops

In this advanced section I describe some uses of R loops that help with writing concise scrips. As these make heavy use of functions, if you are reading the book sequentially, you should skip this section and return to it after reading chapters 6 and 7.

In the same way as we can assign names to numeric, character and other types of objects, we can assign names to functions and expressions. We can also create lists of functions and/or expressions. The R language has a very consistent grammar, with all lists and vectors behaving in the same way. The implication of this is that we can assign different functions or expressions to a given name, and consequently it is possible to write loops over lists of functions or expressions.

In this first example we use a *character vector of function names*, and use function do.call() call them as it accepts both character strings and function names as argument to its first parameter. We obtain a numeric vector with named members with names matching the function names.

```
vct1 <- rnorm(10)
results <- numeric()
fun.names <- c("mean", "max", "min")
for (f.name in fun.names) {
   results[[f.name]] <- do.call(f.name, list(vct1))
}
results
## mean max min
## 0.5453427 2.5026454 -1.1139499</pre>
```

When traversing a *list of functions* in a loop, we face the problem that we cannot access the original names of the functions as what is stored in the list are the code definitions of the functions. In this case, we can hold the function definitions in the loop variable (f in the chunk below) and call the functions by use of the function call notation (f()). We obtain a numeric vector with anonymous members.

```
results <- numeric()
funs <- list(mean, max, min)
for (f in funs) {
  results <- c(results, f(x))
}
results
## [1] 8 8 8</pre>
```

We can use a named list of functions to gain full control of the naming of the results. We obtain a numeric vector with named members with names matching the names given to the list members.

```
results <- numeric()
funs <- list(average = mean, maximum = max, minimum = min)
for (f in names(funs)) {
  results[[f]] <- funs[[f]](x)
}
results
## average maximum minimum
## 8 8 8 8</pre>
```

Next is an example using model formulas. We use a loop to fit three models, obtaining a list of fitted models. We cannot pass to anova() this list of fitted models, as it expects each fitted model as a separate nameless argument to its ... parameter. We can get around this problem using function do.call() to call anova(). Function do.call() passes the members of the list passed as its second argument as individual arguments to the function being called, using their names if present. anova() expects nameless arguments so we need to remove the names present in results.

```
my.data \leftarrow data.frame(x = 1:10, y = 1:10 + rnorm(10, 1, 0.1))
results <- list()
models <- list(linear = y ~ x, linear.orig = y ~ x - 1, quadratic = y ~ x + I(x^2))
for (m in names(models)) {
  results[[m]] <- lm(models[[m]], data = my.data)</pre>
str(results, max.level = 1)
## List of 3
  $ linear
                 :List of 12
    ..- attr(*, "class")= chr "lm"
## $ linear.orig:List of 12
    ..- attr(*, "class")= chr "lm"
## $ quadratic :List of 12
   ..- attr(*, "class")= chr "lm"
do.call(anova, unname(results))
## Analysis of Variance Table
##
## Model 1: y \sim x
## Model 2: y \sim x - 1
## Model 3: y \sim x + I(x^2)
   Res.Df
                RSS Df Sum of Sq
                                            Pr(>F)
## 1
         8 0.05525
## 2
          9 2.31266 -1
                         -2.2574 306.19 4.901e-07 ***
## 3
          7 0.05161 2
                           2.2611 153.34 1.660e-06 ***
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

If we had no further use for results we could simply build a list with nameless members by using positional indexing.

```
results <- list()
models <- list(y ~ x, y ~ x - 1, y ~ x + I(x^2))
for (i in seq(along.with = models)) {
   results[[i]] <- lm(models[[i]], data = my.data)
}
str(results, max.level = 1)
## List of 3
## $ :List of 12
## ..- attr(*, "class")= chr "lm"</pre>
```

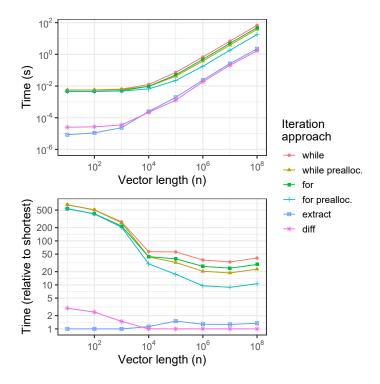
```
$ :List of 12
    ..- attr(*, "class")= chr "lm"
##
   $ :List of 12
    ..- attr(*, "class")= chr "lm"
do.call(anova, results)
## Analysis of Variance Table
##
## Model 1: y \sim x
## Model 2: y \sim x - 1
## Model 3: y \sim x + I(x^2)
               RSS Df Sum of Sq
   Res.Df
                                            Pr(>F)
## 1
         8 0.05525
          9 2.31266 -1 -2.2574 306.19 4.901e-07 ***
          7 0.05161 2 2.2611 153.34 1.660e-06 ***
## Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

# 5.11 Iteration when performance is important

When working with large data sets, or many smaller data sets, one frequently needs to take performance into account. In R, explicit for, while and repeat are considered to be slow to run. Vectorized operations perform in general comparatively faster. As vectorization (see page 30) usually also makes code simpler, it is good style to use vectorization whenever possible. Depending on the case, loops can be replaced using vectorized arithmetic operators, *apply* functions (see section 5.8 on page 154) and functions implementing frequently used operations (see section 5.9 on page 159). Improved performance needs to be balanced against the effort invested in writing faster code, as in most cases our own time is more valuable than computer running time. However, using vectorized operators and optimized functions becomes nearly effortless once one is familiar with them.

To demonstrate the magnitude of the differences in performance that can be expected, I used as a first case the computation of the differences between successive numbers in a vector, applied to vectors of lengths ranging from 10 to 100 million numbers (Figure 5.9). In relative terms the difference in computation time was huge between loops and vectorization for vectors of up to 1 000 numbers (near  $\times 500$ ), but the total times were very short (5  $\times$  10 $^{-3}$  s vs. 10  $\times$  10 $^{-6}$  s). For these vectors, pre-allocation of a vector to collect the results made almost no difference and vectorization with the extraction operator [] together with the minus arithmetic operator – was fastest. There seems to be a significant overhead for explicit loops, as the running time was nearly independent of the length of these short vectors.

For vectors of  $10\,000$  or more numbers there was only a very small advantage in using function diff() over using vectorized arithmetic and extraction operators. For while and for loops pre-allocation of the vector to collect results made an important difference ( $\times 2$  to  $\times 3$ ), larger in the case of for. However, vectorized operators and function diff() remained nearly  $\times 10$  faster than the fastest explicit



#### FIGURE 5.9

Benchmark results for different approaches to computing running differences in numeric (double) vector of different lengths. The data in this figure were obtained in a computer with a 12-years old Xenon E3-1235 CPU with four cores, 32 GB of RAM, Windows 10 and R 4.3.1.

loop. For the longer vectors the time increased almost linearly with their length, with similar slopes for the different approaches. Because of the computation used for this example, *apply()* functions could not be used.

The chunks below show the code for the six approaches compared in Figure 5.9, where a is a numeric vector varying length constructed with function rnorm().

```
b <- numeric() # do not pre-allocate memory
i <- 1
while (i < length(a)) {
   b[i] <- a[i+1] - a[i]
   i <- i + 1
}

b <- numeric(length(a)-1) # pre-allocate memory
i <- 1
while (i < length(a)) {
   b[i] <- a[i+1] - a[i]
   i <- i + 1
}</pre>
```

```
b <- numeric() # do not pre-allocate memory
for(i in seq(along.with = b)) {
   b[i] <- a[i+1] - a[i]
}

b <- numeric(length(a)-1) # pre-allocate memory
for(i in seq(along.with = b)) {
   b[i] <- a[i+1] - a[i]
}

# vectorized using extraction operators
b <- a[2:length(a)] - a[1:length(a)-1]

# vectorized function diff()
b <- diff(a)</pre>
```

In nested iteration loops it is most important to vectorize or otherwise enhance the performance of the innermost loop as it is the one executed most frequently. The code for nested loops (used as example in section 5.7.4 on page 153) can be edited to remove the explicit use of for loops. I assessed the performance of different approaches by collecting timings for square matrix objects with dimensions (rows  $\times$  columns) ranging from  $10 \times 10$ , size =  $10^2$ , to  $10\,000 \times 10\,000$ , size =  $10^8$  (Figure 5.10).

In this second case, pre-allocation of memory to b did not enhance performance in good agreement with the benchmarks for the first example as when largest its length was  $10\,000$ . The two nested loops always took the longest to run irrespective of the size of matrix A. A single loop over rows using a call to sum() for each row, improved performance compared to nested loops, most clearly for large matrices. This approach was out-performed by apply() only for small matrices, from which we can infer that apply() has a much smaller overhead than an explicit for loop. rowsums() was between  $\times 5$  and  $\times 20$  faster than the second fastest approach depending on the size of the matrix.

The chunks below show the code for the six approaches compared in Figure 5.10, where A was a numeric matrix constructed with function rnorm().

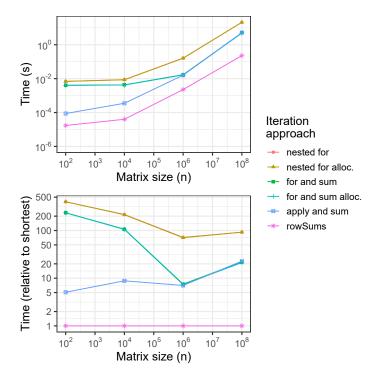
The inner for loop can be replaced by function sum() which returns the sum of a vector. Within the loop A[i, ] extracts whole rows, one at a time.

```
row.sum <- numeric()
for (i in 1:nrow(A)) {
   row.sum[i] <- 0
   for (j in 1:ncol(A))
      row.sum[i] <- row.sum[i] + A[i, j]
}
print(row.sum)

row.sum <- numeric(nrow(A)) # faster
for (i in 1:nrow(A)) {
   row.sum[i] <- sum(A[i, ])
}

The outer loop can be replaced by a call to apply() (see section 5.8 on page 154).</pre>
```

row.sum <- apply(A, MARGIN = 1, sum) # MARGIN=1 indicates rows



#### **FIGURE 5.10**

Benchmark results for different approaches to computing row sums of square numeric (double) matrices of different sizes. The data in this figure were obtained in a computer with a 12-years old Xenon E3-1235 CPU with four cores, 32 GB of RAM, Windows 10 and R 4.3.1.

Calculating row sums is a frequent operation, thus, R provides a built-in function for this.

#### rowSums(A)

The simplest way of measuring the execution time of an R expression is to use function system.time(). Package 'microbenchmark', used for the benchmarks shown in Figures 5.9 and 5.10, provides finer time resolution.

As in these examples the computations in the body of the loop are very simple, the overhead of the iterative loops strongly affects the total computation time in these benchmarks. When the computations at each iteration are time consuming, the overhead of using explicit iteration loops gets diluted. Thus, removing the explicit use of iteration is most helpful, when it is easier to implement vectorized arithmetic or find optimized functions.

The timings in Figures 5.9 and 5.10 are only valid for the specific computer configuration, operating system and R version that I used. They provide only an approximate guide to what can be expected in different conditions. The scripts used are included in package 'learnrbook' in case readers wish to run them on

their computers. As replication is used, the total run time for the script is relatively long.

You may be wandering: how do the faster approaches manage to avoid the overhead of iteration? Of course they do not really avoid iteration, but the loops in functions written in C, C++, or FORTRAN are compiled into machine code as part of R itself or when packages binaries are created. In simpler words, the time required to convert and optimize the code written in these languages into machine code is spent during compilation, usually before we download and install R or packages. Instead, a loop coded in R is interpreted into machine code each time we source our script, and in some cases for each iteration in a loop. The R interpreter does some compilation into virtual machine code, as a preliminary stage which helps improve performance.

The examples in this section use numbers and arithmetic operations, but vectorization and *apply* functions can be also used with vectors of other modes, such as vectors of character strings or logical values.

With modern computer processors, or CPUs, splitting the tasks across multiple cores for concurrent execution can enhance performance. To some extent this happens invisibly due to optimizations in the translation into machine code. Explicit approaches are available in package 'parallel' included in the R distribution and contributed packages such as 'future'. Parallelization is also possible across interconnected computers. However, how to enhance performance based on parallel or distributed execution is beyond the scope of this book.

### 5.12 Object names as character strings

In all assignment examples before this section, we have used object names included as literal character strings in the code expressions. In other words, the names are "decided" as part of the code, rather than at run time. In scripts or packages, the object name to be assigned may need to be decided at run time and, consequently, be available only as a character string stored in a variable. In this case, function assign() must be used instead of the operators <- or ->. The statements below demonstrate its use.

First using a character constant.

```
assign("a", 9.99)
a
## [1] 9.99

Next using a character value stored in a variable.
name.of.var <- "b"
assign(name.of.var, 9.99)
b
## [1] 9.99</pre>
```

The two toy examples above do not demonstrate why one may want to use assign(). Common situations where we may want to use character strings to store

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(future or existing) object names are 1) when we allow users to provide names for objects either interactively or as character data, 2) when in a loop we transverse a vector or list of object names, or 3) we construct at runtime object names from multiple character strings based on data or settings. A common case is when we import data from a text file and we want to name the object according to the name of the file on disk, or a character string read from the header at the top of the file.

Another case is when character values are the result of a computation.

```
for (i in 1:5) {
    assign(paste("square_of_", i, sep = ""), i^2)
}
ls(pattern = "square_of_*")
## [1] "square_of_1" "square_of_2" "square_of_3" "square_of_4" "square_of_5"
```

The complementary operation of *assigning* a name to an object is to *get* an object when we have available its name as a character string. The corresponding function is get().

```
get("a")
## [1] 9.99
get("b")
## [1] 9.99
```

If we have available a character vector containing object names and we want to create a list containing these objects we can use function mget(). In the example below we use function ls() to obtain a character vector of object names matching a specific pattern and then collect all these objects into a list.

```
obj_names <- ls(pattern = "square_of_*")
obj_lst <- mget(obj_names)
str(obj_lst)
## List of 5
## $ square_of_1: num 1
## $ square_of_2: num 4
## $ square_of_3: num 9
## $ square_of_4: num 16
## $ square_of_5: num 25</pre>
```

5.28 Think of possible uses of functions assign(), get() and mget() in scripts you use or could use to analyze your own data (or from other sources). Write a script to implement this, and iteratively test and revise this script until the result produced by the script matches your expectations.

# 5.13 Clean-up

Sometimes we need to make sure that clean-up code is executed even if the execution of a script or function is aborted by the user or as a result of an error condition. A typical example is a script that temporarily sets a disk folder as the working directory or uses a file as temporary storage. Function on.exit() can be used to record that a user supplied expression needs to be executed when the cur-

rent function, or a script, exits. Function on.exit() can also make code easier to read as it keeps creation and clean-up next to each other in the body of a function or in the listing of a script.

```
file.create("temp.file")
## [1] TRUE
on.exit(file.remove("temp.file"))
# code that makes use of the file goes here
```

Function library() attaches the namespace of the loaded packages and in some special cases one may want to detach them at the end of a script. We can use detach() similarly as with attached data.frame objects (see page 110). As an example we detach the packages used in section 5.11. It is important to remember that the order in which they can be detached is determined by their interdependencies.

```
detach(package:patchwork)
detach(package:ggplot2)
detach(package:scales)
```

### 5.14 Further reading

For further readings on the aspects of R discussed in the current chapter, I suggest the books *The Art of R Programming: A Tour of Statistical Software Design* (Matloff 2011) and *Advanced R* (Wickham 2019).

# Base R: Adding New "Words"

Computer Science is a science of abstraction—creating the right model for a problem and devising the appropriate mechanizable techniques to solve it.

Alfred V. Aho and Jeffrey D. Ullman *Foundations of Computer Science*, 1992

## 6.1 Aims of this chapter

In earlier chapters we have only used base R features. In this chapter you will learn how to expand the range of features available. We will start by discussing how to define and use new functions, operators and classes. Later we will focus on using existing packages and touch briefly on how they work. We will not consider the important, but more advanced question of packaging functions and classes into new R packages.

# 6.2 Defining functions and operators

Abstraction can be defined as separating the fundamental properties from the accidental ones. Say obtaining the mean from a given vector of numbers is an actual operation. There can be many such operations on different numeric vectors, each one a specific case. When we describe an algorithm for computing the mean from any numeric vector we have created the abstraction of *mean*. In the same way, each time we separate operations from specific data we create a new abstraction. In this sense, functions are abstractions of operations or actions; they are like "verbs" describing actions separately from actors.

The main role of functions is that of providing an abstraction allowing us to avoid repeating blocks of code (groups of statements) applying the same opera-

tions on different data. The reasons to avoid repetition of similar blocks of code statements are that 1) if the algorithm or implementation needs to be revised—e.g., to fix a bug or error—it is best to make edits in a single place; 2) sooner or later pieces of repeated code can become different leading to inconsistencies and hard-to-track bugs; 3) abstraction and division of a problem into smaller chunks, greatly helps with keeping the code understandable to humans; 4) textual repetition makes the script file longer, and this makes debugging, commenting, etc., more tedious, and error prone.

How do we, in practice, avoid repeating bits of code? We write a function containing the statements that we would need to repeat, and later we *call* ("use") the function in their place. We have been calling R functions or operators in almost every example in this book; what we will next tackle is how to define new functions of our own.

We saw in section 5.3 on page 132 a diagram of a compound statement. A function is a code statement, simple or compound, that is partly isolated from the enclosing environment. The *function* abstraction relies on formal parameters working as placeholders for arguments within the function body. When the function is called (or "used") values are passed as arguments to the parameters, and used when executing the code within the function.

New functions and operators are defined using function function(), and saved like any other object in R by assignment to a variable name. In the example below, x and y are both formal parameters, or names used within the function for objects that will be supplied as *arguments* when the function is called.

Function my.prod() has two formal parameters, x and y.

```
fun1 \leftarrow function(x, y)\{x * y\}
```

When we call fun1() with 4 and 3 as arguments, the computation that takes place is 4 \* 3 and the value returned is 12. In this example it is printed, but we could have assigned it to a variable or used it in further computations within the calling statement.

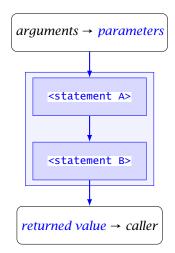
```
fun1(x = 4, y = 3)
## [1] 12
```

**6.1** What is the computation that takes places in this function call? fun1(x = 10, y = 50)

Even though the statements within the function body do have access to the environment in which the function is called, it is safest to pass all input through the function parameters, and return all values to the caller. This ensures that the users of the function can treat it a black box with no side effects.

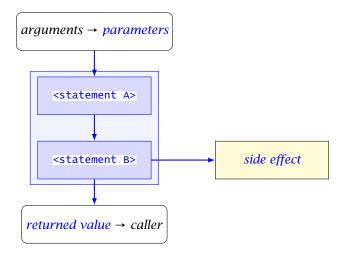
In R, statements within the function usually do not affect directly any variable defined outside the function, the result from the computation is returned as a value. The diagram in Figure 6.1 describes a function that has no *side effects*, as it does not affect its environment, it only returns a value to the caller. A value on which the caller has full control. The statement that calls the function "decides" what to do with the value received from the function.

When a function has a side effect, the caller is no longer in full control (Figure



#### FIGURE 6.1

Diagram of function with no side effects, seen as a compound code statement receiving its input as arguments passed to its formal parameters and returning an object or value to the statement from where it was called or run. The body of the function is represented by the filled box.



#### **FIGURE 6.2**

Diagram of function as a compound code statement receiving its input as arguments passed to its formal parameters and returning an object or value to the statement from where it was called or run. The body of the function is represented by the box filled in blue, while the side effect of the code in the function directly outside is represented by the box filled in yellow.

6.2). Side effects can be actions that do not alter any object in the calling code, like when a call to print() displays text or numbers. Side effects can also be an assignment that modifies an object in the caller's environment, such as assigning a new value to a variable in the caller's environment, i.e., "outside the function".

A function can return only one object, so when multiple results are produced they need to be collected into a single object. In many cases, lists are used to collect all the values to be returned into one R object. For example, model fit functions like Im(), discussed in section 7.9 on page 198, return lists with multiple heterogeneous members, plus ancillary information stored in several attributes. In the case on Im() the returned object's class is Im, and its mode is list.

6.2 When function return() is called within a function, flow of execution within the function stops and the argument passed to return() is the value returned by the function call. In contrast, if function return() is not explicitly called, the value returned by the function call is that returned by the last statement *executed* within the body of the function. Run these examples, and your own variations.

In base R, arguments to functions are passed by copy. This is something important to remember. If code in a function's body modifies the value of a parameter (the placeholder for an argument), its value outside the function is not affected, e.g., if the argument passed was a variable.

```
fn2 <- function(x) {x <- 99}
a <- 1
fn2(a)
a
## [1] 1</pre>
```

In some other computer languages, arguments can be passed by reference, meaning that assignments to a formal parameter within the body of the function are back-referenced to the argument and modify it. It is possible to imitate such behavior in R using some language trickery and consequently, occasionally functions in R use this approach.

Functions have their own *scope*. Any new variables created by normal assignment within the body of a function are visible only within the body of the function and are destroyed when the function returns from the call. In normal use, functions in R do not affect their environment through side effects.

#### 6.2.1 Scope of names

Scoping in R is implemented using *environments* and *name spaces*. We can think of environments as having a boundary with asymmetric visibility. The code within a function runs in its own environment, in isolation from the calling environment in relation to assignments, but the values stored in objects in the calling environment can be retrieved. This protects from unintentional side effects by making difficult to overwrite object definitions in the calling environment. It is possible to override this protection with operator <<- or with function assign(). When used, assignment as side effects, can make the code much more difficult to read and debug, so its best to avoid them.

The visibility of names is determined by the *scoping rules* of a language. The clearest, but not the only situation when scoping rules matter, is when objects with the same name coexist. In such a situation one will be accessible by its unqualified name and the other hidden but possibly accessible by qualifying the name with the namespace where it is defined.

As the R language has few reserved words for which no redefinition is allowed, we should take care not to accidentally reuse names that are part of language. For example pi is a constant defined in R with the value of the mathematical constant  $\pi$ . If we use the same name for one of our variables, the original definition becomes hidden.

```
pi
## [1] 3.141593
pi <- "apple pie"
pi
## [1] "apple pie"
rm(pi)
pi
## [1] 3.141593
exists("pi")
## [1] TRUE</pre>
```

In the example above, the two variables are not defined in the same scope. In the example below we assign a new value to a variable we have earlier created within the same scope, and consequently the second assignment overwrites, rather than hides, the existing definition.

```
my.pie <- "raspberry pie"
my.pie
## [1] "raspberry pie"
my.pie <- "apple pie"
my.pie
## [1] "apple pie"
rm(my.pie)
exists("my.pie")
## [1] FALSE</pre>
```

Name spaces play an important role in avoiding name clashes when contributed packages are attached (see section 6.4.4 on page 182).

Environments can be explicitly created with function environment(). However, environment() is rarely used in scripts while it can be useful within packages.

#### 6.2.2 Ordinary functions

After the toy examples above, we will define a small but useful function: a function for calculating the standard error of the mean from a numeric vector. The standard error is given by  $S_{\hat{x}} = \sqrt{S^2/n}$ . We can translate this into the definition of an R function called SEM.

```
SEM <- function(x){sqrt(var(x) / length(x))}
    We can test our function.
a <- c(1, 2, 3, -5)
a.na <- c(a, NA)
SEM(x = a)
## [1] 1.796988
SEM(a)
## [1] 1.796988
SEM(a.na)
## [1] NA</pre>
```

For example in SEM(a) we are calling function SEM() with a as an argument.

The function we defined above will always give the correct answer because NA values in the input will always result in an NA being returned. The problem is that unlike R's functions like var(), there is no option to omit NA values in the function we defined.

This could be implemented by adding a second parameter na.omit to the definition of our function and passing its argument to the call to var() within the body of SEM(). However, to avoid returning wrong values we need to make sure NA values are also removed before counting the number of observations with length().

A readable way of implementing this in code is to define the function as follows.

```
sem <- function(x, na.omit = FALSE) {
  if (na.omit) {
    x <- na.omit(x)
  }
  sqrt(var(x)/length(x))
}
sem(x = a)
## [1] 1.796988
sem(x = a.na)
## [1] NA
sem(x = a.na, na.omit = TRUE)
## [1] 1.796988</pre>
```

R does not provide a function for standard error, so the function above is generally useful. Its user interface is consistent with that of functionally similar existing functions. We have added a new word to the R vocabulary available to us.

In the definition of sem() we set a default argument for parameter na.omit which is used unless the user explicitly passes an argument to this parameter.

6.3 Define your own function to calculate the mean in a similar way as SEM() was defined above. Hint: function sum() could be of help.

Within an expression, a function name followed by parentheses is interpreted as a call to the function, while the bare name of a function, returns its definition (similarly to any other R object). If the name is entered as a statement at the R console, its value is printed.

We first print (implicitly) the definition of our function from earlier in this section.

```
sem
## function(x, na.omit = FALSE) {
## if (na.omit) {
## x <- na.omit(x)
## }
## sqrt(var(x)/length(x))
## }
## <bytecode: 0x0000021bd92b6a00>
```

Next we print the definition of R's standard deviation function sd().

```
## function (x, na.rm = FALSE)
## sqrt(var(if (is.vector(x) || is.factor(x)) x else as.double(x),
## na.rm = na.rm))
## <bytecode: 0x0000021bd1347b78>
## <environment: namespace:stats>
```

As can be seen at the end of the printouts, these functions written in the R language have been byte-compiled so that they executes faster. We can also see that the definition of sd() resides in namespace:stats because it has been attached from package 'stats'.

Functions that are part of the R language, but that are not coded using the R language, are called primitives and their full definition cannot be accessed through their name (c.f., sem() defined above and sd, with list() below).

```
list
## function (...) .Primitive("list")
```

#### 6.2.3 Operators

Operators are functions that use a different syntax for being called. If their name is enclosed in back ticks they can be called as ordinary functions. Binary operators like + have two formal parameters, and unary operators like unary – have only one formal parameter. The parameters of many binary R operators are named e1 and e2.

```
1 / 2

## [1] 0.5

'/`(1 , 2)

## [1] 0.5

'/`(e1 = 1 , e2 = 2)

## [1] 0.5
```

An important consequence of the possibility of calling operators using ordinary

syntax is that operators can be used as arguments to *apply* functions in the same way as ordinary functions. When passing operator names as arguments to *apply* functions we only need to enclose them in back ticks (see section 5.8 on page 154).

The name by itself and enclosed in back ticks allows us to access the definition of an operator.

```
`/`
## function (e1, e2) .Primitive("/")
```

**Defining a new operator.** We will define a binary operator (taking two arguments) that subtracts from the numbers in a vector the mean of another vector. First we need a suitable name, but we have less freedom as names of user-defined operators must be enclosed in percent signs. We will use %-mean% and as with any *special name*, we need to enclose it in quotation marks for the assignment.

```
"%-mean%" <- function(e1, e2) {
  e1 - mean(e2)
}
We can then use our new operator in a example.</pre>
```

10:15 %-mean% 1:20 ## [1] -0.5 0.5 1.5 2.5 3.5 4.5

To print the definition, we enclose the name of our new operator in back ticks—i.e., we *back quote* the special name.

```
`%-mean%`
## function(e1, e2) {
## e1 - mean(e2)
## }
```

# 6.3 Objects, classes, and methods

New classes are normally defined within packages rather than in user scripts. To be really useful implementing a new class involves not only defining a class but also a set of specialized functions or *methods* that implement operations on objects belonging to the new class. Nevertheless, an understanding of how classes work is important even if only very occasionally a user will define a new method for an existing class within a script.

Classes are abstractions, but abstractions describing the shared properties of "types" or groups of similar objects. In this sense, classes are abstractions of "actors," they are like "nouns" in natural language. What we obtain with classes is the possibility of defining multiple versions of functions (or *methods*) sharing the same name but tailored to operate on objects belonging to different classes. We have already been using methods with multiple *specializations* throughout the book, for example plot() and summary().

We start with a quotation from *S Poetry* (Burns 1998, page 13).

The idea of object-oriented programming is simple, but carries a lot of

weight. Here's the whole thing: if you told a group of people "dress for work," then you would expect each to put on clothes appropriate for that individual's job. Likewise it is possible for S[R] objects to get dressed appropriately depending on what class of object they are.

We say that specific methods are *dispatched* based on the class of the argument passed. This, together with the loose type checks of R, allows writing code that functions as expected on different types of objects, e.g., character and numeric vectors.

R has good support for the object-oriented programming paradigm, but as a system that has evolved over the years, currently R supports multiple approaches. The still most popular approach is called S3, and a more recent and powerful approach, with slower performance, is called S4. The general idea is that a name like "plot" can be used as a generic name, and that the specific version of plot() called depends on the arguments of the call. Using computing terms we could say that the *generic* of plot() dispatches the original call to different specific versions of plot() based on the class of the arguments passed. S3 generic functions dispatch, by default, based only on the argument passed to a single parameter, the first one. S4 generic functions can dispatch the call based on the arguments passed to more than one parameter and the structure of the objects of a given class is known to the interpreter. In S3 functions, the specializations of a generic are recognized/identified only by their name. And the class of an object by a character string stored as an attribute to the object (see section 4.6 on page 114 about attributes).

We first explore one of the methods already available in R. The definition of mean shows that it is the generic for a method.

```
mean
## function (x, ...)
## UseMethod("mean")
## <bytecode: 0x0000021bd07dae78>
## <environment: namespace:base>
```

We can find out which specializations of method are available in the current search path using methods().

mean.POSIXct

## [5] mean.POSIXlt mean.quosure\* mean.vctrs\_vctr\* mean.yearmon\*
## [9] mean.yearqtr\* mean.zoo\*
## see '?methods' for accessing help and source code

We can also use methods() to query all methods, including operators, defined for objects of a given class.

```
methods(class = "list")
## [1] all.equal as.data.frame coerce na.contiguous Ops
## [6] relist sew type.convert within
## see '?methods' for accessing help and source code
```

S3 class information is stored as a character vector in an attribute named "class". The most basic approach to creation of an object of a new S3 class, is to add the new class name to the class attribute of the object. As the implied class

hierarchy is given by the order of the members of the character vector, the name of the new class must be added at the head of the vector. Even though this step can be done as shown here, in practice this step would normally take place within a *constructor* function and the new class, if defined within a package, would need to be registered. We show here this bare-bones example to demonstrate how S3 classes are implemented in R.

```
a <- 123
class(a)
## [1] "numeric"
class(a) <- c("myclass", class(a))
class(a)
## [1] "myclass" "numeric"</pre>
```

Now we create a print method specific to "myclass" objects. Internally we are using function sprintf() and for the format template to work we need to pass a numeric value as an argument—i.e., obviously sprintf() does not "know" how to handle objects of the class we have just created!

```
print.myclass <- function(x) {
    sprintf("[myclass] %.0f", as.numeric(x))
}</pre>
```

Once a specialized method exists for a class, it will be used for objects of this class.

```
print(a)
## [1] "[myclass] 123"
print(as.numeric(a))
## [1] 123
```

The S3 class system is "lightweight" in that it adds very little additional computation load, but it is rather "fragile" in that most of the responsibility for consistency and correctness of the design—e.g., not messing up dispatch by redefining functions or loading a package exporting functions with the same name, etc., is not checked by the R interpreter.

## 6.4 Packages

#### 6.4.1 Sharing of R-language extensions

The most elegant way of adding new features or capabilities to R is through packages. This is without doubt the best mechanism when these extensions to R need to be shared. However, in most situations it is also the best mechanism for managing code that will be reused even by a single person over time. R packages have strict rules about their contents, file structure, and documentation, which makes it possible among other things for the package documentation to be merged into R's help system when a package is loaded. With a few exceptions, packages can be written so that they will work on any computer where R runs.

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Packages can be shared as source or binary package files, sent for example through e-mail. However, for sharing packages widely, it is best to submit them to a repository. The largest public repository of R packages is called CRAN (https://cran.r-project.org/), an acronym for Comprehensive R Archive Network. Packages available through CRAN are guaranteed to work, in the sense of not failing any tests built into the package and not crashing or aborting prematurely. They are tested daily, as they may depend on other packages whose code will change when updated. The number of packages available through CRAN at the time of printing was 19906.

A key repository for bioinformatics with R is Bioconductor (https://www.bioconductor.org/), containing packages that pass strict quality tests, adding an additional 3 400 packages. ROpenScience has established guidelines and a system for code peer review for R packages. These peer-reviewed packages are available through CRAN or other repositories and listed at the ROpenScience website (https://ropensci.org/). In some cases you may need or want to install less stable code from Git repositories such as versions still under development not yet submitted to CRAN. Using the package 'devtools' we can install packages directly from GitHub, Bitbucket and other code repositories based on Git. Installations from code repositories are always installations from sources (see below). It is of course also possible to install packages from local files (e.g., after a manual download).

One good way of learning how the extensions provided by a package work, is by experimenting with them. When using a function we are not yet familiar with, looking at its help to check all its features will expand your "toolbox." How much documentation is included with packages varies, while documentation of exported objects is enforced, many packages include, in addition, comprehensive user guides or articles as *vignettes*. It is not unusual to decide which package to use from a set of alternatives based on the quality of available documentation. In the case of packages adding extensive new functionality, they may be documented in depth in a book. Well-known examples are *Mixed-Effects Models in S and S-Plus* (Pinheiro and Bates 2000), *Lattice: Multivariate Data Visualization with R* (Sarkar 2008) and *gaplot2: Elegant Graphics for Data Analysis* (Wickham and Sievert 2016).

#### 6.4.2 Download, installation and use

In R speak, "library" is the location where packages are installed. Packages are sets of functions, and data, specific for some particular purpose, that can be loaded into an R session to make them available so that they can be used in the same way as built-in R functions and data. Function library() is used to load and attach packages that are already installed in the local R library. In contrast, function install.packages() is used to install packages.

# **?** How to install or update a package from CRAN?

CRAN is the default repository for R packages. If you use RStudio or another IDE as front end on any operating system or RGUI under MS-Windows, installation and updates can be done through a menu or GUI 'button'. These menus use calls to install.packages() and update.packages() behind the scenes.

Alternatively, at the R command line, or in a script, install.packages() can

called with the name of the package as argument. For example, to install package 'learnrbook' we use.

```
install.packages("learnrbook")
```

Already installed packages are updated with function update.packages().

R packages can be installed either from sources, or from already built "binaries". Installing from sources, depending on the package, may require additional software to be available. Under MS-Windows, the needed shell, commands and compilers are not available as part of the operating system. Installing them is not difficult as they are available prepackaged in installers (you will need RTools, and MiKTeX). It is easier to install packages from binary .zip files under MS-Windows. Under Linux most tools will be available, or very easy to install, so it is usual to install packages from sources. For OS X (Apple Mac) the situation is somewhere in-between. If the tools are available, packages can be very easily installed from sources from within RStudio. However, binaries are for most packages also readily available.

6.4 Use help to look up the help page for install.packages(), and explore how to control whether the package is installed from a source or a binary file. Also explore, how to install a package from a file in a local disk instead of from a repository like CRAN.

Frequently the README file of a package includes instructions on how to install it from CRAN or another on-line repository. Exceptionally, packages may require additionally the installation of software outside R before their installation and/or use. When present, these rather exceptional requirements are always listed in the DESCRIPTION under SystemRequirements: and explained in more detail in the README file.

# **3** How to change the repository used to install packages?

Function setRepositories() can be used to enable other repositories than CRAN interactively. In recent versions of R the default list of repositories is taken from R option "repos" if defined. Consult help("setRepositories") for the details.

# **1** How to use an installed package?

To use the functions and other objects defined in a package, the package must first be loaded, and for the names of these objects to be visible in the user's workspace, the package needs to be attached. Function library() loads and attaches one package at a time. For example, to load and attach package 'learnrbook' we use.

```
library("learnrbook")
```

As packages are contributed by independent authors, they should be cited in addition to citing R itself when they are used to obtain results or plots included in publications. R function citation() when called with the name of a package as its argument provides the reference that should be cited for the package, and without an explicit argument, the reference to cite for the version of R in use as shown below.

```
citation()
## To cite R in publications use:
##
```

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```
R Core Team (2023). _R: A Language and Environment for Statistical
##
##
     Computing_. R Foundation for Statistical Computing, Vienna, Austria.
##
     <https://www.R-project.org/>.
##
## A BibTeX entry for LaTeX users is
##
##
     @Manual{,
##
       title = {R: A Language and Environment for Statistical Computing},
##
       author = {{R Core Team}},
       organization = {R Foundation for Statistical Computing},
##
##
       address = {Vienna, Austria},
       year = \{2023\},\
##
##
       url = {https://www.R-project.org/},
##
##
## We have invested a lot of time and effort in creating R, please cite it
## when using it for data analysis. See also 'citation("pkgname")' for
## citing R packages.
```

6.5 Look at the help page for function citation() for a discussion of why it is important for users to cite R and packages when using them.

Conflicts among packages can easily arise, for example, when they use the same names for objects or functions. These are reported when the packages are attached (see section 6.4.4 on page 182 for a workaround). In addition, many packages use functions defined in packages in the R distribution itself or other independently developed packages by importing them. Updates to depended-upon packages can "break" (make non-functional) the dependent packages or parts of them. The rigorous testing by CRAN detects such problems in most cases when package revisions are submitted, forcing package maintainers to fix problems before distribution through CRAN is possible. However, if you use other repositories, I recommend that you make sure that revised (especially if under development) versions do work with your own code, before their use in "production" (important) data analyses.

#### 6.4.3 Finding suitable packages

Due to the large number of contributed R packages it can sometimes be difficult to find a suitable package for a task at hand. It is good to first check if the necessary capability is already built into base R. Base R plus the recommended packages (installed when R is installed) cover a lot of ground. To analyze data using almost any of the more common statistical methods does not require the use of special packages. Sometimes, contributed packages duplicate or extend the functionality in base R with advantage. When one considers the use of novel or specialized types of data analysis, the use of contributed packages can be unavoidable. Even in such cases, it is not unusual to have alternatives to choose from within the available contributed packages. Sometimes groups or suites of packages are designed to work well together.

The CRAN repository has very broad scope and includes a section called "views." R views are web pages providing annotated lists of packages frequently used within

a given field of research, engineering or specific applications. These views are edited and updated by different editors. They can be found at https://cran.r-project.org/web/views/.

The Bioconductor repository specializes in bioinformatics with R. It also has a section with "views" and within it, descriptions of different data analysis workflows. The workflows are especially good as they reveal which sets of packages work well together. These views can be found at https://www.bioconductor.org/packages/release/BiocViews.html.

Although ROpenSci does not keep a separate package repository for the peer-reviewed packages, they do keep an index of them at https://ropensci.org/packages/.

The CRAN repository keeps an archive of earlier versions of packages, on an individual package basis. METACRAN (https://www.r-pkg.org/) is an archive of repositories, that keeps a historical record as snapshots from CRAN. METACRAN uses a different search engine than CRAN itself, making it easier to search the whole repository.

### 6.4.4 How packages work

The development of packages is beyond the scope of the current book, and thoroughly explained in the book *R Packages* (Wickham 2015). However, it is still worthwhile mentioning a few things about the development of R packages. Using RStudio it is relatively easy to develop your own packages. Packages can be of very different sizes and complexity. Packages use a relatively rigid structure of folders for storing the different types of files, including documentation compatible with R's built-in help system. This allows documentation for contributed packages to be seamlessly linked to R's help system when packages are loaded. In addition to R code, packages can call functions and routines written in C, C++, FORTRAN, Java, Python, etc., but some kind of "glue" is needed, as function call conventions and name mangling depend on the programming language, and in many cases also on the compiler used. For C++, the 'Rcpp' R package makes the "gluing" relatively easy (Eddelbuettel 2013). In the case of Python, R package 'reticulate' makes calling of Python methods and exchange of data easy, and it is well supported by RStudio. In the case of Java we can use package 'RJava' instead. For C and FORTRAN, R provides the functionality needed, but the interface needs some ad hoc coding in most cases.

Only objects exported by a package that has been attached are visible outside its own namespace. Loading and attaching a package with library() makes the exported objects available. Attaching a package adds the objects exported by the package to the search path so that they can be accessed without prepending the name of the namespace. Most packages do not export all the functions and objects defined in their code; some are kept internal, in most cases because they may change or be removed in future versions. Package namespaces can be detached and also unloaded with function detach() using a slightly different notation for the argument from that which we described for data frames in section 4.4.5 on page 109.

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An additional important thing to remember is that R packages define all objects within a *namespace* with the same name as the package itself. This means that when we reuse a name defined in a package, its definition in the package does not get overwritten, but instead, only hidden and still accessible using the name *qualified* by prepending the name of the package followed by two colons.

If two packages define objects with the same name, then which one is visible depends on the order in which the packages were attached. To avoid confusion in such cases, in scripts it is best to use the qualified names for calling all the objects defined with the same name in the two package, or attaching only one of the packages and using qualified names for all the objects exported by the other package.

If one uses a qualified name for an object but does not attach the package with a call to library, the package is only loaded. In other words, the names of the objects are not added to the search pass, but the code defining them is retrieved and available using qualified names.

Some functions that are part of R are collected into packages grouped by category: 'stats', 'datasets', etc., and can be called when needed using qualified names. even functions like list() can be called as base::list() if they cannot be accessed directly because of the presence of other objects with the same name being present in the global environment, or having priority. We can find out the search order by calling search(), with the search starting at the ".GlobalEnv" for statements evaluated at the R command line.

Namespaces isolate the names defined within them from those in other namespaces. This helps prevent name clashes, and makes it possible to access objects even when they are "hidden" by a different object with the same name.

```
head(cars, 3) # first three rows
     speed dist
## 1
         4
             2
## 2
         4
             10
         7
              4
getAnywhere("cars")$where # defined in package
## [1] "package:datasets"
cars <- "my car is blue"
getAnywhere("cars")$where # the first visible definition is in the global en-
                          "package:datasets"
## [1] ".GlobalEnv"
cars # prints cars defined in the global environment
## [1] "my car is blue"
head(datasets::cars, 3) # first three rows
     speed dist
##
## 1
        4
             2
         4
             10
## 2
## 3
         7
             4
rm(cars) # clean up
```

In the example above I used a data frame object, but the same mechanisms apply to all R objects including functions. The situation when one of the definitions is a function and the other is not, is slightly different in that a call using parenthe-

sis notation will distinguish between a function and an object of the same name that is not a function. Relying on this distinction is anyway a bad idea.

```
## function (x, ...)
## UseMethod("mean")
## <bytecode: 0x0000021bd07dae78>
## <environment: namespace:base>
mean \leftarrow mean(1:5)
mean
## [1] 3
mean(8:9)
## [1] 8.5
getAnywhere("mean")$where
## [1] ".GlobalEnv"
                         "package:base"
                                            "namespace:base"
rm(mean)
getAnywhere("mean")$where
## [1] "package:base"
                         "namespace:base"
```

In this last example we removed with rm(mean) the variable we had assigned a value to. Package namespaces also prevent deletion or overwriting of objects defined in the package. This is different to defining a new object with the same name, which is allowed. The two statements below trigger errors and are not evaluated when typesetting the book.

```
datasets::cars <- "my car is green"
rm(datasets::cars)</pre>
```

We looked at only one member of the value returned by getAnywhere(), do have a look at its help page for more details as it contains additional information.

### 6.5 Further reading

An in-depth discussion of object-oriented programming in R is outside the scope of this book. For the non-programmer user, a basic understanding of R classes can be useful, even if he or she does not intend to create new classes. This basic knowledge is what we covered in this chapter. Several books describe in detail the different class systems available and how to use them in R packages. For an indepth treatment of the subject please consult the books *Advanced R* (Wickham 2019) and *Extending R* (Chambers 2016).

The development of packages is thoroughly described in the book R Packages (Wickham 2015) and an in-depth description of R from the programming perspective is given in the book  $Advanced\,R$  (Wickham 2019). The book Extending R (Chambers 2016) covers both subjects.

# Base R: "Verbs" and "Nouns" for Statistics

The purpose of computing is insight, not numbers.

Richard W. Hamming Numerical Methods for Scientists and Engineers, 1987

## 7.1 Aims of this chapter

This chapter aims to give the reader an introduction to the approach used in base R for the computation of statistical summaries, the fitting of models to observations and tests of hypothesis. This chapter does *not* explain data analysis methods, statistical principles or experimental designs. There are many good books on the use of R for different kinds of statistical analyses (see further reading on page 239) but most of them tend to focus on specific statistical methods rather than on the commonalities among them. Although base R's model fitting functions target specific statistical procedures, they use a common approach to model specification and for returning the computed estimates and test outcomes. This approach, also followed by many contributed extension packages, can be considered as part of the philosophy behind the R language. In this chapter you will become familiar with the approaches used in R for calculating statistical summaries, generating (pseudo-)random numbers, sampling, fitting models and carrying out tests of significance. We will use linear correlation, t-test, linear models, generalized linear models, non-linear models and some simple multivariate methods as examples. The focus is on how to specify statistical models, contrasts and observations, how to access different components of the objects returned by the corresponding fit and summary functions, and how to use these extracted components in further computations or for customized printing and formatting.

Function	Symbol	Formulation	Name
mean()	$\bar{X}$	$\sum x/n$	mean
var()	$s^2$	$\sum (x_i - \hat{x})^2 / (n-1)$	sample variance
sd()	S	$\sqrt[2]{S^2}$	sample standard deviation
<pre>median()</pre>	M or $\tilde{x}$		median
mad()	MAD	median $ x_i - \hat{x} $	median absolute deviation
<pre>mode()</pre>	MOD		mode
max()	$x_{ ext{max}}$		maximum
min()	$x_{\min}$		minimum
range()	$x_{\min}, x_{\max}$		range

**TABLE 7.1** Frequently used simple statistical summaries and the corresponding R functions.

#### 7.2 Statistical summaries

Being the main focus of the R language in data analysis and statistics, R provides functions both for simple and complex calculations, going from means and variances to fitting very complex models. Table 7.1 lists some frequently used functions. All these methods accept numeric vectors and/or matrices as arguments. In addition function quantile() can be used to simultaneously compute multiple arbitrary quantiles for a vector of observations, and method summary() produces a summary that depends on the class of the argument passed to it. Please, see section 6.2.2 on page 174 for how to define your own functions.)

By default, if the argument contains NAs these functions return NA. The logic behind this is that if one value exists but is unknown, the true result of the computation is unknown (see page 33 for details on the role of NA in R). However, an additional parameter called na.rm allows us to override this default behavior by requesting any NA in the input to be removed (or discarded) before calculation,

```
x <- c(1:20, NA)
mean(x)
## [1] NA
mean(x, na.rm = TRUE)
## [1] 10.5</pre>
```

Function mean() can be used to compute the mean from all values, as in the example above, as well as trimmed means, i.e., means computed after discarding extreme values. The argument passed to parameter trim decides the fraction of the observations to discard at *each extreme* of the vector of values after ordering them from smallest to largest.

```
x <- c(1:20, 100)
mean(x)
## [1] 14.7619
mean(x, trim = 0.05)
## [1] 11</pre>
```

**TABLE 7.2** Standard probability distributions in R. Partial list of base R functions related to probability distributions. The full list can be obtained by executing the command help(Distributions).

Distribution	Symbol	Density	<i>P</i> -value	Quantiles	Draws
Normal	N	dnorm()	pnorm()	qnorm()	rnorm()
Student's	t	dt()	pt()	qt()	rt()
F	F	df()	pf()	qf()	rf()
binomial	B	dbinom()	<pre>pbinom()</pre>	qbinom()	rbinom()
multinomial	M	<pre>dmultinom()</pre>	pmultinom()	qmultinom()	rmultinom()
Poisson		dpois()	ppois()	<pre>qpois()</pre>	rpois()
X-squared	$X^2$	<pre>dchisq()</pre>	<pre>pchisq()</pre>	qchisq()	rchisq()
lognormal		dlnorm()	plnorm()	qlnorm()	rlnorm()
uniform		dunif()	punif()	qunif()	runif()

7.1 In contrast to the use of other functions, I do not provide examples of the use of all the functions listed in Table 7.1. Construct numeric vectors with artificial data or use real data to play with the remaining functions. Study the help pages to learn about the different parameters and their uses.

Other more advanced functions are also available in R, such as boxplot.stats() that computes the values needed to draw boxplots (see section 9.6.6 on page 318).

In many cases you will want to compute statistical summaries by group or treatment in addition or instead of for a whole data set or vector. See section 4.4.2 on page 104 for details on how to compute summaries of data stored in data frames using base R functions, and section 8.7 on page 256 for alternative functions from contributed packages.

# 7.3 Standard probability distributions

Density, distribution functions, quantile functions and generation of pseudorandom values for several different standard (theoretical) probability distributions are part of the R language. Entering help(Distributions) at the R prompt will open a help page describing all the distributions available in base R. For each distribution the different functions contain the same "root" in their names: norm for the normal distribution, unif for the uniform distribution, and so on. The "head" of the name indicates the type of values returned: "d" for density, "q" for quantile, "r" (pseudo-)random draws, and "p" for probability (Table 7.2).

Theoretical distributions are defined by mathematical functions that accept parameters that control the exact shape and location. In the case of the Normal distribution, these parameters are the *mean* (mean) controlling location and (standard deviation) (sd) controlling the spread around the center of the distribution. The

four different functions differ in which values are calculated (the unknowns) and which values are supplied as arguments (the known inputs).

In what follows we use the normal distribution as an example, but with differences in their parameters, the functions for other theoretical distributions follow a similar naming pattern.

#### 7.3.1 Density from parameters

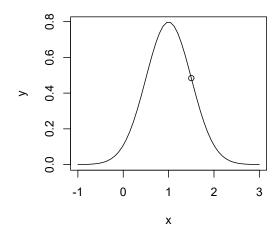
To obtain a single point from the distribution curve we pass a vector of length one as an argument for x.

```
dnorm(x = 1.5, mean = 1, sd = 0.5)
## [1] 0.4839414
```

To obtain multiple values we can pass a longer vector as an argument.

```
dnorm(x = seq(from = -1, to = 1, length.out = 5), mean = 1, sd = 0.5)
## [1] 0.0002676605 0.0088636968 0.1079819330 0.4839414490 0.7978845608
```

With 50 equally spaced values for x we can plot a line (type = "1") that shows that the 50 generated data points give the illusion of a continuous curve. We also add a point showing the value for x = 1.5 calculated above.



#### 7.3.2 Probabilities from parameters and quantiles

If we have a known quantile value we can look up the corresponding p-value from the Normal distribution, i.e., the area under the curve, either to the right or to the left of a given value of x. When working with observations, the quantile, mean

and standard deviation are in most cases computed from the same observations under the null hypothesis. In the example below, we use invented values for all parameters q, the quantile, mean, and sd, the standard deviation.

```
pnorm(q = 4, mean = 0, sd = 1)
## [1] 0.9999683
pnorm(q = 4, mean = 0, sd = 1, lower.tail = FALSE)
## [1] 3.167124e-05
pnorm(q = 4, mean = 0, sd = 4, lower.tail = FALSE)
## [1] 0.1586553
pnorm(q = c(2, 4), mean = 0, sd = 1, lower.tail = FALSE)
## [1] 2.275013e-02 3.167124e-05
```

In tests of significance, empirical z-values and t-values are computed by subtracting from the observed mean for one group or raw quantile, the "expected" mean (possibly a hypothesized theoretical value, the mean of a control condition used as reference, or the mean computed over all treatments under the assumption of no effect of treatments) and then dividing by the standard deviation. Consequently, the p-values corresponding to these empirical z-values and t-values need to be looked up using mean = 0 and sd = 1 when calling pnorm() or pt() respectively. These frequently used values are the defaults.

### 7.3.3 Quantiles from parameters and probabilities

The reverse computation from that in the previous section is to obtain the quantile corresponding to a known p-value or area under one of the tails of the distribution curve. These quantiles are equivalent to the values in the tables of precalculated quantiles used in earlier times to assess significance with statistical tests.

```
qnorm(p = 0.01, mean = 0, sd = 1)
## [1] -2.326348
qnorm(p = 0.05, mean = 0, sd = 1)
## [1] -1.644854
qnorm(p = 0.05, mean = 0, sd = 1, lower.tail = FALSE)
## [1] 1.644854
```

Quantile functions like qnorm() and probability functions like pnorm() always do computations based on a single tail of the distribution, even though it is possible to specify which tail we are interested in. If we are interested in obtaining simultaneous quantiles for both tails, we need to do this manually. If we are aiming at quantiles for P = 0.05, we need to find the quantile for each tail based on P/2 = 0.025.

```
qnorm(p = 0.025, mean = 0, sd = 1)
## [1] -1.959964
qnorm(p = 0.025, mean = 0, sd = 1, lower.tail = FALSE)
## [1] 1.959964
```

We see above that in the case of a symmetric distribution like the Normal, the quantiles in the two tails differ only in sign. This is not the case for asymmetric distributions.

When calculating a *p*-value from a quantile in a test of significance, we need to first decide whether a two-sided or single-sided test is relevant, and in the case of a single sided test, which tail is of interest. For a two-sided test we need to multiply the returned value by 2.

```
pnorm(q = 4, mean = 0, sd = 1) * 2
## [1] 1.999937
```

#### 7.3.4 "Random" draws from a distribution

True random sequences can only be generated by physical processes. All "pseudorandom" sequences of numbers generated by computation are really deterministic although they share some properties with true random sequences (e.g., in relation to autocorrelation).

It is possible to compute not only pseudo-random draws from a uniform distribution but also from the Normal, t, F and other distributions. In each case, the probability with which different values are "drawn" approximates the probabilities set by the corresponding theoretical distribution. Parameter n indicates the number of values to be drawn, or its equivalent, the length of the vector returned.

```
rnorm(5)
## [1] -0.8248801  0.1201213 -0.4787266 -0.7134216  1.1264443
rnorm(n = 10, mean = 10, sd = 2)
## [1] 12.394190  9.697729  9.212345 11.624844 12.194317 10.257707 10.082981
## [8] 10.268540 10.792963  7.772915
```

**7.2** Edit the examples in sections 7.3.2, 7.3.3 and 7.3.4 to do computations based on different distributions, such as Student's *t*, *F* or uniform.

It is impossible to generate truly random sequences of numbers by means of a deterministic process such as a mathematical computation. "Random numbers" as generated by R and other computer programs are *pseudo random numbers*, long deterministic series of numbers that resemble random draws. Random number generation uses a *seed* value that determines where in the series we start. The usual way of automatically setting the value of the seed is to take the milliseconds or similar rapidly changing set of digits from the real time clock of the computer. However, in cases when we wish to repeat a calculation using the same series of pseudo-random values, we can use <code>set.seed()</code> with an arbitrary integer as an argument to reset the generator to the same point in the underlying (deterministic) sequence.

7.3 Execute the statement rnorm(3) by itself several times, paying attention to the values obtained. Repeat the exercise, but now executing set.seed(98765) immediately before each call to rnorm(3), again paying attention to the values obtained. Next execute set.seed(98765), followed by c(rnorm(3), rnorm(3)), and then execute set.seed(98765), followed by rnorm(6) and compare the output. Repeat the exercise using a different argument in the call to set.seed(). analyze

the results and explain how setseed() affects the generation of pseudo-random numbers in R.

### 7.4 Observed probability distributions

It is common to estimate the value of the parameters for a standard distribution like Student's t or Normal distributions from observational data, assuming a priori the suitability of the distribution. If we compute the and standard deviation for a large sample, these two parameters define a specific Normal distribution curve. If we add the estimate of the degrees of freedom, v = n - 1, the three parameters define a specific t-distribution curve. Thus it is possible to use the functions described in section 7.3 on page 7.3, in statistical inference.

Package 'mixtools' provides tools for fitting and analysing *mixture models* such as the mix of two or more univariate Normal distributions. An example of its use could be to estimate mean and standard deviations for males and females in a dataset where the gender was not recorded at the time of observation.

It is also possible to describe the observed shape of the distribution, or empirical distribution, for a data set without relying on a standard distribution. The fitted empirical distribution can later be used to compute probabilities, quantiles, and random draws similarly as from standard distributions. This also allows statistical inference, using methods such as the bootstrap or some additive models.

Function density() computes kernel density estimates, using different methods. A curve is used to describe the shape, and the bandwith determines how flexible this curve is. The curve is a flexible smoother that adapts to the observed shape. The object returned is a complex list that can be used to plot the estimate shape.

In the example below we estimate the empirical distribution for the waiting time in minutes between eruptions of the Old Faithful geyser at Yelowstone, a dataset from R.

```
d <- density(faithful$waiting, bw = "sj")</pre>
```

Using str() we can explore the structure of the object returned by function density().

The object saved as d is a list with seven members. The two numeric vectors,

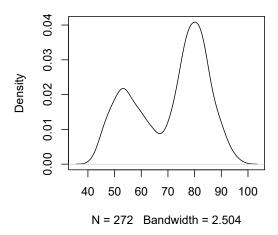
x and y describe the estimated probability distribution and produce the curve in the plot below. The numerical bandwidth estimated using method "sj" is in bw, and the length of vector faithful\$waiting, the data used, is in n. Member call is the command used to call the function, the remaining two members have self explanatory names. The returned object belongs to class density. The overall pattern is similar, but simpler than for the model fitting functions that we will see later in the chapter. The class name of the object is the same as the name of the function that created it, call provides a *trace* of how the object was created. Other members, facilitate computation of derived quantities and plotting. Being a list, the individual members can be extracted by name.

d\$n ## [1] 272

As a plot() method is available for class density we can easily produce a plot of the estimated empirical density distribution. In this case a bimodal curve, with two maxima, and thus, far from Normal.

plot(d)

#### density(x = faithful\$waiting, bw = "sj")



Observed probability distributions, especially empirical ones, nowadays play a central role in data visualization including 1D and 2D empirical density plots based on the use of functions like density(), as well as traditional histograms (see section 9.6.5 on page 317 for examples of more elaborate and elegant plots).

# 7.5 "Random" sampling

In addition to drawing values from a theoretical distribution, we can draw values from an existing set or collection of values. We call this operation (pseudo-)random sampling. The draws can be done either with replacement or without replacement.

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In the second case, all draws are taken from the whole set of values, making it possible for a given value to be drawn more than once. In the default case of not using replacement, subsequent draws are taken from the values remaining after removing the values chosen in earlier draws.

```
sample(x = LETTERS)
## [1] "Z" "N" "Y" "R" "M" "E" "W" "J" "H" "G" "U" "O" "S" "T" "L" "F" "X" "P" "K"
## [20] "V" "D" "A" "B" "C" "I" "Q"
sample(x = LETTERS, size = 12)
## [1] "M" "S" "L" "R" "B" "D" "Q" "W" "V" "N" "J" "P"
sample(x = LETTERS, size = 12, replace = TRUE)
## [1] "K" "E" "V" "N" "A" "O" "L" "C" "T" "L" "H" "U"
```

In practice, pseudo-random sampling is useful when we need to select subsets of observations. One such case is assigning treatments to experimental units in an experiment or selecting persons to interview in a survey. Another use is in bootstrapping to estimate variation in parameter estimates using empirical distributions.

# How to sample random rows from a data frame?

As described in section 4.4 on page 94, data frames are commonly used to store one observation per row. To sample a subset of rows we need to generate a random set of indices to use with the extraction operator ([ ]). Here we sample four rows from data frame cars included in R. These data consist of stopping distances for cars moving at different speeds as described in the documentation available by entering help(cars)).

```
cars[sample(x = 1:nrow(cars), size = 4),]
##  speed dist
## 33    18    56
## 31    17    50
## 50    25    85
## 36    19    36
```

**7.4** Consult the documentation of sample() and explain why the code below is equivalent to that in the example immediately above.

```
cars[sample(x = nrow(cars), size = 4),]
```

#### 7.6 Correlation

Both parametric (Pearson's) and non-parametric robust (Spearman's and Kendall's) methods for the estimation of the (linear) correlation between pairs of variables are available in base R. The different methods are selected by passing arguments to a single function. While Pearson's method is based on the actual values of the observations, non-parametric methods are based on the ordering or rank of the observations, and consequently less affected by observations with extreme values.

#### 7.6.1 Pearson's $\gamma$

Function cor() can be called with two vectors of the same length as arguments. In the case of the parametric Pearson method, we do not need to provide further arguments as this method is the default one. We use data set cars.

```
cor(x = cars$speed, y = cars$dist)
## [1] 0.8068949
```

It is also possible to pass a data frame (or a matrix) as the only argument. When the data frame (or matrix) contains only two columns, the returned value is equivalent to that of passing the two columns individually as vectors.

When the data frame or matrix contains more than two numeric vectors, the returned value is a matrix of estimates of pairwise correlations between columns. We here use rnorm() described above to create a long vector of pseudo-random values drawn from the Normal distribution and matrix() to convert it into a matrix with three columns (see page 71 for details about R matrices).

**7.5** Modify the code in the chunk immediately above constructing a matrix with six columns and then computing the correlations.

While cor() returns and estimate for r the correlation coefficient, cor.test() also computes the t-value, p-value, and confidence interval for the estimate.

```
cor.test(x = cars$speed, y = cars$dist)
##
## Pearson's product-moment correlation
##
## data: cars$speed and cars$dist
## t = 9.464, df = 48, p-value = 1.49e-12
## alternative hypothesis: true correlation is not equal to 0
## 95 percent confidence interval:
## 0.6816422 0.8862036
## sample estimates:
## cor
## 0.8068949
```

Above we passed two numeric vectors as arguments, one to parameter x and one to parameter y. Alternatively, we can pass a data frame as argument to data, and a *model formula* to parameter formula. The argument passed to formula determines which variables from data are to be used, and in which role. Briefly, the variabel(s) to the left of the tilde ( ) are response variables, and those to the right independent variables. In the case of correlation, no assumption is made on cause and effect, and both variables appear to the right of the tilde. The code below is equivalent to

*t-test* 195

that above. See section 7.13 on page 224 for details on the use of model formulas and section 7.8 on page 197 for examples of their use in model fitting.

```
cor.test(formula = ~ speed + dist, data = cars)
```

7.6 Functions cor() and cor.test() return R objects, that when using R interactively get automatically "printed" on the screen. One should be aware that print() methods do not necessarily display all the information contained in an R object. This is almost always the case for complex objects like those returned by R functions implementing statistical tests. As with any R object we can save the result of an analysis into a variable. As described in section 4.3 on page 86 for lists, we can peek into the structure of an object with method str(). We can use class() and attributes() to extract further information. Run the code in the chunk below to discover what is actually returned by cor().

```
mat1 <- cor(cars)
class(mat1)
attributes(mat1a)
str(mat1)</pre>
```

Methods class(), attributes() and str() are very powerful tools that can be used when we are in doubt about the data contained in an object and/or how it is structured. Knowing the structure allows us to retrieve the data members directly from the object when predefined extractor methods are not available.

#### 7.6.2 Kendall's $\tau$ and Spearman's $\rho$

We use the same functions as for Pearson's r but explicitly request the use of one of these methods by passing and argument.

```
cor(x = cars$speed, y = cars$dist, method = "kendall")
## [1] 0.6689901
cor(x = cars$speed, y = cars$dist, method = "spearman")
## [1] 0.8303568
```

Function cor.test(), described above, also allows the choice of method with the same syntax as shown for cor().

7.7 Repeat the exercise in the playground immediately above, but now using non-parametric methods. How does the information stored in the returned matrix differ depending on the method, and how can we extract information about the method used for calculation of the correlation from the returned object.

#### 7.7 *t*-test

The t-test is based on Student's t-distribution. It can be applied to any parameter estimate for which its standard deviation is available, and the t-distribution is a plausible assumption. It is most frequently used to compare an estimate of the mean against a constant value, or the estimate of a difference between two means

and a target difference, usually no difference. In R these can be computed manually using functions mean(), sd(), and pt() or with t.test().

Although rarely presented is such a way, the t-test can be thought of as a special case of a linear model fit. Consistently with functions used to fit models to observations we can use a *formula* to describe a t-test. A formula such as  $y \sim x$  is read as y is explained by x. We use *lhs* (left-hand-side) and *rhs* (right-hand-side) to signify all terms to the left and right of the tilde ( $\sim$ ), respectively ( $<1hs>\sim<rhs>$ ). (See section 7.13 on page 224 for a detailed discussion of model formulas, and section 7.8 on page 197 for examples of their use in model fitting.)

The formula some.size~1 is read as "the mean of variable some.size is explained by a constant value". The value estimated from observations,  $\bar{x}$ , is compared against the value of  $\mu$  set as the null hypothesis, where  $\mu$  is the *unknown* mean of the sampled population. By default, t.test() applies a two-sided test (alternative = "two.sided") against mu = 0, but here we use mu = 2 instead.

```
t.test(some.size ~ 1, mu = 2, data = df1)
##
## One Sample t-test
##
## data: some.size
## t = 1.078, df = 19, p-value = 0.2945
## alternative hypothesis: true mean is not equal to 2
## 95 percent confidence interval:
## 1.741200 2.808479
## sample estimates:
## mean of x
## 2.27484
```

The same test can be calculated step by step. In this case this approach is not needed, but it is useful when we have a parameter estimate (not just mean) and its standard error available, as in model fits (see the advanced playground on page 205 for an example).

The same function, with a different formula, tests the for the difference between the means of two groups or treatments,  $H_o$ :  $\mu_A - \mu_B = 0$ . We read the formula some.size~group as "differences in some.size are explained by factor group". The difference between the means for the two groups is estimated and compared against the hypothesis. (In this case, the value of the argument passed to mu, zero by default, describes this difference.) By default variances in the two groups are not to assumed equal,

```
t.test(some.size ~ group, data = df1)
##
## Welch Two Sample t-test
##
```

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**TABLE 7.3** R functions implementing frequently used statistical tests. Student's t-test and correlation tests are described on pages 195 and 193, respectively.

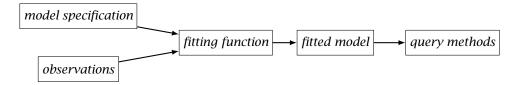
Statistical test	Function name
Student's $t$ -test (1 and 2 samples) Wilcoxon rank sum and signed rank tests Kolmogorov-Smirnov tests Correlation tests (Pearson, Kendall, Spearman) F-test to compare two variances Fisher's exact test for count data Pearson's Chi-squared ( $\chi^2$ ) test for count data Exact Binomial Test	<pre>t.test() wilcox.test ks.test() cor.test() var.test() fisher.test() chisq.test() binom.test()</pre>
Test of equal or given proportions	<pre>prop.test()</pre>

```
## data: some.size by group
## t = 1.5864, df = 17.666, p-value = 0.1304
## alternative hypothesis: true difference in means between group A and group B is not equal to 0
## 95 percent confidence interval:
   -0.2538836 1.8108119
## sample estimates:
## mean in group A mean in group B
          2.664072
                          1.885608
   and with var.equal = TRUE pooling the variances of groups A and B.
t.test(some.size ~ group, var.equal = TRUE, data = df1)
##
##
   Two Sample t-test
##
## data: some.size by group
## t = 1.5864, df = 18, p-value = 0.1301
## alternative hypothesis: true difference in means between group A and group B is not equal to 0
## 95 percent confidence interval:
   -0.2524857 1.8094140
## sample estimates:
## mean in group A mean in group B
          2.664072
                          1.885608
```

The t-test serves as an example of how statistical tests are usually carried out in R. Table 7.3 lists R functions for frequently used statistical tests.

# 7.8 Model fitting in R

The general approach to model fitting in R is to separate the actual fitting of a model from the inspection of the fitted model. A model fitting function minimally requires a description of the model to fit, as a model formula and a data frame or vectors with the data or observations to which to fit the model. These functions



#### FIGURE 7.1

Model fitting in R is done in steps, and can be represented schematically as a flow of information.

in R return a model fit object. This object contains the data, the model formula, call and the result of fitting the model. Several methods are available for querying it. The diagram in Figure 7.1 summarises the approach used in R for data analysis based on fitted models.

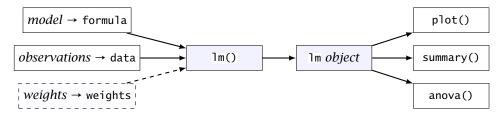
Models are described using model formulas such as  $y \sim x$  which we read as y is explained by x. We use *lhs* (left-hand-side) and *rhs* (right-hand-side) to signify all terms to the left and right of the tilde ( $\sim$ ), respectively ( $<1hs>\sim<rhs>$ ). Model formulas are used in different contexts: fitting of models, plotting, and tests like t-test. The syntax of model formulas is consistent throughout base R and numerous independently developed packages. However, their use is not universal, and several packages extend the basic syntax to allow the description of specific types of models. As most things in R, model formulas are objects and can be stored in variables. See section 7.13 on page 224 for a detailed discussion of model formulas.

Although there is some variation, especially for fitted model classes defined in extension packages, in most cases the *query functions* bulked together in the rightmost box in the diagram include methods summary(), anova() and plot(), with several other methods such as coef(), residuals(), fitted(), predict(), AIC(), BIC() usually also available. Additional methods may be available. However, as model fit objects are derived from class list, these and other components can be extract or computed programmatically when needed. Consequently, the examples in this chapter can be adapted to the fitting of types of models not described here.

Fitted model objects in R are self contained and include a copy of the data to which the model was fit, as well as residuals and possibly even intermediate results of computations. Although this can make the size of these objects large, it allows querying and even updating them in the absence of the data in the current R workspace.

### 7.9 Fitting linear models

Regression, analysis of variance (ANOVA) and analysis of covariance (ANCOVA) are all linear models, differing only on the type of explanatory variables included in the statistical model fitted. If in the fitted model all explanatory variables are continuous, i.e., numeric, vectors, the model is a regression model. If all explana-



#### FIGURE 7.2

Linear model fitting in R is done in steps. Generic diagram from Figure 7.1 redrawn to show a linear model fit. Non-filled boxes are shared with fitting of other types of models, and filled ones are specific to lm(). Only the three most frequently used query methods are shown, while both response and explanatory variables are under *observations*. Dashed boxes and arrows are optional as defaults are provided.

tory variables are discrete, i.e., factors, the model is ANOVA. Finally, if the model contains but numeric variables and factors it is named ANCOVA. As in all cases the fitting approach is the same, based on ordinary least squares (OLS), in R, they are all implemented in function lm().

There is another meaning of ANOVA, referring only to the tests of significance rather than to an approach to model fitting. Consequently, rather confusingly, results for tests of significance can both in the case of regression, ANOVA and ANCOVA, be presented in an ANOVA table. In this second, stricter meaning, ANOVA means a test of significance based on the ratios between pairs of variances.

If you do not clearly remember the difference between numeric vectors and factors, or how they can be created, please, revisit chapter 3 on page 23.

Figure 7.2 shows the steps needed to fit a linear model and extract the estimates and test results. The observations are stored in a data frame, one case or event per row, with values for both response and explanatory variables in variables or columns. The model formula is used to indicate which variables in the data frame are to be used and in which role: either response or explanatory, and when explanatory how they contribute to the estimated response. The object containing the results from the fit is queried to assess validity and make conclusions or predictions.

Weights are multiplicative factors used to alter the *weight* given to individual residuals when fitting a model to observations that are not equally informative. A frequent case is fitting a model to observations that are means of drastically different numbers of individual measurements. Some model fit functions compute the weights, but in most cases they are supplied as an argument to parameter weights. By default, weights have a value of 1 and thus do not affect the resulting model fit, when supplied or computed, the weights are saved to the model fit object.

#### 7.9.1 Regression

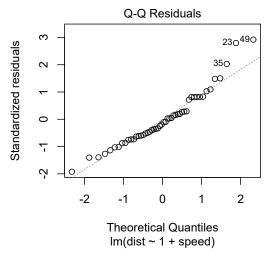
In this section we continue using the cars data set, which contains two numeric variables.

A simple linear model  $y = \alpha \cdot 1 + \beta \cdot x$  where y corresponds to stopping distance (dist) and x to initial speed (speed) is formulated in R as dist  $\sim 1$  + speed. The fitted model object is assigned to variable fm1 (a mnemonic for fitted-model one).

```
fm1 <- lm(dist ~ 1 + speed, data=cars)
class(fm1)
## [1] "lm"</pre>
```

The next step is diagnosis of the fit. Are assumptions of the linear model procedure used reasonably close to being fulfilled? In R it is most common to use plots to this end. We show here only one of the plots normally produced. This quantile vs. quantile plot is used to assess how much the distribution of the residuals deviates from the assumed Normal distribution.

```
plot(fm1, which = 2)
```



In the case of a regression, calling summary() with the fitted model object as argument is most useful as it provides a table of coefficient estimates and their errors. Remember that as is the case for most R functions, the value returned by summary() is printed when we call this method at the R prompt.

```
summary(fm1)
##
##
  lm(formula = dist ~ 1 + speed, data = cars)
##
##
  Residuals:
##
                1Q Median
       Min
                                30
                                        Max
##
  -29.069 -9.525
                    -2.272
                              9.215
                                     43.201
##
  Coefficients:
##
               Estimate Std. Error t value Pr(>|t|)
## (Intercept) -17.5791
                            6.7584 -2.601
```

```
## speed 3.9324 0.4155 9.464 1.49e-12 ***
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 15.38 on 48 degrees of freedom
## Multiple R-squared: 0.6511,Adjusted R-squared: 0.6438
## F-statistic: 89.57 on 1 and 48 DF, p-value: 1.49e-12
```

The summary is organized in sections. "Call:" shows dist  $\sim 1 + \text{speed}$  or the specification of the model fitted, plus the data used. "Residuals:" displays the extremes, quartiles and median of the residuals, or deviations between observations and the fitted line. "Coefficients:" contains estimates of the model parameters and their variation plus corresponding t-tests. In the last three lines there is information on overall standard error and its degrees of freedom and overall coefficient of determination ( $R^2$ ) and F-statistic.

Replacing  $\alpha$  and  $\beta$  in  $y = \alpha \cdot 1 + \beta \cdot x$  by the estimates for the intercept, a = -17.6, and slope, b = 3.93, we obtain an estimate for the regression line y = -17.6 + 3.93x. However, given the nature of the problem, we *know based on first principles* that stopping distance must be zero when speed is zero. This suggests that we should not estimate the value of  $\alpha$  but instead set  $\alpha = 0$ , or in other words, fit the model  $y = \beta \cdot x$ .

In R models, the intercept is included by default, so the model fitted above can be formulated as dist ~ speed—i.e., the missing + 1 does not change the model. To exclude the intercept we need to specify it as dist ~ speed - 1 (or its equivalent dist ~ speed + 0), for a straight line passing through the origin (x = 0, y = 0). In the summary for this model there is an estimate for the slope but not for the intercept.

```
fm2 \leftarrow 1m(dist \sim speed - 1, data = cars)
summary(fm2)
##
## Call:
## lm(formula = dist ~ speed - 1, data = cars)
##
## Residuals:
##
       Min
                1Q Median
                                3Q
                                        Max
  -26.183 -12.637
                   -5.455
                             4.590
                                    50.181
##
##
## Coefficients:
##
         Estimate Std. Error t value Pr(>|t|)
## speed
         2.9091
                    0.1414
                               20.58 <2e-16 ***
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
## Residual standard error: 16.26 on 49 degrees of freedom
## Multiple R-squared: 0.8963, Adjusted R-squared: 0.8942
## F-statistic: 423.5 on 1 and 49 DF, p-value: < 2.2e-16
```

The equation for fm2 is y = 2.91x. From the residuals, it can be seen that it is inadequate, as the straight line does not follow the curvature of the cloud of observations.

**7.8** You will now fit a second-degree polynomial, a different linear model:  $y = \alpha \cdot 1 + \beta_1 \cdot x + \beta_2 \cdot x^2$ . The function used is the same as for linear regression, lm(). We only need to alter the formulation of the model. The identity function **I**() is used to protect its argument from being interpreted as part of the model formula. Instead, its argument is evaluated beforehand and the result is used as the, in this case second, explanatory variable.

```
fm3 <- lm(dist ~ speed + I(speed^2), data = cars)
plot(fm3, which = 3)
summary(fm3)</pre>
```

The "same" fit using an orthogonal polynomial can be specified using function poly(). Polynomials of different degrees can be obtained by supplying as the second argument to poly() the corresponding positive integer value. In this case, the different terms of the polynomial are bulked together in the summary.

```
fm3a <- lm(dist ~ poly(speed, 2), data = cars)
summary(fm3a)</pre>
```

It is possible to compare two model fits using <code>anova()</code>, testing whether one of the models describes the data better than the other. It is important in this case to take into consideration the nature of the difference between the model formulas, most importantly if they can be interpreted as nested—i.e., interpreted as a base model vs. the same model with additional terms.

```
anova(fm2, fm1)
```

Three or more models can also be compared in a single call to anova(). However, care is needed, as the order of the arguments matters.

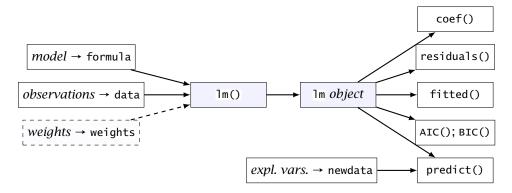
```
anova(fm2, fm3, fm3a)
anova(fm2, fm3a, fm3)
```

Different criteria can be used to choose the "best" model: significance based on *p*-values or information criteria (AIC, BIC). AIC (Akaike's "An Information Criterion") and BIC ("Bayesian Information Criterion" = SBC, "Schwarz's Bayesian criterion") that penalize the resulting "goodness" based on the number of parameters in the fitted model. In the case of AIC and BIC, a smaller value is better, and values returned can be either positive or negative, in which case more negative is better. Estimates for both BIC and AIC are returned by anova(), and on their own by BIC() and AIC()

```
BIC(fm2, fm1, fm3, fm3a)
AIC(fm2, fm1, fm3, fm3a)
```

Once you have run the code in the chunks above, you will be able see that these three criteria do not necessarily agree on which is the "best" model. Find in the output p-value, BIC and AIC estimates, for the different models and conclude which model is favored by each of the three criteria. In addition you will notice that the two different formulations of the quadratic polynomial are equivalent.

Additional query methods give easy access to different aspects of fitted models: vcov() returns the variance-covariance matrix, coef() and its alias coefficients() return the estimates for the fitted model coefficients, fitted() and its alias fitted.values() extract the fitted values, and resid() and its alias residuals()



#### **FIGURE 7.3**

Diagram including additional methods used to query fitted model objects using linear models as an example. For other details please see the legend to Figure 7.2.

the corresponding residuals (or deviations) (Figure 7.3). Less frequently used accessors are getCall(), effects(), terms(), model.frame() and model.matrix().

7.9 Familiarize yourself with these extraction and summary methods by reading their documentation and use them to explore fm1 fitted above or model fits to other data of your interest.

The objects returned by model fitting functions contain the full information, including the data to which the model was fit to. Their structure resembles a nested list. In most cases the class of the objects returned by model fit functions agrees in name with the name of the model-fit function ("1m" in this example) but is not derived from R class "list". The different functions described above, either extract parts of the object or do additional calculations and formatting based on them. There are different specializations of these methods which are called depending on the class of the model-fit object. (See section 6.3 on page 176.)

```
class(fm1)
## [1] "lm"
names(fm1)
## [1] "coefficients" "residuals" "effects" "rank"
## [5] "fitted.values" "assign" "qr" "df.residual"
## [9] "xlevels" "call" "terms" "model"
```

The structure of model-fit objects is of interest only when the query or accessor functions do not provide the needed information and when we are interested to learn how model fitting works in R. As with any other R object str() shows the structure. Calling str() with no.list = TRUE, give.attr = FALSE, vec.len = 2 as arguments restricts the output to an overview of the structure of fm1.

```
str(fm1, no.list = TRUE, give.attr = FALSE, vec.len = 2)
## $ coefficients : Named num [1:2] -17.58 3.93
  $ residuals
                : Named num [1:50] 3.85 11.85 ...
  $ effects
                 : Named num [1:50] -304 146 ...
##
  $ rank
                 : int 2
  $ fitted.values: Named num [1:50] -1.85 -1.85 ...
  $ assign
                 : int [1:2] 0 1
##
                  :List of 5
    ..$ qr : num [1:50, 1:2] -7.071 0.141 ...
##
##
    ..$ qraux: num [1:2] 1.14 1.27
##
    ..$ pivot: int [1:2] 1 2
##
    ..$ tol : num 1e-07
##
    ..$ rank : int 2
##
   $ df.residual : int 48
##
   $ xlevels
                 : Named list()
##
   $ call
                  : language lm(formula = dist ~ 1 + speed, data = cars)
                  :Classes 'terms', 'formula' language dist ~ 1 + speed
##
   $ terms
                  :'data.frame': 50 obs. of 2 variables:
   $ model
    ..$ dist : num [1:50] 2 10 4 22 16 ...
    ..$ speed: num [1:50] 4 4 7 7 8 ...
```

Member call contains the function call and arguments used to create object fm1.

```
str(fm1$call)
## language lm(formula = dist ~ 1 + speed, data = cars)
```

It is usual to only look at the value returned by anova() and summary() as implicitly displayed by print(). However, both anova() and summary() return complex objects, derived from list, containing some members not displayed by print(). Access to members of these objects can be necessary to use them in further calculations or to print them in a format different to the default.

The class of the object returned by anova() does not depend on the class of the model fit object, while its structure does depend.

```
anova(fm1)
## Analysis of Variance Table
##
## Response: dist
            Df Sum Sq Mean Sq F value
## speed
            1 21186 21185.5 89.567 1.49e-12 ***
## Residuals 48 11354
                        236.5
## Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
class(anova(fm1))
## [1] "anova"
                   "data.frame"
str(anova(fm1))
## Classes 'anova' and 'data.frame': 2 obs. of 5 variables:
  $ Df
           : int 1 48
## $ Sum Sq : num 21185 11354
## $ Mean Sq: num 21185 237
   $ F value: num 89.6 NA
   Pr(>F) : num 1.49e-12 NA
## - attr(*, "heading")= chr [1:2] "Analysis of Variance Table\n" "Response: dist"
```

The class of the summary objects depends on the class of the model fit object; summary() is a generic method with multiple specializations.

```
class(summary(fm1))
## [1] "summary.lm"
```

One case where we need to extract individual members is when adding annotations to plots. Another case is when writing reports to include programmatically the computed values within the text. str() can be used to display the structure in a simplified way, and later of one member as above.

```
str(summary(fm1), no.list = TRUE, give.attr = FALSE, vec.len = 2)
##
   $ call
                  : language lm(formula = dist ~ 1 + speed, data = cars)
                  :Classes 'terms', 'formula' language dist ~ 1 + speed
   $ terms
   $ residuals : Named num [1:50] 3.85 11.85 ...
   $ coefficients : num [1:2, 1:4] -17.58 3.93 ...
   $ aliased
                  : Named logi [1:2] FALSE FALSE
   $ sigma
                  : num 15.4
##
   $ df
                  : int [1:3] 2 48 2
                : num 0.651
##
   $ r.squared
   $ adj.r.squared: num 0.644
##
   $ fstatistic : Named num [1:3] 89.6 1 ...
  $ cov.unscaled : num [1:2, 1:2] 0.1931 -0.0112 ...
  Extraction of members follows the usual R rules using $, [ ], or [[ ]].
```

```
summary(fm1)$adj.r.squared
## [1] 0.6438102
```

The coefficients estimates in the summary are accompanied by estimates for the corresponding standard errors, *t*-value and *P*-value, while in the model object fm1 these are not included.

```
coef(fm1)
## (Intercept)
                     speed
   -17.579095
                  3.932409
str(fm1$coefficients)
   Named num [1:2] -17.58 3.93
   - attr(*, "names")= chr [1:2] "(Intercept)" "speed"
print(summary(fm1)$coefficients)
##
                 Estimate Std. Error
                                       t value
                                                   Pr(>|t|)
## (Intercept) -17.579095 6.7584402 -2.601058 1.231882e-02
                3.932409 0.4155128 9.463990 1.489836e-12
str(summary(fm1)$coefficients)
   num [1:2, 1:4] -17.579 3.932 6.758 0.416 -2.601 ...
   - attr(*, "dimnames")=List of 2
##
    ..$ : chr [1:2] "(Intercept)" "speed"
##
     ..$ : chr [1:4] "Estimate" "Std. Error" "t value" "Pr(>|t|)"
##
```

As an example of the use of values extracted from the summary. Im object, I show how to test if the slope from a linear regression fit deviates significantly from a constant value different from the usual zero, which tests for the presence of an "effect" of the explanatory variable. When testing for deviations from a calibration by comparing two instruments or an instrument and a reference, a null hypothesis of one for the slope tests for deviations from the true readings. In some cases, when comparing the effectiveness of interventions we may be interested to test if

a new approach surpasses that in current use by at least a specific margin. There exist practical situations where testing if a response exceeds a threshold is of interest.

When using anova() and summary() the null hypothesis is no effect or no response. The equivalent test with a null hypothesis of slope = 1 is easy to implement if we consider how we calculate a t-value (see section 7.7 on page 195). To compute the t-value we need an estimate for slope and an estimate of the standard error for slope, and the degrees of freedom. All these values are available as members of the summary object of a fitted model.

```
est.slope.value <- summary(fm1)$coefficients["speed", "Estimate"]
est.slope.se <- summary(fm1)$coefficients["speed", "Std. Error"]
degrees.of.freedom <- summary(fm1)$df[2]</pre>
```

The t-value is computed based on the difference between the estimate for the slope and the null hypothesis and the standard error. A probability is obtained based on computed t-value, or quantile, and the t distribution with matching degrees of freedom with a call to pt() (see section 7.3 on page 187.) For a two-tail test we multiply by two the one-tail P estimate.

```
hyp.null <- 1
t.value <- (est.slope.value - hyp.null) / est.slope.se
p.value <- 2 * pt(q = t.value, df = degrees.of.freedom, lower.tail = FALSE)
cat("slope =", signif(est.slope.value, 3),
    "with s.e. =", signif(est.slope.se, 3),
    "\nt.value =", signif(t.value, 3),
    "and P-value =", signif(p.value, 3))
## slope = 3.93 with s.e. = 0.416
## t.value = 7.06 and P-value = 6.01e-09</pre>
```

This example is for a linear model fitted with function <code>lm()</code> but the same approach can be applied to other model fit procedures for which parameter estimates and their corresponding standard error estimates can be extracted or computed.

7.10 Check that the computations above after replacing hyp.null <- 1 by hyp.null <- 0 agree with the output of printing summary().

Modify the example above so as to test whether the intercept is significantly larger than 5 feet, doing a one-sided test.

Method predict() uses the fitted model together with new data for the independent variables to compute predictions. As predict() accepts new data as input, it allows interpolation and extrapolation to values of the independent variables not present in the original data. In the case of fits of linear- and some other models, method predict() returns, in addition to the prediction, estimates of the confidence and/or prediction intervals. The new data must be stored in a data frame with columns using the same names for the explanatory variables as in the data used for the fit, a response variable is not needed and additional columns are ignored. (The explanatory variables in the new data can be either continuous or factors, but they must match in this respect those in the original data.)

**7.11** Predict using both fm1 and fm2 the distance required to stop cars moving at 0, 5, 10, 20, 30, and 40 mph. Study the help page for the predict

method for linear models (using help(predict.lm)). Explore the difference between "prediction" and "confidence" bands: why are they so different?

# 7.9.2 Analysis of variance, ANOVA

In ANOVA the explanatory variable is categorical, and in R, must be a factor or ordered factor (see section 3.12 on page 79). As a linear model, the fitting approach is the same as for linear and polynomial regression (Figure 7.2). The InsectSprays data set used in the next example, gives insect counts in plots sprayed with different insecticides. In these data, spray is a factor with six levels.

What determines that this is an ANOVA is that spray, the explanatory variable, is a factor.

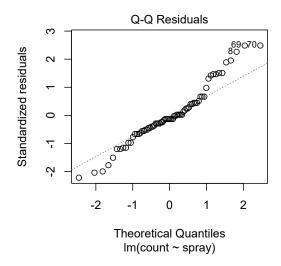
```
data(InsectSprays)
is.numeric(InsectSprays$spray)
## [1] FALSE
is.factor(InsectSprays$spray)
## [1] TRUE
levels(InsectSprays$spray)
## [1] "A" "B" "C" "D" "E" "F"
```

By using a factor instead of a numeric vector, a different model matrix is built from an equivalent formula.

```
fm4 <- lm(count ~ spray, data = InsectSprays)</pre>
```

Diagnostic plots are obtained in the same way as for linear regression. We show only the quantile-quantile plot for simplicity, but during data analysis it is very important to check all the diagnostics plots. As many of the residuals deviate from the one-to-one line we have to conclude the residuals do not follow the Normal distribution, and a different approach to model fitting should be used (see section 7.10 on page 215).

```
plot(fm4, which = 2)
```



In ANOVA, most frequently the interest is in testing hypotheses with function anova(), that implements the *F*-test for main effects of factors and their interactions. In this example, with a single explanatory variable there is only one effect of interest, that of sprays.

Function summary() can be used to extract parameter estimates informing of the size of the effects, but meaningfully only by using contrasts different to the default ones. Function aov() is a wrapper on lm() that returns an object that by default displays the output of anova() also with summary(), but even in this case it can be preferable to change the default contrasts (see help(aov)).

The contrasts used affect the estimates returned by coef() and summary() applied to an ANOVA model fit. The default used in R, contr.treatment, is different to that used in S, contr.helmert. With contr.treatment the first level of the factor (assumed to be a control) is used as reference for estimation of coefficients and testing of their significance. With contr.helmert the contrasts are of the second level with the first, the third with the average of the first two, and so on. These contrasts depend on the order of factor levels. Instead, contr.sum uses as reference the mean of all levels, i.e., using as condition that the sum of the coefficient estimates is equal to zero. Obviously what type of contrast is used changes what the coefficient estimates describe, and, consequently, how the *p*-values should be interpreted.

- The approach used by default for model fits and ANOVA calculations vary among programs. There exist different so-called "types" of sums of squares, usually called I, II, and III. In orthogonal designs the choice is of no consequence, but differences can be important for unbalanced designs, even leading to different conclusions. R's default, type I, is usually considered to suffer milder problems than type III, the default used by SPSS and SAS. In any case, for unbalanced data it is preferable to use the approach implemented in package 'nlme'.
- The most straightforward way of setting a different default for contrasts for a whole series of model fits is by setting R option contrasts, which we here only print.

```
options("contrasts")
## $contrasts
## unordered ordered
## "contr.treatment" "contr.poly"
```

The option is set to a named character vector of length two, with the first value, named unordered giving the name of the function used when the explanatory variable is an unordered factor (created with factor()) and the second value, named

ordered, giving the name of the function used when the explanatory variable is an ordered factor (created with ordered()).

It is also possible to select the contrast to be used in the call to aov() or lm().

In fm4trea we used contr.treatment(), thus contrasts for individual treatments are done against spray1 taking it as the control or reference, as can be inferred from the generated contrasts matrix. For this reason, there is no row for Spray1 in the summary table. Each of the rows Spray2 to Spray6 is a test comparing these treatments individually against Spray1.

```
contr.treatment(length(levels(InsectSprays$spray)))
   2 3 4 5 6
## 1 0 0 0 0 0
## 2 1 0 0 0 0
## 3 0 1 0 0 0
## 4 0 0 1 0 0
## 5 0 0 0 1 0
## 6 0 0 0 0 1
summary(fm4trea)
##
## Call:
## lm(formula = count ~ spray, data = InsectSprays, contrasts = list(spray = contr.treatment))
##
## Residuals:
##
             1Q Median
                           30
    Min
                                 Max
## -8.333 -1.958 -0.500 1.667 9.333
##
## Coefficients:
             Estimate Std. Error t value Pr(>|t|)
## (Intercept) 14.5000 1.1322 12.807 < 2e-16 ***
## sprayB
               0.8333
                         1.6011 0.520
                                            0.604
              -12.4167 1.6011 -7.755 7.27e-11 ***
## sprayC
## sprayD
              -9.5833 1.6011 -5.985 9.82e-08 ***
              -11.0000
## sprayE
                           1.6011 -6.870 2.75e-09 ***
## sprayF
               2.1667
                           1.6011 1.353
                                            0.181
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 3.922 on 66 degrees of freedom
## Multiple R-squared: 0.7244, Adjusted R-squared: 0.7036
## F-statistic: 34.7 on 5 and 66 DF, p-value: < 2.2e-16
```

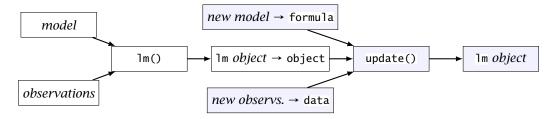
In fm4sum we used contr.sum() with the sum constrained to be zero, thus estimates for the last treatment level are determined by the sum of the previous ones, and not tested for significance.

```
contr.sum(length(levels(InsectSprays$spray)))
     [,1] [,2] [,3] [,4] [,5]
## 1
             0
                  0
## 2
        0
            1
                  0
                       0
                            0
## 3
            0
       0
                 1
                       0
                            0
       0
           0
                 0
                            0
## 4
                      1
## 5
       0
            0
                 0
                       0
                            1
       -1
            -1
                -1
                      -1
                           -1
summary(fm4sum)
##
## Call:
## lm(formula = count ~ spray, data = InsectSprays, contrasts = list(spray = contr.sum))
##
## Residuals:
             1Q Median
##
                            30
     Min
                                  Max
## -8.333 -1.958 -0.500 1.667
                                9.333
##
## Coefficients:
               Estimate Std. Error t value Pr(>|t|)
##
## (Intercept) 9.5000
                         0.4622 20.554 < 2e-16 ***
                5.0000
                            1.0335
                                    4.838 8.22e-06 ***
## spray1
## spray2
                5.8333
                            1.0335
                                     5.644 3.78e-07 ***
                            1.0335 -7.176 7.87e-10 ***
## spray3
                -7.4167
                -4.5833
                            1.0335 -4.435 3.57e-05 ***
## spray4
                -6.0000
                            1.0335 -5.805 2.00e-07 ***
## spray5
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
## Residual standard error: 3.922 on 66 degrees of freedom
## Multiple R-squared: 0.7244, Adjusted R-squared: 0.7036
## F-statistic: 34.7 on 5 and 66 DF, p-value: < 2.2e-16
```

7.12 Explore how taking the last level as reference in contr.sas() instead of the first one as in contr.treatment() affects the estimates. Reorder the levels of factor spray so that the test using contr.sas() becomes equivalent to that obtained above with contr.treatment(). Consider why contr.poly() is the default for ordered factors and when contr.helmert() could be most useful.

Contrasts, on the other hand, do not affect the table returned by anova() as this table does not deal with the effects of individual factor levels. The overall estimates shown at the bottom of the summary table remain unchanged. In other words, when using different contrasts what changes is how the total variation explained by the fitted model is partitioned into components to be tested for specific contributions to the overall model fit.

Post-hoc test with contrasts and multiple comparisons tests are most frequently applied after an ANOVA to test for differences among pairs of treatments or specific combinations of treatments. R function tukey.test() implements tukey's HSD (honestly significant difference) test for pairwise tests. Function tukey.test() supports different correction methods for the tukey.test() supports different correction methods for the tukey.test() significant difference) adjustments to tukey.test() applies adjustments to tukey.test() applies adjustments to tukey.test() and can be used when the test procedure does not apply them. The most comprehensive implementation of multiple comparisons is available in package 'multcomp'.



#### **FIGURE 7.4**

Diagram showing the steps for updating a fitted model (in filled boxes) together with the previous steps in unfilled boxes. Please, see Figure 7.2 for other details.

Function glht() (general linear hypothesis testing) from this package supports different contrasts and adjustment methods.

Contrasts and their interpretation are discussed in detail by Venables and Ripley (2002) and Crawley (2012).

# 7.9.3 Analysis of covariance, ANCOVA

When a linear model includes both explanatory factors and continuous explanatory variables, we may call it *analysis of covariance* (ANCOVA). The formula syntax is the same for all linear models and, as mentioned in previous sections, what determines the type of analysis is the nature of the explanatory variable(s). As the formulation remains the same, no specific example is given. The main difficulty of ANCOVA is in the selection of the covariate and the interpretation of the results of the analysis (e.g. Smith 1957).

# 7.9.4 Model update and selection

Model fit objects can be updated, i.e., modified, because they contain not only the results of the fit but also the data to which the model was fit (see page 203). Given that the call is also stored, all the information needed to recalculate the same fit is available. Method update() makes possible to recalculate the fit with changes to the call, without passing again all the arguments to a new call to lm() (Figure 7.4). We can modify different arguments, including selecting part of the data by passing a new argument to formal parameter subset.

Method update() retrieves the call from the model fit object using getcall(), modifies it and, by default, evaluates it. The default update() method works as long as the model-fit object contains a member named call or if a specialization of getcall() is available. Thus, method update() can be used with models fitted with other functions in addition to lm().

For the next example we recreate the model fit object fm4 from page 207.

```
fm4 <- lm(count ~ spray, data = InsectSprays)
anova(fm4)
## Analysis of Variance Table
##
## Response: count</pre>
```

```
##
            Df Sum Sq Mean Sq F value
                                        Pr(>F)
## spray
            5 2668.8 533.77 34.702 < 2.2e-16 ***
## Residuals 66 1015.2
                       15.38
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
fm4a <- update(fm4, formula = log10(count + 1) ~ spray)</pre>
anova(fm4a)
## Analysis of Variance Table
##
## Response: log10(count + 1)
            Df Sum Sq Mean Sq F value
           5 7.2649 1.45297 46.007 < 2.2e-16 ***
## spray
## Residuals 66 2.0844 0.03158
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
```

**7.13** Print fm4\$call and fm4a\$call. These two calls differ in the argument to formula. What other members have been updated in fm4a compared to fm4?

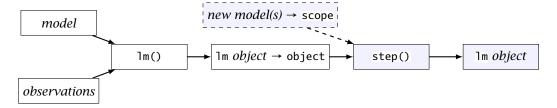
In the chunk above we replaced the argument passed to formula. This is a frequent use, but for example to fit the same model to a subset of the data we can pass a suitable argument to parameter subset.

7.14 When having many treatments with long names, which is not the case here, instead of listing the factor levels for which to subset the data, it can be convenient to use regular expressions for pattern matching (see section 3.4 on page 46). Run the code below, and investigate why anova(fm4b) and anova(fm4c) produce the same ANOVA table printout, but the fit model objects are not identical. You can use str() to explore if any members differ between the two objects.

```
fm4c <- update(fm4, subset = !grepl("[AB]", spray))
anova(fm4c)
identical(fm4b, fm4c)</pre>
```

Method update() plays an additional role when fitting is done by numerical approximation, as the previously computed estimates are used as the starting values for the numerical calculations required for fitting the updated model (see section 7.11 on page 218 as an example). This can drastically decrease computation time, or even easy the task of finding suitable starting values for parameter estimates by fitting increasingly more complex nested models.

Method update() used together with AIC() (or anova()) gives us the tools to compare nested models, and select one out a group of them as shown above. When comparing several models doing the comparisons manually is tedious, and



#### FIGURE 7.5

Diagram showing the steps used for stepwise model selection among nested models (in filled boxes) together with the previous steps in unfilled boxes. The range of models to select from can be set by the user. Please, see Figure 7.2 for other details.

in scripts, in many cases difficult to write code that is flexible (or abstract) enough. Method step() automates stepwise selection of nested models such as the selection among polynomials of different degrees or which variables to retain in multiple regression. After fitting a model, method step() is used to update this model using an automatic stopping criterion (Figure 7.5).

Step-wise model selection, either in the *forward* direction from simpler to more complex models, in the backward direction from more complex to simpler models or in both directions is implemented in base R's *method* step() using Akaike's information criterion (AIC) as the selection criterion. Use of method step() from R is possible, for example, with lm() and glm fits. AIC is described on page 202.

For the next example we use fm3 from page 202, a linear model for a polynomial regression. If as shown here, no models are passed through formal parameter scope, the previously fit model will be simplified, if possible. Method step() by default prints to the console a trace of the models tried and the corresponding AIC estimates.

```
fm3 <- lm(dist \sim speed + I(speed^2), data = cars)
fm3a <- step(fm3)</pre>
## Start: AIC=274.88
## dist ~ speed + I(speed^2)
##
##
                Df Sum of Sq
                                RSS
## - speed
                 1 46.42 10871 273.09
                              10825 274.88
## <none>
  - I(speed^2) 1
                      528.81 11354 275.26
##
## Step: AIC=273.09
## dist ~ I(speed^2)
##
##
                Df Sum of Sq
                                RSS
## <none>
                              10871 273.09
## - I(speed^2) 1
                       21668 32539 325.91
```

Method summary() reveals the differences between the original and updated models.

```
summary(fm3)
##
## Call:
```

```
## lm(formula = dist ~ speed + I(speed^2), data = cars)
##
## Residuals:
##
      Min
                1Q Median
                                3Q
                                       Max
## -28.720 -9.184
                   -3.188
                             4.628
                                   45.152
##
## Coefficients:
##
               Estimate Std. Error t value Pr(>|t|)
## (Intercept) 2.47014
                         14.81716
                                     0.167
                                              0.868
## speed
                0.91329
                           2.03422
                                     0.449
                                              0.656
## I(speed^2)
                0.09996
                           0.06597
                                     1.515
                                              0.136
##
## Residual standard error: 15.18 on 47 degrees of freedom
## Multiple R-squared: 0.6673, Adjusted R-squared: 0.6532
## F-statistic: 47.14 on 2 and 47 DF, p-value: 5.852e-12
summary(fm3a)
##
## lm(formula = dist ~ I(speed^2), data = cars)
##
## Residuals:
##
      Min
                1Q Median
                                3Q
                                       Мах
## -28.448 -9.211 -3.594
                             5.076
                                   45.862
##
## Coefficients:
##
              Estimate Std. Error t value Pr(>|t|)
## (Intercept) 8.86005
                          4.08633
                                   2.168
                                           0.0351 *
## I(speed^2)
               0.12897
                           0.01319
                                    9.781 5.2e-13 ***
## --
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
## Residual standard error: 15.05 on 48 degrees of freedom
## Multiple R-squared: 0.6659, Adjusted R-squared: 0.6589
## F-statistic: 95.67 on 1 and 48 DF, p-value: 5.2e-13
```

If we pass a model with additional terms through parameter scope this model will be taken as the most complex model to be assessed. If, instead of one model, we pass two nested models in a list and name them lower and upper, they will delimit the scope of the stepwise search. In the next example we see that first a backward search is done and term speed is removed as removal decreases AIC. Subsequently a forward search is done unsuccessfully for a model with smaller AIC.

```
fm3b <-
       scope = dist \sim speed + I(speed^2) + I(speed^3) + I(speed^4)
## Start: AIC=274.88
## dist ~ speed + I(speed^2)
##
##
                Df Sum of Sq
                               RSS
                                      AIC
## - speed
                 1
                      46.42 10871 273.09
## <none>
                             10825 274.88
## - I(speed^2) 1
                      528.81 11354 275.26
## + I(speed^4) 1
                      233.62 10591 275.79
## + I(speed^3) 1
                      190.35 10634 275.99
##
## Step: AIC=273.09
```

```
## dist ~ I(speed^2)
##
               Df Sum of Sq
##
                             RSS
                                     AIC
## <none>
                            10871 273.09
## + speed
                       46.4 10825 274.88
## + I(speed^3) 1
                        5.6 10866 275.07
## + I(speed^4)
                1
                        0.0 10871 275.09
## - I(speed^2) 1
                    21667.8 32539 325.91
summary(fm3b)
##
## Call:
## lm(formula = dist ~ I(speed^2), data = cars)
## Residuals:
               1Q Median
##
      Min
                               30
                                      Max
## -28.448 -9.211 -3.594
                            5.076 45.862
##
## Coefficients:
##
              Estimate Std. Error t value Pr(>|t|)
## (Intercept) 8.86005
                         4.08633 2.168
                                          0.0351 *
## I(speed^2) 0.12897
                          0.01319 9.781 5.2e-13 ***
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 15.05 on 48 degrees of freedom
## Multiple R-squared: 0.6659, Adjusted R-squared: 0.6589
## F-statistic: 95.67 on 1 and 48 DF, p-value: 5.2e-13
```

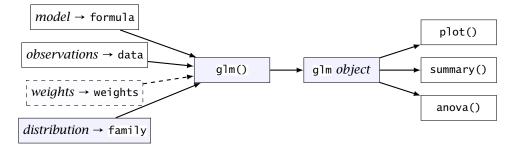
**7.15** Explain why the stepwise model selection in the code below differs from those in the two previous examples. Consult help(step) is necessary.

Functions update() and step() are *convenience functions* as they provide direct and/or simpler access to operations available through other functions or combined use of multiple functions.

#### 7.10 Generalized linear models

Linear models make the assumption of normally distributed residuals. Generalized linear models, fitted with function glm() are more flexible, and allow the assumed distribution to be selected as well as the link function (defaults are as in lm()). Figure 7.6 shows that the steps used to fit a model with glm() are the same as with lm() except that we can select the probability distribution assumed to describe the variation among observations. Frequently used probability distributions are binomial and Poisson (see help(family)) for the variations and additional ones).

For count data, GLMs are preferred over LMs. In the example below we fit the



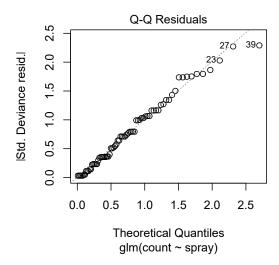
#### **FIGURE 7.6**

Generalized linear model fitting in R is done in steps similar to those used for linear models. Generic diagram from Figure 7.1 redrawn to show a generalized linear model fit. Non-filled boxes are shared with fitting of other types of models, and filled ones are specific to glm(). Only the three most frequently used query methods are shown, while both response and explanatory variables are under *observations*. Dashed boxes and arrows are optional as defaults are provided.

same model as above, but assuming a quasi-Poisson distribution instead of the Normal. An argument passed to family selects the assumed error distribution. The InsectSprays data set used in the next example, gives insect counts in plots sprayed with different insecticides. In these data, spray is a factor with six levels. fm10 <- glm(count ~ spray, data = InsectSprays, family = quasipoisson)

Method plot() as for linear-model fits, produces diagnosis plots. We show as above the q-q-plot of residuals. The Normal distribution assumed in the linear model fit was not a good approximation (section 7.9.2 on page 207), as count data are known to follow a different distribution. This is clear by comparing the quantile-quantile plot for fm4 (page 207) and the plot below for the model fit under the assumption of a Quasi-Poisson distribution.

plot(fm10, which = 2)



The printout from the anova() method for GLM fits has some differences to that for LM fits. In R versions previous to 4.4.0 no test statistics or P-values were computed unless requested by passing an argument to parameter test. In newer versions of R either a chi-squared test or an F-test are computed by default depending on whether the dispersion is fixed or free. We here use "F" as an argument to request an F-test.

```
anova(fm10, test = "F")
## Analysis of Deviance Table
##
## Model: quasipoisson, link: log
##
## Response: count
##
## Terms added sequentially (first to last)
##
##
        Df Deviance Resid. Df Resid. Dev
##
                                                    Pr(>F)
                            71
                                   409.04
## NULL
## spray 5
              310.71
                            66
                                    98.33 41.216 < 2.2e-16 ***
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
```

We can extract different components similarly as described for linear models (see section 7.9 on page 198).

```
class(fm10)
## [1] "glm" "lm"
summary(fm10)
##
## Call:
## glm(formula = count ~ spray, family = quasipoisson, data = InsectSprays)
## Coefficients:
##
              Estimate Std. Error t value Pr(>|t|)
## (Intercept) 2.67415
                          0.09309
                                   28.728 < 2e-16 ***
               0.05588
                           0.12984
                                    0.430
                                              0.668
## sprayB
                                   -7.388 3.30e-10 ***
               -1.94018
                           0.26263
## sprayC
               -1.08152
                                   -5.847 1.70e-07 ***
                           0.18499
## sprayD
## sprayE
               -1.42139
                           0.21110
                                   -6.733 4.82e-09 ***
## sprayF
               0.13926
                           0.12729
                                    1.094
                                              0.278
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
## (Dispersion parameter for quasipoisson family taken to be 1.507713)
##
##
      Null deviance: 409.041 on 71 degrees of freedom
## Residual deviance: 98.329 on 66 degrees of freedom
## AIC: NA
## Number of Fisher Scoring iterations: 5
head(residuals(fm10))
           1
                                  3
                                            4
## -1.2524891 -2.1919537 1.3650439 -0.1320721 -0.1320721 -0.6768988
head(fitted(fm10))
         2
               3
     1
## 14.5 14.5 14.5 14.5 14.5 14.5
```

If we use str() or names() we can see that there are some differences with respect to linear model fits. The returned object is of a different class and contains some members not present in linear models. Two of these have to do with the iterative approximation method used, iter contains the number of iterations used and converged the success or not in finding a solution.

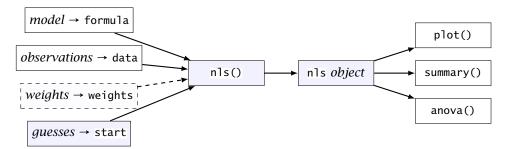
```
class(fm10)
## [1] "glm" "lm"
names(fm10)
    [1] "coefficients"
                              "residuals"
                                                    "fitted.values"
        "effects"
                              "R"
                                                    "rank"
    [4]
        "qr"
                              "family"
    [7]
                                                    "linear.predictors"
##
                              "aic"
        "deviance"
##
   [10]
                                                    "null.deviance"
        "iter"
                              "weights"
                                                    "prior.weights"
##
   [13]
                              "df.null"
        "df.residual"
        "converged"
                              "boundary"
                                                    "model"
   Г197
        "call"
                              "formula"
                                                    "terms"
   Γ221
        "data"
                              "offset"
                                                    "control"
   T251
## [28] "method"
                              "contrasts"
                                                    "xlevels"
fm10$converged
## [1] TRUE
fm10$iter
## [1] 5
```

Methods update() and step(), described for lm() in section 7.9.4 on page 211, can be also used with models fitted with glm().

# 7.11 Non-linear regression

By *non-linear* it is meant non-linear *in the parameters* whose values are being estimated through fitting the model to observations. This is different from the shape of the function when plotted—i.e., polynomials of any degree are linear models. In contrast, the Michaelis-Menten equation used in chemistry and the Gompertz equation used to describe growth are models non-linear in their parameters.

While analytical algorithms exist for finding estimates for the parameters of linear models, in the case of non-linear models, the estimates are obtained by approximation. For analytical solutions, estimates can always be obtained (except in pathological cases affected by the limitations of floating point numbers described on page 27). For approximations obtained through iteration, cases when the algorithm fails to *converge* onto an answer are relatively common. Iterative algorithms attempt to improve an initial guess for the values of the parameters to be estimated, a guess frequently supplied by the user. In each iteration the estimate obtained in the previous iteration is used as the starting value, and this process is repeated one time after another. The expectation is that after a finite number of iterations the algorithm will converge into a solution that "cannot" be improved further. In real life we stop iteration when the improvement in the fit is smaller than a certain threshold, or when no convergence has been achieved after a certain



#### **FIGURE 7.7**

Non-linear model fitting in R is done in steps. Generic diagram from Figure 7.1 redrawn to show a non-linear model fit. Non-filled boxes are shared with fitting of other types of models, and filled ones are specific to nls(). Only the three most frequently used query methods are shown, while both response and explanatory variables are under *observations*. Dashed boxes and arrows are optional as defaults are provided.

maximum number of iterations. In the first case, we usually obtain good estimates; in the second case, we do not obtain usable estimates and need to look for different ways of obtaining them.

When convergence fails, the first thing to do is to try different starting values and if this also fails, switch to a different computational algorithm. These steps usually help, but not always. Good starting values are in many cases crucial and in some cases "guesses" can be obtained using either graphical or analytical approximations.

Function nls() is R's workhorse for fitting non-linear models. The step to its use are similar to those for LM and GLM (Figure 7.7). One difference is that starting values are needed, and another difference is in how the model to be fitted is specified: the user provides the names of the parameters and an a model equation that includes in the *rhs* a call to an R function.

In cases when algorithms exist for "guessing" suitable starting values, R provides a mechanism for packaging the R function to be fitted together with the R function generating the starting values. These functions go by the name of *self-starting functions* and relieve the user from the burden of guessing and supplying suitable starting values. The self-starting functions available in R are SSasymp(), SSasympOff(), SSasympOrig(), SSbiexp(), SSfol(), SSfpl(), SSgompertz(), SSlogis(), SSmicmen(), and SSweibull(). Function selfstart() can be used to define new ones. All these functions can be used when fitting models with nls or nlme. Please, check the respective help pages for details.

As example the Michaelis-Menten equation describing reaction kinetics in biochemistry and chemistry is fitted to the Puromycin data set. The mathematical formulation is given by

$$v = \frac{d[P]}{dt} = \frac{V_{\text{max}}[S]}{K_{\text{M}} + [S]}$$
 (7.1)

and is implemented in R under the name ssmicmen() as a self-starting function.

As for other fitted models we use query methods (see section 7.9 on page 198).

```
class(fm21)
## [1] "nls"
summary(fm21)
##
## Formula: rate ~ SSmicmen(conc, Vm, K)
##
## Parameters:
      Estimate Std. Error t value Pr(>|t|)
##
## Vm 2.127e+02 6.947e+00 30.615 3.24e-11 ***
## K 6.412e-02 8.281e-03
                           7.743 1.57e-05 ***
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
## Residual standard error: 10.93 on 10 degrees of freedom
## Number of iterations to convergence: 0
## Achieved convergence tolerance: 1.929e-06
residuals(fm21)
   [1] 25.4339971 -3.5660029 -5.8109605
                                            4.1890395 -11.3616075
                                                                   4.6383925
   [7] -5.6846886 -12.6846886   0.1670798   10.1670798   6.0311723   -0.9688277
## attr(,"label")
## [1] "Residuals"
fitted(fm21)
   [1] 50.5660 50.5660 102.8110 102.8110 134.3616 134.3616 164.6847 164.6847
   [9] 190.8329 190.8329 200.9688 200.9688
## attr(,"label")
## [1] "Fitted values"
```

Methods str() and names() can reveal differences with respect to linear and generalized linear models. The the fitted model object is of class nls contains additional members but lacks others. Two members are related to the iterative approximation method used, control containing nested members holding iteration settings, and convinfo (convergence information) with nested members with information on the outcome of the iterative algorithm.

```
fm21$convInfo
## $isConv
## [1] TRUE
##
## $finIter
## [1] 0
##
## $finTol
## [1] 1.928554e-06
##
## $stopCode
## [1] 0
##
## $stopMessage
## [1] "converged"
```

Method update(), described for lm() in section 7.9.4 on page 211, can be also used with models fitted with nls(). Reuse of previous estimates as guesses for updates is an important feature.

# 7.12 Splines and local regression

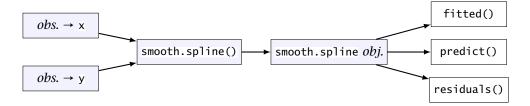
The name "spline" derives from the tool used by draftsmen to draw smooth curves. Originally, a spline of soft wood was used as a flexible guide to draw arbitrary curves. Later the wood splines were replaced by a rod of flexible metal, such as lead, encased in plastic or similar material but the original name persisted. In mathematics, splines are functions that describe smooth and flexible curves.

Most of the model fits given above as examples produce estimates for parameters that are interpretable in the real world, directly in the case of mechanistic models like the estimate of reaction constants or at least indicating broadly a relationship between two variables as in the case of linear regression. In the case of polynomials with degree higher than 2, parameter estimates no longer directly describe features of the data.

Splines take this a step farther and parameter estimates have no practical interest. The interest resides in the overall shape and position of the predicted curve. Splines consist in knots (or connection points) joined by straight or curved fitted lines, i.e., they are functions that are *piecewise*. The simplest splines, are piece-wise linear, given by chained straight line segments connecting knots.

In more complex splines the segments are polynomials, frequently cubic polynomials, that fulfil certain constraints at the knots. For example, that the slope or first derivative is the same for the two connected curve "pieces" at the knot where they are connected. This constraint ensures that the curve is smooth. In some cases similar constraints are imposed on higher order derivatives, for example to the second derivative to ensure that the curve of the first derivative is also smooth at the knots.

Splines are used in free-hand drawing with computers to draw arbitrary smooth curves. They are also be used for interpolation, in which case observations, as-



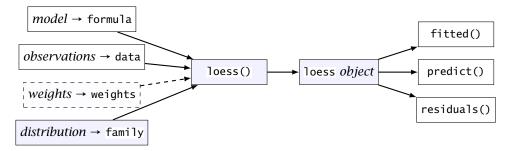
#### **FIGURE 7.8**

Fitting of smooth splines in R. Generic diagram from Figure 7.1 redrawn to show the fitting of splines. Non-filled boxes are shared with fitting of other types of models, and filled ones are specific to smooth.spline(). Only the three most frequently used query methods are shown, while response and explanatory variables are passed separately to x and y.

sumed to be error-free, become the knots of a spline used to approximate intermediate values. Finally, splines can be used as models to be fit to observations subject to random variation. In this case splines fulfil the role of smoothers, as a curve that broadly describes a relationship among variables.

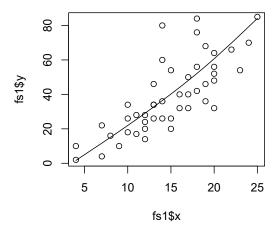
Splines are frequently used as smooth curves in plots as described in section 9.6.3 on page 311. Function spline() is used for interpolation and function smooth.spline() for smoothing by fitting a cubic spline (a spline where the knots are connected by third degree polynomials). Function smooth.spline() has a different user interface than that we used for model fit functions described above, as it only accepts numeric vectors as arguments to parameters x and y (Figure 7.8). Additional parameters make it possible to override the defaults for number of knots and adjust the stiffness or tendency towards a straight line. The plot() method differently to other fit functions produces a plot of the prediction. As no model formula is used only one curve at a time is fitted and no statistical tests involving groups are possible. The most commonly used query functions are thus not the same as for linear and non-linear models.

```
fs1 <- smooth.spline(x = cars$speed, y = cars$dist)
print(fs1)
## Call:
## smooth.spline(x = cars$speed, y = cars$dist)
##
## Smoothing Parameter spar= 0.7801305 lambda= 0.1112206 (11 iterations)
## Equivalent Degrees of Freedom (Df): 2.635278
## Penalized Criterion (RSS): 4187.776
## GCV: 244.1044
plot(fs1, type = "l")
points(x = cars$speed, y = cars$dist)</pre>
```



#### **FIGURE 7.9**

Loess model fitting in R is done in steps. Generic diagram from Figure 7.1 redrawn to show local polynomial regression model fitting. Non-filled boxes are shared with fitting of other types of models, and filled ones are specific to loess(). Only the three most frequently used query methods are shown, while both response and explanatory variables are under *observations*. Dashed boxes and arrows are optional as defaults are provided.



Function loess implements *local polynomial regression*. It fits a polynomial curve or surface (i.e., more than one explanatory variable can be included in the model formula) using local-weighted fitting. Its user interface is rather similar to that of glm() with formula, family and data formal parameters (Figure 7.9). Additional parameters control "stiffness" or the extent of the local data used for fitting (how much weight is given to observations as a function of their distance). The type of fit local or not used for individual explanatory variables can be controlled through parameter parametric.

```
floc <- loess(dist ~ speed, data = cars)
class(floc)
## [1] "loess"
summary(floc)
## call:</pre>
```

```
## loess(formula = dist ~ speed, data = cars)
##
## Number of Observations: 50
## Equivalent Number of Parameters: 4.78
## Residual Standard Error: 15.29
## Trace of smoother matrix: 5.24 (exact)
## Control settings:
##
     span
             : 0.75
##
     degree
                 2
##
     family
                 gaussian
                               cell = 0.2
##
     surface :
                 interpolate
##
    normalize:
                 TRUE
##
   parametric:
                 FALSE
## drop.square:
                 FALSE
```

- Function anova() can be used to compare two or more loess fits, but not on a single one.
- Several modern approaches to data analysis, which do provide estimates of effects' significance and sizes, are based on the use of splines to describe the responses and even variance. Among them are additive models such as GAM and related methods (see Wood 2017) and functional data analysis (FDA) (Ramsay 2009). These methods are outside the scope of this book and implemented in specialized extension packages.

#### 7.13 Model formulas

Model formulas, such as  $y \sim x$  are widely used in R, both in model fitting as exemplified in previous sections of this chapter and in plotting when using base R plot() methods.

R is consistent and flexible in how it treats various objects, to a extent that can be surprising to those familiar with other computer languages. Model formulas are objects of class formula and mode call and can be manipulated and stored similarly to objects of other classes.

```
class(y ~ x)
## [1] "formula"
mode(y ~ x)
## [1] "call"
```

Like any other R object formulas can be assigned to variables and be members of lists and vectors. Consequently, the first linear model fit example from page 200 can be rewritten as follows.

```
my.formula <- dist ~ 1 + speed
fm1 <- lm(my.formula, data=cars)</pre>
```

In some situations, e.g., calculation of correlations, models lacking a *lhs* term (a

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term on the left hand side of ~) are used. At least one term must be present in the *rhs* of model formulas, as an expression ending in ~ is syntactically incomplete.

```
class(~ x + y)
## [1] "formula"
mode(~ x + y)
## [1] "call"
is.empty.model(~ x + y)
## [1] FALSE
```

Some details of R formulas can be important in advanced scripts. Two kinds of "emptiness" are possible for formulas. As with other classes, empty objects or vectors of length zero are valid and can be created with the class constructor. In the case of formulas there is an additional kind of emptiness, a formula describing a model with no explanatory terms on its *rhs*.

An "empty" object of class formula can be created by a call to formula() with no arguments, similarly as a numeric vector of length zero is created by the call numeric(). The last, commented out, statement in the code below triggers an error as the argument passed to is.empty.model() is of length zero. (This behaviour is not consistent with numeric vectors of length zero; see for example the value returned by is.finite(numeric()).)

```
class(formula())
## [1] "formula"
mode(formula())
## [1] "list"
length(formula())
## [1] 0
# is.empty.model(formula())
```

A model formula describing a model with no explanatory terms on the rhs, is considered empty even if it is a valid object of class formula and, thus, not missing. While  $y \sim 1$  describes a model with only an intercept (estimating  $a = \bar{x}$ ),  $y \sim 0$  or its equivalent  $y \sim -1$ , describes an empty model that cannot be fitted to data.

```
class(y ~ 0)
## [1] "formula"
mode(y ~ 0)
## [1] "call"
is.empty.model(y ~ 0)
## [1] TRUE
is.empty.model(y ~ 1)
## [1] FALSE
is.empty.model(y ~ x)
```

The value returned by length() on a single formula is not always 1, the number of formulas in the vector of formulas, but instead the number of components in the formula. For longer vectors, it does return the number of member formulae. Because of this, it is better to store model formulas in objects of class list than in vectors, as length() consistently returns the expected value on lists.

```
length(formula())
## [1] 0
length(y ~ 0)
## [1] 3
length(y ~ 1)
## [1] 3
length(y ~ x)
## [1] 3
length(c(y ~ 1, y ~ x))
## [1] 2
length(list(y ~ 1))
## [1] 1
length(list(y ~ 1, y ~ x))
## [1] 2
```

As described above, length() applied to a single formula and to a list of formulas behaves differently. To call length() on each member of a list of formulas, we can use sapply() (see section 5.8 on page 154). As function is.empty.model() is not vectorized, we also have to use sapply() with a list of formulas.

```
sapply(list(y ~ 0, y ~ 1, y ~ x), length)
## [1] 3 3 3
sapply(list(y ~ 0, y ~ 1, y ~ x), is.empty.model)
## [1] TRUE FALSE FALSE
```

In the examples in previous sections we fitted simple models. More complex ones can be easily formulated using the same syntax. First of all, one can avoid use of operator \* and explicitly define all individual main effects and interactions using operators + and : . The syntax implemented in base R allows grouping by means of parentheses, so it is also possible to exclude some interactions by combining the use of \* and parentheses.

The same symbols as for arithmetic operators are used for model formulas. Within a formula, symbols are interpreted according to formula syntax. When we mean an arithmetic operation that could be interpreted as being part of the model formula we need to "protect" it by means of the identity function I(). The next two examples define formulas for models with only one explanatory variable. With formulas like these, the explanatory variable will be computed on the fly when fitting the model to data. In the first case below we need to explicitly protect the addition of the two variables into their sum, because otherwise they would be interpreted as two separate explanatory variables in the model. In the second case, log() cannot be interpreted as part of the model formula, and consequently does not require additional protection, neither does the expression passed as its argument.

```
y \sim I(x1 + x2)

y \sim log(x1 + x2)
```

R formula syntax allows alternative ways for specifying interaction terms. They allow "abbreviated" ways of entering formulas, which for complex experimental designs saves typing and can improve clarity. As seen above, operator \* saves us from having to explicitly indicate all the interaction terms in a full factorial model.

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```
y \sim x1 + x2 + x3 + x1:x2 + x1:x3 + x2:x3 + x1:x2:x3
Can be replaced by a concise equivalent.
y \sim x1 * x2 * x3
```

When the model to be specified does not include all possible interaction terms, we can combine the concise notation with parentheses. Below, equivalent formulas are shown using concise and verbose notation.

```
y \sim x1 + (x2 * x3)

y \sim x1 + x2 + x3 + x2:x3

y \sim x1 * (x2 + x3)

y \sim x1 + x2 + x3 + x1:x2 + x1:x3
```

The ^ operator provides a concise notation to limit the order of the interaction terms included in a formula.

```
y \sim (x1 + x2 + x3)^2

y \sim x1 + x2 + x3 + x1:x2 + x1:x3 + x2:x3
```

Operator %in% can also be used as a shortcut for including only some of all the possible interaction terms in a formula.

```
y \sim x1 + x2 + x1 \% in\% x2
```

**7.16** Whether two model formulas above are equivalent or not, can be investigated using function terms().

```
terms(y ~ x1 + (x2 * x3))
terms(y ~ x1 * (x2 + x3))
terms(y ~ (x1 + x2 + x3)^2)
terms(y ~ x1 + x2 + x1 %in% x2)
```

**P** 7.17 For operator ^ to behave as expected, its first operand should be a formula with no interactions! Compare the result of expanding these two formulas with terms().

```
y \sim (x1 + x2 + x3)^2

y \sim (x1 * x2 * x3)^2
```

**P** 7.18 Run the code examples below using the npk data set from R. They demonstrate the use of different model formulas in ANOVA. Use these examples plus your own variations on the same theme to build your understanding of the syntax of model formulas. Based on the terms displayed in the ANOVA tables, first work out what models are being fitted in each case. In a second step, write each of the models using a mathematical formulation. Finally, think how model choice may affect the conclusions from an analysis of variance.

```
data(npk)
anova(lm(yield ~ N * P * K, data = npk))
anova(lm(yield ~ (N + P + K)^2, data = npk))
anova(lm(yield ~ N + P + K + P %in% N + K %in% N, data = npk))
anova(lm(yield ~ N + P + K + N %in% P + K %in% P, data = npk))
```

Nesting of factors in experiments using hierarchical designs such as split-plots or repeated measures, results in the need to compute additional error terms, differing in their degrees of freedom. In such a design, different effects are tested based on different error terms. Whether nesting exists or not is a feature of the design

of an experiment, resulting from the randomization approach used for treatment assignment to experimental units. In base-R model-formulas, nesting needs to be described by explicit definition of error terms by means of Error() within the formula. Nowadays, linear mixed-effects (LME) models are most frequently used with data from experiments and surveys using hierarchical designs, as implemented in packages 'nlme' (Pinheiro and Bates 2000) and 'lme4' (Bates et al. 2015). These two packages use their own extensions to the model formula syntax to describe nesting and distinguishing fixed and random effects.

Additive models have required other extensions, most of them specific to individual packages. These extensions fall outside the scope of this book and are described by Wood (2017) and Zuur (2012).

R will accept any syntactically correct model formula, even when the results of the fit are not interpretable. It is *the responsibility of the user to ensure that models are meaningful*. The most common, and dangerous, mistake is specifying for factorial experiments, models that are missing lower-order terms.

Fitting models like those below to data from an experiment based on a three-way factorial design should be avoided. In both cases simpler terms are missing, while higher-order interaction(s) that include the missing term are included in the model. Such models are not interpretable, as the variation from the missing term(s) ends being "disguised" within the remaining terms, distorting their apparent significance and parameter estimates.

```
y ~ A + B + A:B + A:C + B:C
y ~ A + B + C + A:B + A:C + A:B:C
```

In contrast to those above, the models below are interpretable, even if not "full" models (not including all possible interactions).

```
y ~ A + B + C + A:B + A:C + B:C
y ~ (A + B + C)^2
y ~ A + B + C + B:C
y ~ A + B * C
```

Manipulation of model formulas. Because this is a book about the R language, it is pertinent to describe how formulas can be manipulated. Formulas, as any other R objects, can be saved in variables including lists. Why is this useful? For example, if we want to fit several different models to the same data, we can write a for loop that walks through a list of model formulas (see section 5.10 on page 160). Obviously, user-defined functions can accept formulas as arguments as Im() and other model fitting functions do. In addition, it is relatively simple for user code to programmatically create and edit R formulas, in the same way as functions update() and step() do under the hood.

To start with, as could be expected, a conversion constructor is available with name as.formula(). It is useful when formulas are input interactively by the user or read from text files. With as.formula() we can convert a character string into a formula.

```
as.formula("y ~ x") ## y ~ x
```

As there are many functions for the manipulation of character strings available

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in base R and through extension packages, it is easiest to build model formulas as strings. We can use functions like paste() to assemble a formula as text, and then use as.formula() to convert it to an object of class formula, usable for fitting a model.

```
paste("y", "x", sep = "~") |> as.formula()
## y ~ x
```

For the reverse operation of converting a formula into a string, we have available methods as.character() and format(). The first of these methods returns a character vector containing the components of the formula as individual strings, while format() returns a single character string with the formula formatted for printing.

```
as.character(y ~ x)
## [1] "~" "y" "x"
format(y ~ x)
## [1] "y ~ x"
```

This conversion makes it possible to edit a formula as a character string.

```
format(y \sim x) |> gsub("x", "x + z", x = _) |> as.formula() ## y \sim x + z
```

It is also possible to *edit* formula objects with method <code>update()</code>. In the replacement formula, a dot can replace either the left-hand side (lhs) or the right-hand side (rhs) of the existing formula in the replacement formula. We can also remove terms as can be seen below. In some cases the dot corresponding to the lhs can be omitted, but including it makes the syntax clearer.

```
my.formula <- y ~ x1 + x2
update(my.formula, . ~ . + x3)
## y ~ x1 + x2 + x3
update(my.formula, . ~ . - x1)
## y ~ x2
update(my.formula, . ~ x3)
## y ~ x3
update(my.formula, z ~ .)
## z ~ x1 + x2
update(my.formula, . + z ~ .)
## y + z ~ x1 + x2</pre>
```

As R provides high-level functions for model selection editing model formulas is not very frequently needed for model fitting.

A model matrix of dummy coefficients is used in the actual computations. This matrix can be derived from a model formula, a contrast name, and the data for the explanatory variables using function model.matrix().

#### 7.14 Time series

Longitudinal data consist of repeated measurements, usually done over time, on the same experimental units. Longitudinal data, when replicated on several experimental units at each time point, are called repeated measurements, while when not replicated, they are called time series. Base R provides special support for the analysis of time series data, while repeated measurements can be analyzed with nested linear models, mixed-effects models, and additive models.

Time series data are data collected in such a way that there is only one observation, possibly of multiple variables, available at each point in time. This brief section introduces only the most basic aspects of time-series analysis. In most cases time steps are of uniform duration and occur regularly, which simplifies data handling and storage. R not only provides methods for the analysis and manipulation of time-series, but also a specialized class for their storage, "ts". Regular time steps allow more compact storage—e.g., a ts object does not need to store time values for each observation but instead a combination of two of start time, step size and end time.

By now, you surely guessed that to create an object of class "ts" one needs to use a constructor called ts() or a conversion constructor called as.ts() and that you can look up the arguments they accept by consulting help using help(ts).

```
my.ts \leftarrow ts(1:10, start = 2019, deltat = 1/12)
```

The print() method for ts objects is special, and adjusts the printout according to the time step or deltat of the series.

The structure of the ts object is simple. Its mode is numeric but its class is ts. It is similar to a numeric vector with the addition of one attribute named tsp describing the time steps, as a numeric vector of length 3, giving start and end time and the size of the steps.

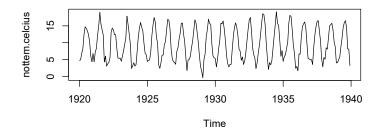
Data set nottem, included in R, contains meteorological data for Nottingham.

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The annual cycle of mean air temperatures (in degrees Fahrenheit) as well variation among years are clear when data are plotted.

Reexpression of the temperatures in the time-series from degrees Fahrenheit into degrees Celsius can be achieved as in numeric vectors using vectorized arithmetic and recycling.

```
nottem.celcius <- (nottem - 32) * 5 / 9
is.ts(nottem.celcius)
## [1] TRUE
plot(nottem.celcius)</pre>
```



7.19 Explore the structure of the nottem.celcius object (or the nottem object), and consider how and why it differs or not from that of the object my.ts that we created above. Similarly explore time series ausres, another of the data sets included in R.

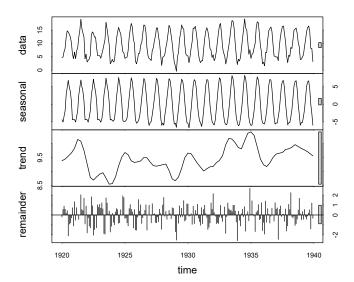
```
str(nottem.celcius)
attributes(nottem.celcius)
```

Many time series of observations display cyclic variation at different frequencies. Outdoors, air temperature varies cyclically between day and nigh and through the year. Superimposed on these regular cycles there can be faster random variation and long-term trends. One approach to the analysis of time series data is to estimate the separate contribution of these components.

An efficient approach to time series decomposition, based on LOESS (see section 7.12 on 221), is STL (Seasonal and Trend decomposition using Loess).

A seasonal window of 7 months, the minimum accepted, allows the extraction of the annual cycles and a long-term trend leaving as reminder unexplained variation. In the plot is important to be aware that the scale limits in the different panels are different, and re-set for each plot.

```
nottem.stl <- stl(nottem.celcius, s.window = 7)
plot(nottem.stl)</pre>
```



It is interesting to explore the class and structure of the object returned by stl(), as we may want to extract components. We can see that the structure of this object is rather similar to model-fit objects of classes lm and glm.

```
class(nottem.stl)
## [1] "stl"
str(nottem.stl, no.list = TRUE, give.attr = FALSE, vec.len = 2)
   $ time.series: Time-Series [1:240, 1:3] from 1920 to 1940: -4.4 -5.08 ...
               : num [1:240] 1 1 1 1 1 ...
   $ weights
                : language stl(x = nottem.celcius, s.window = 7)
   $ call
   $ win
                : Named num [1:3] 7 23 13
                 : Named int [1:3] 0 1 1
   $ deg
   $ jump
                : Named num [1:3] 1 3 2
                 : int 2
   $ inner
   $ outer
                 : int 0
```

As with other fit methods, method summary() is available. However, this method for class stl returns the stl object received as argument and displays a summary. In other words, it behaves similarly to print() methods with respect to the returned object, but produces a different printout than print() as its side effect.

```
summary(nottem.stl)
##
   call:
    stl(x = nottem.celcius, s.window = 7)
##
##
    Time.series components:
##
##
       seasonal
                             trend
                                               remainder
##
           :-6.693714
                        Min.
                                : 8.548340
                                             Min.
                                                    :-2.5950749
    1st Qu.:-4.413237
                        1st Qu.: 9.201837
                                             1st Qu.:-0.6907277
    Median :-0.650109
                        Median: 9.456694
                                             Median: 0.0593786
    Mean
          : 0.001867
                        Mean
                                : 9.462835
                                             Mean
                                                    : 0.0017326
##
    3rd Qu.: 4.595458
                        3rd Qu.: 9.779625
                                             3rd Qu.: 0.6445627
##
          : 8.215818
                        Max.
                                :10.424848
                                                    : 2.6914745
##
        STL.seasonal STL.trend STL.remainder data
##
```

```
##
        9.0087
                      0.5778
                                1.3353
                                               8.5833
##
      % 105.0
                        6.7
                                 15.6
                                               100.0
##
##
    Weights: all == 1
##
##
    Other components: List of 5
##
    $ win : Named num [1:3] 7 23 13
##
    $ deg
          : Named int [1:3] 0 1 1
##
    $ jump : Named num [1:3] 1 3 2
##
    $ inner: int 2
    $ outer: int 0
##
```

**7.20** Consult help(stl) and help(plot.stl) and create different plots and decompositions by passing different arguments to the formal parameters of these methods.

Method print() shows the different components. Extract the seasonal component and plot is on its own against time.

More advanced time-series analysis and forecasting methods are beyond the scope of this book, and mostly implemented in contributed packages. The text-book *Forecasting: principles and practice* (Hyndman and Athanasopoulos 2021) is comprehensive starting with an introduction to time series and continuing all the way to the description of modern forecasting methods, using R throughout.

# 7.15 Multivariate statistics

All the methods presented above are univariate, as even if in some cases we considered multiple explanatory variables on the rhs of model formulas, the lhs contained at most one response variable. There are many different multivariate methods available, and a few of them are implemented in base R functions. The current section does not describe these methods in depth, it only provides a few simple examples for some of the frequently used ones.

# 7.15.1 Multivariate analysis of variance

Multivariate methods take into account several response variables simultaneously, as part of a single analysis. In practice it is usual to use contributed packages for multivariate data analysis in R, except for simple cases. We will look first at *multivariate* ANOVA or MANOVA. In the same way as aov() is a wrapper that uses internally lm(), manova() is a wrapper that uses internally aov().

Multivariate model formulas in base R require the use of column binding (cbind()) on the left-hand side (lhs) of the model formula. For the next examples we use the well-known iris data set, containing size measurements for flowers of two species of *Iris*.

```
mmf2 <- manova(cbind(Petal.Length, Petal.Width) ~ Species, data = iris)
anova(mmf2)
## Analysis of Variance Table</pre>
```

class(pc)

```
##
               Df Pillai approx F num Df den Df
##
                                                   Pr(>F)
                1 0.98786
                           5939.2
                                     2
                                             146 < 2.2e-16 ***
## (Intercept)
## Species
                2 1.04645
                              80.7
                                       4
                                             294 < 2.2e-16 ***
## Residuals
              147
## --
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
summary(mmf2)
             Df Pillai approx F num Df den Df
## Species
             2 1.0465
                         80.661
                                          294 < 2.2e-16 ***
## Residuals 147
## Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

7.21 Modify the example above to use aov() instead of manova() and save the result to a variable named mmf3. Use class(), attributes(), names(), str() and extraction of members to explore objects mmf1, mmf2 and mmf3. Are they different?

# 7.15.2 Principal components analysis

Principal components analysis (PCA) is used to simplify a data set by combining variables with similar and "mirror" behavior into principal components. At a later stage, we frequently try to interpret these components in relation to known and/or assumed independent variables. Base R's function prcomp() computes the principal components and accepts additional arguments for centering and scaling.

By printing the returned object we can see the loadings of each variable in the principal components P1 to P4.

```
## [1] "prcomp"
pc
## Standard deviations (1, .., p=4):
## [1] 1.7083611 0.9560494 0.3830886 0.1439265
##
## Rotation (n x k) = (4 x 4):
## PC1 PC2 PC3
```

## Sepal.Length 0.5210659 -0.37741762 0.7195664 0.2612863
## Sepal.width -0.2693474 -0.92329566 -0.2443818 -0.1235096
## Petal.Length 0.5804131 -0.02449161 -0.1421264 -0.8014492
## Petal.width 0.5648565 -0.06694199 -0.6342727 0.5235971

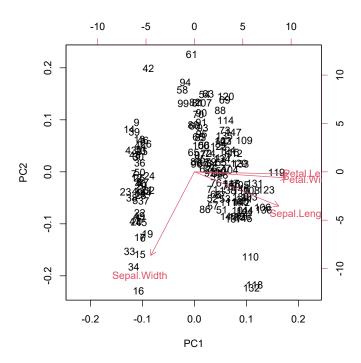
In the summary, the rows "Proportion of Variance" and "Cumulative Proportion" are most informative of the contribution of each principal component (PC) to explaining the variation among observations.

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## Cumulative Proportion 0.7296 0.9581 0.99482 1.00000

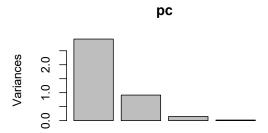
Method biplot() produces a plot with one principal component (PC) on each axis, plus arrows for the loadings.

biplot(pc)



Method plot() generates a bar plot of variances corresponding to the different components.

plot(pc)



Visually more elaborate plots of the principal components and their loadings can be obtained using package 'ggplot' described in chapter 9 on page 265. Package 'ggfortify' extends 'ggplot' so as to make it easy to plot principal components and their loadings.

7.22 For growth and morphological data, a log-transformation can be suitable given that variance is frequently proportional to the magnitude of the values measured. We leave as an exercise to repeat the above analysis using transformed values for the dimensions of petals and sepals. How much does the use of transformations change the outcome of the analysis?

**7.23** As for other fitted models, the object returned by function prcomp() is list-like with multiple components and belongs to a class of the same name as the function, not derived from class "list".

```
class(pc)
str(pc, max.level = 1)
```

# 7.15.3 Multidimensional scaling

The aim of multidimensional scaling (MDS) is to visualize in 2D space the similarity between pairs of observations. The values for the observed variable(s) are used to compute a measure of distance among pairs of observations. The nature of the data will influence what distance metric is most informative. For MDS we start with a matrix of distances among observations. We will use, for the example, distances in kilometers between geographic locations in Europe from data set eurodist.

```
loc <- cmdscale(eurodist)</pre>
```

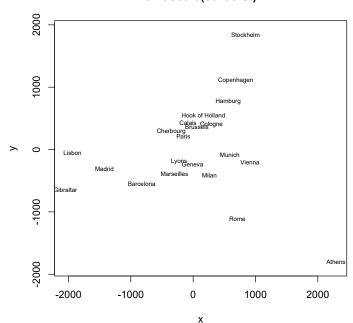
We can see that the returned object loc is a matrix, with names for one of the dimensions.

```
class(loc)
## [1] "matrix" "array"
dim(loc)
## [1] 21 2
dimnames(loc)
## [[1]]
##
    [1]
        "Athens"
                            "Barcelona"
                                               "Brussels"
                                                                  "Calais"
                            "Cologne"
                                                                  "Geneva"
        "Cherbourg"
                                               "Copenhagen"
##
    [5]
                                                                  "Lisbon"
        "Gibraltar"
                                               "Hook of Holland"
##
   [9]
                            "Hamburg"
                                                                  "Milan"
        "Lyons"
                            "Madrid"
                                               "Marseilles"
## [13]
        "Munich"
                            "Paris"
                                               "Rome"
                                                                  "Stockholm"
## [17]
## [21] "Vienna"
##
## [[2]]
## NULL
head(loc)
##
                    [,1]
              2290.27468 1798.8029
## Athens
## Barcelona -825.38279
                          546.8115
                59.18334 -367.0814
## Brussels
## Calais
               -82.84597 -429.9147
## Cherbourg -352.49943 -290.9084
               293.68963 -405.3119
## Cologne
```

To make the code easier to read, two vectors are first extracted from the matrix and named x and y. We force aspect to equality so that distances on both axes are comparable.

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#### cmdscale(eurodist)



7.24 Find data on the mean annual temperature, mean annual rainfall and mean number of sunny days at each of the locations in the eurodist data set. Next, compute suitable distance metrics, for example, using function dist. Finally, use MDS to visualize how similar the locations are with respect to each of the three variables. Devise a measure of distance that takes into account the three climate variables and use MDS to find how distant the different locations are.

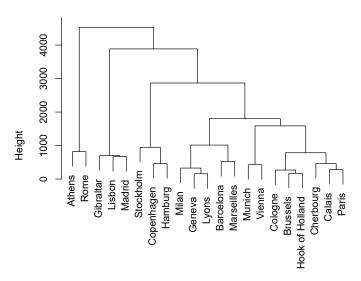
# 7.15.4 Cluster analysis

In cluster analysis, the aim is to group observations into discrete groups with maximal internal homogeneity and maximum group-to-group differences. In the next example we use function hclust() from the base-R package 'stats'. We use, as above, the eurodist data which directly provides distances. In other cases a matrix of distances between pairs of observations needs to be first calculated with function dist which supports several methods.

```
hc <- hclust(eurodist)
print(hc)
##
## Call:
## hclust(d = eurodist)
##</pre>
```

```
## Cluster method : complete
## Number of objects: 21
plot(hc)
```

### **Cluster Dendrogram**



eurodist hclust (\*, "complete")

We can use cutree() to limit the number of clusters by directly passing as an argument the desired number of clusters or the height at which to cut the tree.

```
cutree(hc, k = 5)
##
            Athens
                          Barcelona
                                             Brussels
                                                                Calais
                                                                              Cherbourg
##
                  1
                                   2
                                                     3
                                                                      3
                                                                                       3
##
           Cologne
                         Copenhagen
                                               Geneva
                                                             Gibraltar
                                                                                Hamburg
##
                  3
                                                     2
                                                                      5
                                                                                       4
## Hook of Holland
                              Lisbon
                                                Lyons
                                                                Madrid
                                                                             Marseilles
                                                                                       2
##
                  3
                                   5
                                                    2
                                                                      5
##
             Milan
                              Munich
                                                                              Stockholm
                                                Paris
                                                                  Rome
##
                  2
                                   3
                                                     3
                                                                      1
                                                                                       4
##
             Vienna
##
                   3
```

The object returned by hclust() contains details of the result of the clustering, which allows further manipulation and plotting.

```
str(hc)
## List of 7
                 : int [1:20, 1:2] -8 -3 -6 -4 -16 -17 -5 -7 -2 -12 ...
    $ merge
    $ height
                 : num [1:20] 158 172 269 280 328 428 460 460 521 668 ...
                 : int [1:21] 1 19 9 12 14 20 7 10 16 8 ...
   $ order
   $ labels
                 : chr [1:21] "Athens" "Barcelona" "Brussels" "Calais" ...
                 : chr "complete"
   $ method
                 : language hclust(d = eurodist)
    $ call
    $ dist.method: NULL
   - attr(*, "class")= chr "hclust"
```

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# 7.16 Further reading

R and its extension packages provide implementations of most known statistical methods. For some methods alternative implementations exist in different packages. The present chapter only attempts to shown how some of the most used implementations are used, as this knowledge is frequently taken for granted in specialized books, several of which I list here. Two recent text books on statistics, following a modern approach, and using R for examples, are OpenIntro Statistics (Diez et al. 2019) and Modern Statistics for Modern Biology (Holmes and Huber 2019). They differ in the subjects emphasized, with the second one focusing more on genetic and molecular biology. Three examples of books introducing statistical computations in R are Introductory Statistics with R (Dalgaard 2008), A Handbook of Statistical Analyses Using R (B. S. Everitt and Hothorn 2010) and A Beginner's Guide to R (Zuur et al. 2009). The book Biometry for Forestry and Environmental Data with Examples in R (Mehtätalo and Lappi 2020) presents both the statistical theory and code examples. The comprehensive *The R Book* (Crawley 2012) and the classic reference Modern Applied Statistics with S (Venables and Ripley 2002) both present statistical theory in parallel with the R code examples. More specific books are also available from which a few suggestions for further reading are An Introduction to Applied Multivariate Analysis with R (B. Everitt and Hothorn 2011), Linear Models with R (Faraway 2004), Extending the linear model with R: generalized linear, mixed effects and nonparametric regression models (Faraway 2006), Forecasting: principles and practice (Hyndman and Athanasopoulos 2021), An Introduction to Statistical Learning: with Applications in R (James et al. 2013), Mixed-Effects Models in S and S-Plus (Pinheiro and Bates 2000) and Generalized Additive Models (Wood 2017).

# R Extensions: Data Wrangling

Essentially everything in S[R], for instance, a call to a function, is an S[R] object. One viewpoint is that S[R] has self-knowledge. This self-awareness makes a lot of things possible in S[R] that are not in other languages.

Patrick J. Burns S Poetry, 1998

# 8.1 Aims of this chapter

Base R and the recommended extension packages (installed by default) include many functions for manipulating data. The R distribution supplies a complete set of functions and operators that allow all the usual data manipulation operations. These functions have stable and well-described behavior, so in my view they should be preferred unless some of their limitations justify the use of alternatives defined in contributed packages. In the present chapter I describe the new syntax introduced by the most popular contributed R extension packages aiming at changing (usually improving one aspect at the expense of another) in various ways how we can manipulate data in R. These independently developed packages extend the R language not only by adding new "words" to it but by supporting new ways of meaningfully connecting "words"—i.e., providing new "grammars" for data manipulation. While at the current stage of development of base R not breaking existing code has been the priority, several of the still "young" packages in the 'tidyverse' have prioritized experimentation with enhanced features over backwards compatibility. The development of 'tidyverse' packages seems to have emphasized users' convenience more than encouraging safe/error-free user code. The design of package 'data.table' has prioritized performance at the expense of easy of use. I do not describe in depth these new approaches but instead only briefly compare them to base R highlighting the most important differences.

### 8.2 Introduction

By reading previous chapters, you have already become familiar with base R classes, methods, functions and operators for storing and manipulating data. Most of these had been originally designed to perform optimally on rather small data sets (see Matloff 2011). The R implementation has been improved over the years significantly in performance, and random-access memory in computers has become cheaper, making constraints imposed by the original design of R less limiting. On the other hand, the size of data sets has also increased.

Some contributed packages have aimed at improving performance by relying on different compromises between usability, speed and reliability than used for base R. Package 'data.table' is the best example of an alternative implementation of data storage and manipulation that maximizes the speed of processing for large data sets using a new semantics and requiring a new syntax. We could say that package 'data.table' is based on a theoretical abstraction, or "grammar of data", that is different from that in the R language. The compromise in this case has been the use of a less intuitive syntax, and by defaulting to passing arguments by reference instead of by copy, increasing the "responsibility" of the programmer or data analyst with respect to not overwriting or corrupting data. This focus on performance has made obvious performance bottlenecks in base R which have been subsequently alleviated while maintaining backwards compatibility for users' code.

Another recent development is the 'tidyverse', which is a formidable effort to redefine how data analysis operations are expressed in R code and scripts. In many ways it is also a new abstraction, or "grammar of data". With respect to its implementation, it can also be seen as a new language built on-top of the R language. It is still young and evolving, and the developers from Posit still remain relentless about fixing what they consider earlier misguided decisions in the design of the packages comprising the 'tidyverse'. This is a wise decision for the future, but can be annoying to occasional users who may not be aware of the changes that have taken place between uses. As a user I highly value long-term stability and backwards compatibility of software. Older systems like base R provide this, but their long development history shows up as occasional inconsistencies and quirks. The 'tidyverse' as a paradigm is nowadays popular among data analysts while among users for whom data analysis is not the main focus, it is more common to make use of only individual packages as the need arises, e.g., using the new grammar only for some stages of the data analysis work flow.

When a computation included a chain of sequential operations, until R 4.1.0, using base R by itself we could either store the returned value in a temporary variable at each step in the computation, or nest multiple function calls. The first approach is verbose, but allows readable scripts, especially if the names used for temporary variables are wisely chosen. The second approach becomes very difficult too read as soon as there is more than one nesting level. Attempts to find an alternative syntax have borrowed the concept of data *pipes* from Unix shells (Kernigham and Plauger 1981). Interestingly, that it has been possible to write packages that define

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the operators needed to "add" this new syntax to R is a testimony to its flexibility and extensibility. Two packages, 'magrittr' and 'wrapr', define operators for pipebased syntax. In year 2021 a pipe operator was added to the R language itself and more recently its features enhanced.

In much of my work I emphasize reproducibility and reliability, preferring base R over extension packages, except for plotting, whenever practical. For run once and delete or quick-and-dirty data analyses I tend to use the *tidyverse*. However, with modern computers and some understanding of what are the performance bottlenecks in R code, I have rarely found it worthwhile the effort needed for improved performance by using extension packages. The benefit to effort balance will be different for those readers who analyze huge data sets.

The definition of the *tidyverse* is rather vague, as package 'tidyverse' loads and attaches a set of packages of which most but not all follow a consistent design and support this new grammar. In this chapter you will become familiar with packages 'tibble', 'dplyr' and 'tidyr'. Package 'ggplot2' will be described in chapter 9 as it implements the grammar of graphics and has little in common with other members of the 'tidyverse'. As many of the functions in the *tidyverse* can be substituted by existing base R functions, recognizing similarities and differences between them has become important since both approaches are now in common use, and frequently even coexist within R scripts.

In any design, there is a tension between opposing goals. In software for data analysis a key pair of opposed goals are usability, including concise but expressive code, and avoidance of ambiguity. Base R function subset() has an unusual syntax, as it evaluates the expression passed as the second argument within the namespace of the data frame passed as its first argument (see 4.4.5 on page 109). This saves typing, enhancing usability, at the expense of increasing the risk of bugs, as by reading the call to subset, it is not obvious which names are resolved in the environment of the call to subset() and which ones within its first argument—i.e., as column names in the data frame. In addition, changes elsewhere in a script can change how a call to subset is interpreted. In reality, subset is a wrapper function built on top of the extraction operator [ ] (see section 3.10 on page 64). It is a convenience function, mostly intended to be used at the console, rather than in scripts or package code. To extract columns or rows from a data frame it is always safer to use the [ , ] or [[ ]] operators at the expense of some verbosity.

Package 'dplyr', and much of the 'tidyverse', relies on a similar approach as subset to enhance convenience at the expense of ambiguity. Package 'dplyr' has undergone quite drastic changes during its development history with respect to how to handle the dilemma caused by "guessing" of the environment where names should be looked up. There is no easy answer; a simplified syntax leads to ambiguity, and a fully specified syntax is verbose. Recent versions of the package introduced a terse syntax to achieve a concise way of specifying where to look up names. I do appreciate the advantages of the grammar of data that is implemented in the 'tidyverse'. However, the actual implementation, can result in ambiguities and subtleties that are even more difficult to deal by inexperienced or occasional users than those caused by inconsistencies in base R. My opinion is that for code that needs to be highly reliable and produce reproducible results in the future,

we should for the time being prefer base R constructs. For code that is to be used once, or for which reproducibility can depend on the use of a specific (old or soon to become old) version of packages like 'dplyr', or which is not a burden to thoroughly test and update regularly, the conciseness and power of the new syntax can be an advantage.

Package 'poorman' re-implements many of the functions in 'dplyr' and a few from 'tidyr' using pure R code instead of compiled C++ code and with no dependencies on other extension packages. This light-weight approach can be useful when R's data frames rather than tibbles are preferred or when the possible enhanced performance with large data sets is not needed.

# 8.3 Packages used in this chapter

install.packages(learnrbook::pkgs\_ch\_data)

To run the examples included in this chapter, you need first to load and attach some packages from the library (see section 6.4 on page 178 for details on the use of packages).

library(learnrbook)
library(tibble)
library(magrittr)
library(wrapr)
library(stringr)
library(dplyr)
library(tidyr)
library(lubridate)

### 8.4 Replacements for data. frame

## 8.4.1 Package 'data.table'

The function call semantics of the R language is that arguments are passed to functions by copy. If the arguments are modified within the code of a function, these changes are local to the function. If implemented naively, this semantic would impose a huge toll on performance, however, R in most situations only makes a copy in memory if and when the value changes. Consequently, for modern versions of R which are very good at avoiding unnecessary copying of objects, the normal R semantics has only a moderate negative impact on performance. However, this impact can still be a problem as modification is detected at the object level, and consequently R may make copies of large objects such as a whole data frame when only values in a single column or even just an attribute have changed.

Functions and methods from package 'data.table' pass arguments by reference, avoiding making any copies. However, any assignments within these functions and

methods modify the variables passed as arguments. This simplifies the needed tests for delayed copying and also by avoiding the need to make a copy of arguments, achieves the best possible performance. This is a specialized package but extremely useful when dealing with very large data sets. Writing user code, such as scripts, with 'data.table' requires a good understanding of the pass-by-reference semantics. Obviously, package 'data.table' makes no attempt at backwards compatibility with base-R data.frame.

In contrast to the design of package 'data.table', the focus of the 'tidyverse' is not only performance. The design of this grammar has also considered usability. Design compromises have been resolved differently than in base R or 'data.table' and in some cases code written using base R can significantly outperform the 'tidyverse' and vice versa. There exist packages that implement a translation layer from the syntax of the 'tidyverse' into that of 'data.table' or relational database queries.

### 8.4.2 Package 'tibble'

The authors of package 'tibble' describe their tbl class as nearly backwards compatible with data.frame and make it a derived class. This backwards compatibility is only partial so in some situations data frames and tibbles are not equivalent.

The class and methods that package 'tibble' defines lift some of the restrictions imposed by the design of base R data frames at the cost of creating some incompatibilities due to changed (improved) syntax for member extraction. Tibbles simplify the creation of "columns" of class list and remove support for columns of class matrix. Handling of attributes is also different, with no row names added by default. There are also differences in default behavior of both constructors and methods.

Although, objects of class tb1 can be passed as arguments to functions that expect data frames as input, these functions are not guaranteed to work correctly with tibbles as a result of the differences in syntax of some methods.

It is easy to write code that will work correctly both with data frames and tibbles by avoiding constructs that behave differently. However, code that is syntactically correct according to the R language may fail to work as expected if a tibble is used in place of a data frame. Only functions tested to work correctly with both tibbles and data frames can be relied upon as compatible.

Being newer and not part of the R language, the packages in the 'tidyverse' are evolving fast with rather frequent changes that require edits to the code of scripts and packages that use them. For example, whether attributes set in tibbles by users are copied or not to returned values has changed with updates.

That it has been possible to define tibbles as objects of a class derived from data.frame reveals one of the drawbacks of the simple implementation of S3 object classes in R. Allowing this is problematic because the promise of compatibility implicit in a derived class is not always fulfilled. An independently developed method designed for data frames will not necessarily work correctly with tibbles,

but in the absence of a specialized method for tibbles it will be used (dispatched) when the generic method is called with a tibble as argument.

One should be aware that although the constructor tibble() and conversion function as\_tibble(), as well as the test is\_tibble() use the name tibble, the class attribute is named tbl. This is inconsistent with base R conventions, as it is the use of an underscore instead of a dot in the name of these methods.

```
my.tb <- tibble(numbers = 1:3)
is_tibble(my.tb)
## [1] TRUE
inherits(my.tb, "tibble")
## [1] FALSE
class(my.tb)
## [1] "tbl_df" "tbl" "data.frame"</pre>
```

Furthermore, to support tibbles based on different underlying data sources such as data.table objects or databases, a further derived class is needed. In our example, as our tibble has an underlying data.frame class, the most derived class of my.tb is tbl\_df.

We define a function that concisely reports the class of the object passed as argument and of its members (*apply* functions are described in section 5.8 on page 154).

The tibble() constructor by default does not convert character data into factors, while the data.frame() constructor did before R version 4.0.0. The default can be overridden through an argument passed to these constructors, and in the case of data.frame() also by setting an R option. This new behaviour extends to function read.table() and its wrappers (see section 10.6 on page 372).

```
my.df <- data.frame(codes = c("A", "B", "C"), numbers = 1:3, integers = 1L:3L)
is.data.frame(my.df)
## [1] TRUE
is_tibble(my.df)
## [1] FALSE
show_classes(my.df)
## data.frame containing:
## codes: character, numbers: integer, integers: integer</pre>
```

Tibbles are, or pretend to be (see above), data frames—or more formally class tibble is derived from class data.frame. However, data frames are not tibbles.

```
my.tb <- tibble(codes = c("A", "B", "C"), numbers = 1:3, integers = 1L:3L)
is.data.frame(my.tb)
## [1] TRUE</pre>
```

```
is_tibble(my.tb)
## [1] TRUE
show_classes(my.tb)
## tbl_df containing:
## codes: character, numbers: integer, integers: integer
```

The print() method for tibbles differs from that for data frames in that it outputs a header with the text "A tibble:" followed by the dimensions (number of rows × number of columns), adds under each column name an abbreviation of its class and instead of printing all rows and columns, a limited number of them are displayed. In addition, individual values are formatted more compactly and using color to highlight, for example, negative numbers in red.

```
print(my.df)
     codes numbers integers
## 1
                  1
                  2
                            2
## 2
         В
## 3
         C
                  3
                            3
print(my.tb)
## # A tibble: 3 x 3
     codes numbers integers
     <chr>
              <int>
## 1 A
                  1
                            1
## 2 B
                  2
                            2
## 3 C
                  3
                            3
```

The default number of rows printed depends on R option tibble.print\_max that can be set with a call to options(). This option plays for tibbles a similar role as option max.print plays for base R print() methods.

```
options(tibble.print_max = 3, tibble.print_min = 3)
```

8.1 Print methods for tibbles and data frames differ in their behaviour when not all columns fit in a printed line. 1) Construct a data frame and an equivalent tibble with at least 50 rows and then test how the output looks when they are printed. 2) Construct a data frame and an equivalent tibble with more columns than will fit in the width of the R console and then test how the output looks when they are printed.

Data frames can be converted into tibbles with as\_tibble().

```
my_conv.tb <- as_tibble(my.df)
is.data.frame(my_conv.tb)
## [1] TRUE
is_tibble(my_conv.tb)
## [1] TRUE
show_classes(my_conv.tb)
## tbl_df containing:
## codes: character, numbers: integer, integers: integer

Tibbles can be converted into "real" data.frames with as.data.frame().
my_conv.df <- as.data.frame(my.tb)
is.data.frame(my_conv.df)
## [1] TRUE
is_tibble(my_conv.df)</pre>
```

```
## [1] FALSE
show_classes(my_conv.df)
## data.frame containing:
## codes: character, numbers: integer, integers: integer
```

P Not all conversion functions work consistently when converting from a derived class into its parent. The reason for this is disagreement between authors on what the *correct* behavior is based on logic and theory. You are not likely to be hit by this problem frequently, but it can be difficult to diagnose.

We have already seen that calling as.data.frame() on a tibble strips the derived class attributes, returning a data frame. We will look at the whole character vector stored in the "class" attribute to demonstrate the difference. We also test the two objects for equality, in two different ways. Using the operator == tests for equivalent objects. Objects that contain the same data. Using identical() tests that objects are exactly the same, including attributes such as "class", which we retrieve using class().

```
class(my.tb)
## [1] "tbl_df"
                    "tb1"
                                  "data.frame"
class(my_conv.df)
## [1] "data.frame"
my.tb == my_conv.df
        codes numbers integers
## [1,] TRUE
                 TRUE
## [2,] TRUE
                 TRUE
                          TRUE
## [3,] TRUE
                 TRUE
                          TRUE
identical(my.tb, my_conv.df)
## [1] FALSE
```

Now we derive from a tibble, and then attempt a conversion back into a tibble.

```
my.xtb <- my.tb
class(my.xtb) <- c("xtb", class(my.xtb))</pre>
class(my.xtb)
                                   "tb1"
## [1] "xtb"
                     "tbl df"
                                                 "data.frame"
my_conv_x.tb <- as_tibble(my.xtb)</pre>
class(my_conv_x.tb)
## [1] "tbl_df"
                     "tb1"
                                   "data.frame"
my.xtb == my_conv_x.tb
        codes numbers integers
## [1,]
        TRUE
                  TRUE
## [2,]
        TRUE
                  TRUE
## [3,] TRUE
                  TRUE
                           TRUE
identical(my.xtb, my_conv_x.tb)
## [1] FALSE
```

The two viewpoints on conversion functions are as follows. 1) The conversion function should return an object of its corresponding class, even if the argument is an object of a derived class, stripping the derived class. 2) If the object is of the class to be converted to, including objects of derived classes, then it should remain untouched. Base R follows, as far as I have been able to work out, approach 1). Some packages in the 'tidyverse' sometimes follow, or have followed in the past,

approach 2). If in doubt about the behavior of some function, then you will need to do a test similar to the one used in this box.

As tibbles have been defined as a class derived from data.frame, if methods have not been explicitly defined for tibbles, the methods defined for data frames are called, and these are likely to return a data frame rather than a tibble. Even a frequent operation like column binding is affected, at least at the time of writing.

```
class(my.df)
## [1] "data.frame"
class(my.tb)
## [1] "tbl_df"
                    "tb1"
                                  "data.frame"
class(cbind(my.df, my.tb))
## [1] "data.frame"
class(cbind(my.tb, my.df))
## [1] "data.frame"
class(cbind(my.df, added = -3:-1))
## [1] "data.frame"
class(cbind(my.tb, added = -3:-1))
## [1] "data.frame"
identical(cbind(my.tb, added = -3:-1), cbind(my.df, added = -3:-1))
## [1] TRUE
```

There are additional important differences between the constructors tibble() and data.frame(). One of them is that in a call to tibble(), member variables ("columns") being defined can be used in the definition of subsequent member variables.

```
tibble(a = 1:5, b = 5:1, c = a + b, d = letters[a + 1])
## # A tibble: 5 x 4
##
                     c d
        a
               h
##
    <int> <int> <int> <chr>
## 1
        1
               5
                     6 b
## 2
         2
               4
                     6 c
## 3
        3
               3
## # i 2 more rows
```

**8.2** What is the behavior if you replace tibble() by data.frame() in the statement above?

While objects passed directly as arguments to the data.frame() constructor to be included as "columns" can be factors, vectors or matrices (with the same number of rows as the data frame), arguments passed to the tibble() constructor can be factors, vectors or lists (with the same number of members as rows in the tibble). As we saw in section 4.4 on page 94, base R's data frames can contain columns of classes list and matrix. The difference is in the need to use I(), the identity function, to protect these variables during construction and assignment to true data.frame objects as otherwise list members and matrix columns will be assigned to multiple individual columns in the data frame.

```
tibble(a = 1:5, b = 5:1, c = list("a", 2, 3, 4, 5))
## # A tibble: 5 x 3
##
         a
               h c
##
     <int> <int> <ist>
## 1
        1
               5 <chr [1]>
## 2
         2
               4 <dbl [1]>
         3
               3 <dbl [1]>
## # i 2 more rows
   A list of lists or a list of vectors can be directly passed to the constructor.
tibble(a = 1:5, b = 5:1, c = list("a", 1:2, 0:3, letters[1:3], letters[3:1]))
## # A tibble: 5 x 3
         a
               b c
     <int> <int> <liist>
##
## 1
        1
               5 <chr [1]>
## 2
         2
               4 <int [2]>
## 3
        3
               3 <int [4]>
## # i 2 more rows
```

# 8.5 Data pipes

The first obvious difference between scripts using 'tidyverse' packages is the frequent use of *pipes*. This is, however, mostly a question of preferences, as pipes can be as well used with base R functions. In addition, since version 4.0.0, R has a native pipe operator |>, described in section 5.5 on page 134. Here we describe other earlier implementations of pipes, and the differences among these and R's pipe operator.

### 8.5.1 'magrittr'

A set of operators for constructing pipes of R functions is implemented in package 'magrittr'. It preceded the native R pipe by several years. The pipe operator defined in package 'magrittr', %>%, is imported and re-exported by package 'dplyr', which in turn defines functions that work well in data pipes.

Operator %>% plays a similar role as R's |>.

```
data.in <- 1:10
data.in %>% sqrt() %>% sum() -> data0.out
```

The value passed can be made explicit using a dot as placeholder passed as an argument by name and by position to the function on the *rhs* of the %>% operator. Thus . in 'magrittr' plays a similar but not identical role as \_ in base R pipes.

```
data.in %>% sqrt(x = .) %>% sum(.) -> data1.out
all.equal(data0.out, data1.out)
## [1] TRUE
```

R's native pipe operator requires, consistently with R in all other situations, that functions that are to be evaluated use the parenthesis syntax, while 'magrittr'

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allows the parentheses to be missing when the piped argument is the only one passed to the function call on *rhs*.

```
data.in %>% sqrt %>% sum -> data5.out
all.equal(data0.out, data5.out)
## [1] TRUE
```

Package 'magrittr' provides additional pipe operators, such as "tee" (%T>%) to create a branch in the pipe, and %<>% to apply the pipe by reference. These operators are much less frequently used than %>%.

### 8.5.2 'wrapr'

The %.>%, or "dot-pipe", operator from package 'wrapr', allows expressions both on the rhs and lhs, and *enforces the use of the dot* (.), as placeholder for the piped object. Given the popularity of 'dplyr' the pipe operator from 'magrittr' has been the most used.

Rewritten using the dot-pipe operator, the pipe in the previous chunk becomes

```
data.in %.>% sqrt(.) %.>% sum(.) -> data2.out
all.equal(data0.out, data2.out)
## [1] TRUE
```

However, as operator %>% from 'magrittr' recognizes the . placeholder without enforcing its use, the code below where %.>% is replaced by %>% returns the same value as that above.

```
data.in %>% sqrt(.) %>% sum(.) -> data3.out
all.equal(data0.out, data3.out)
## [1] TRUE
```

To use operator |> from R, we need to edit the code using (\_) as placeholder and passing it as argument to parameters by name in the function calls on the *rhs*.

```
data.in |> sqrt(x = _) |> sum(x = _) -> data4.out
all.equal(data0.out, data4.out)
## [1] TRUE
```

We can, in this case, simply use no placeholder, and pass the arguments by position to the first parameter of the functions.

```
data.in |> sqrt() |> sum() -> data4.out
all.equal(data0.out, data4.out)
## [1] TRUE
```

The dot-pipe operator %.>% from 'wrapr' allows us to use the placeholder . in expressions on the *rhs* of operators in addition to in function calls.

```
data.in %.>% (.^2) -> data7.out
```

In contrast, operators |> and %>% do not support expressions, only function call syntax on their *rhs*, forcing us to call operators with parenthesis syntax and named arguments

```
data.in |> `^`(e1 = _, e2 = 2) -> data8.out
all.equal(data7.out, data8.out)
## [1] TRUE
```

```
data.in %>% `^`(e1 = ., e2 = 2) -> data9.out
all.equal(data7.out, data9.out)
## [1] TRUE
```

In conclusion, R syntax for expressions is preserved when using the dot-pipe operator from 'wrapr', with the only caveat that because of the higher precedence of the %.>% operator, we need to "protect" bare expressions containing other operators by enclosing them in parentheses. In the examples above we showed a simple expression so that it could be easily converted into a function call. The %.>% operator supports also more complex expressions, even with multiple uses of the placeholder.

```
data.in %.>% (.^2 + sqrt(. + 1))
## [1] 2.414214 5.732051 11.000000 18.236068 27.449490 38.645751
## [7] 51.828427 67.000000 84.162278 103.316625
```

### 8.5.3 Comparing pipes

Under-the-hood, the implementations of operators |> and %>% and %.>% are different, with |> expected to have the best performance, followed by %.>% and %>% being slowest. As implementations evolve, performance may vary among versions. However, |> being part of R is likely to remain the fastest.

Being part of the R language, |> will remain available and most likely also backwards compatible, while packages could be abandoned or redesigned by their maintainers. For this reason, it is preferable to use the |> in scripts or code expected to be reused, unless compatibility with R versions earlier than 4.2.0 is needed.

In the rest of the book when possible I will use R's pipes and use in examples the \_ placeholder to facilitate understanding. In most cases the examples can be easily rewritten using operator %>%.

Pipes can be used with any R function, but how elegant can be their use depends on the order of formal parameters. This is especially the case when passing arguments implicitly to the first parameter of the function on the *rhs*. Several of the functions and methods defined in 'tidyr', 'dplyr', and a few other packages from the 'tidyverse' fit this need.

Writing a series of statements and saving intermediate results in temporary variables makes debugging easiest. Debugging pipes is not as easy, as this usually requires splitting them, with one approach being the insertion of calls to print(). This is possible, because print() returns its input invisibly in addition to displaying it.

```
data.in |> print() |> sqrt() |> print() |> sum() |> print() -> data10.out
## [1] 1 2 3 4 5 6 7 8 9 10
## [1] 1.000000 1.414214 1.732051 2.000000 2.236068 2.449490 2.645751 2.828427
## [9] 3.000000 3.162278
## [1] 22.46828
data10.out
## [1] 22.46828
```

Debugging nested function calls is the most difficult as well as code using such

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calls is difficult to read. So, in general, it is good to use pipes instead of nested function calls. However, it is best to avoid very long pipes. Normally while writing scripts or analysing data it is important to check the correctness of intermediate results, so saving them to variables can save time and effort.

The design of R's native pipes has benefited from the experience gathered by earlier implementations and being now part the language, we can expect it to become the reference one once its implementation is stable. The designers of the three implementations have to some extent disagreed in their design decisions. Consequently, some differences are more than aesthetic. R pipes are simpler, easier to use and expected to be fastest. Those from 'magrittr' are the most feature rich, but not as safe to use, and purportedly given a more complex implementation, the slowest. Package 'wrapr' is an attempt to enhance pipes compared to 'magrittr' focusing in syntactic simplicity and performance. R's |> operator has been enhanced since its addition in R only two years ago. These enhancements have all been backwards compatible.

The syntax of operators  $|\cdot|$  and %>% is not identical. With R's  $|\cdot|$  (as of R 4.3.0) the placeholder \_ can be only passed to parameters by name, while with 'magrittr's %>% the placeholder . can be used to pass arguments both by name and by position. With operator %.>% the use of the placeholder . is mandatory, and it can be passed by name or by position to the function call on the rhs. Other differences are deeper like those related to the use in the rhs of the extraction operator or support or not for expressions that are not explicit function calls.

In the case of R, the pipe is conceptually a substitution with no alteration of the syntax or evaluation order. This avoids *surprising* the user and simplifies implementation. In other words, R pipes are an alternative way of writing nested function calls. Quoting R documentation:

Currently, pipe operations are implemented as syntax transformations. So an expression written as  $x \mid > f(y)$  is parsed as f(x, y). It is worth emphasizing that while the code in a pipeline is written sequentially, regular R semantics for evaluation apply and so piped expressions will be evaluated only when first used in the rhs expression.

While frequently the different pipe operators can substitute for each other by adjusting the syntax, in some cases the differences among them in the order and timing of evaluation of the terms needs to be taken into account.

In some situations operator %>% from package 'magrittr' can behave unexpectedly. One example is the use of assign() in a pipe. With R's operator |> assignment takes place as expected.

```
data.in |> assign(x = "data6.out", value = _)
all.equal(data.in, data6.out)
## [1] TRUE
```

Named arguments are also supported with the dot-pipe operator from 'wrapr'.

```
data.in %.>% assign(x = "data7.out", value = .)
all.equal(data.in, data7.out)
## [1] TRUE
```

However, the pipe operator (%>%) from package 'magrittr' silently and unexpectedly fails to assign the value to the name.

```
data.in %>% assign(x = "data8.out", value = .)
if (exists("data8.out")) {
   all.equal(data.in, data8.out)
} else {
   print("'data8.out' not found!")
}
## [1] "'data8.out' not found!"
```

Although there are usually alternatives to get the computations done correctly, unexpected silent behaviour is not easy to deal with.

# 8.6 Reshaping with 'tidyr'

Data stored in table-like formats can be arranged in different ways. In base R most model fitting functions and the plot() method using (model) formulas and when accepting data frames, expect data to be arranged in "long form" so that each row in a data frame corresponds to a single observation (or measurement) event on a subject. Each column corresponds to a different measured feature, or ancillary information like the time of measurement, or a factor describing a classification of subjects according to treatments or features of the experimental design (e.g., blocks). Covariates measured on the same subject at an earlier point in time may also be stored in a column. Data arranged in *long form* has been nicknamed as "tidy" and this is reflected in the name given to the 'tidyverse' suite of packages. However, this longitudinal arrangement of data has been the R and S preferred format since their inception. Data in which columns correspond to measurement events is described as being in a *wide form*.

Although long-form data is and has been the most commonly used arrangement of data in R, manipulation of such data has not always been possible with concise R statements. The packages in the 'tidyverse' provide convenience functions to simplify coding of data manipulation, which in some cases, have, in addition, improved performance compared to base R—i.e., it is possible to code the same operations using only base R, but this may require more and/or more verbose statements.

Real-world data is rather frequently stored in wide format or even ad hoc formats, so in many cases the first task in data analysis is to reshape the data. Package 'tidyr' provides functions for reshaping data from wide to long form and *vice versa*.

Package 'tidyr' replaced 'reshape2' which in turn replaced 'reshape', while additionally the functions implemented in 'tidyr' have been replaced by new ones with different syntax and name. So, using these functions although convenient, has over a period of several years made necessary to revise or rewrite scripts and relearn how to carry out these operations. If one is a data analyst and uses these functions every day, then the cost involved is frequently tolerable or even desirable given the improvements. However, if as is the case with many users of R in applied fields, to whom this book is targeted, in the long run using stable features from

base R is preferable. This does not detract from the advantages of using a clear workflow as emphasized by the proponents of the *tidyverse*.

We use in examples below the iris data set included in base R. Some operations on R data.frame objects with 'tidyverse' packages will return data.frame objects while others will return tibbles—i.e., "tb" objects. Consequently it is safer to first convert into tibbles the data frames we will work with.

```
iris.tb <- as_tibble(iris)</pre>
```

Function pivot\_longer() from 'tidyr' converts data from wide form into long form (or "tidy"). We use it here to obtain a long-form tibble. By comparing iris.tb with long\_iris.tb we can appreciate how pivot\_longer() reshaped its input.

```
long_iris.tb <-</pre>
  pivot_longer(iris.tb,
               cols = -Species,
               names_to = "part"
               values_to = "dimension")
long_iris.tb
## # A tibble: 600 x 3
                           dimension
    Species part
##
    <fct>
             <chr>
                               <dbl>
## 1 setosa Sepal.Length
                                 5.1
## 2 setosa Sepal.Width
                                 3.5
## 3 setosa Petal.Length
## # i 597 more rows
```

Differently to base R, in most functions from the 'tidyverse' packages we can use bare column names preceded by a minus sign to signify "all other columns".

Function pivot\_wider() does not directly implement the exact inverse operation of pivot\_longer(). With multiple rows with shared codes, i.e., replication, in our case within each species and flower part, the returned tibble has columns that are lists of vectors. We need to expand these columns with function unnest() in a second step.

```
wide_iris.tb <-
  pivot_wider(long_iris.tb,
              names_from = "part",
              values_from = "dimension",
              values_fn = list) |>
  unnest(cols = -Species)
wide_iris.tb
## # A tibble: 150 x 5
     Species Sepal.Length Sepal.Width Petal.Length Petal.Width
##
     <fct>
                    <dbl>
                                <fdb>>
                                             <dbl>
                                                          <fdb>>
                                  3.5
## 1 setosa
                      5.1
                                               1.4
                                                            0.2
                      4.9
                                  3
                                                            0.2
## 2 setosa
                                               1.4
                      4.7
                                  3.2
                                                1.3
                                                            0.2
## 3 setosa
## # i 147 more rows
```

8.3 Is wide\_iris.tb equal to iris.tb, the tibble we converted into long shape and back into wide shape? Run the comparisons below, and print the tibbles to find out.

```
identical(iris.tb, wide_iris.tb)
all.equal(iris.tb, wide_iris.tb)
all.equal(iris.tb, wide_iris.tb[, colnames(iris.tb)])
```

What has changed? Would it matter if our code used indexing with a numeric vector to extract columns? or if it used column names as character strings?

Starting from version 1.0.0 of 'tidyr', functions gather() and spread() are deprecated and replaced by functions pivot\_longer() and pivot\_wider(). These new functions, described above, use a different syntax than the old ones.

8.4 Functions pivot\_longer() and pivot\_wider() from package 'poorman' attempt to replicate the behaviour of the same name functions from package 'tidyr'. In some edge cases, the behaviour differs. Test if the two code chunks above return identical or equal values when poorman:: is prepended to the names of these two functions. First, ensure than package 'poorman' is installed, then run the code below.

```
poor_long_iris.tb <-
  poorman::pivot_longer(
    iris,
    cols = -Species,
    names_to = "part",
    values_to = "dimension")
identical(long_iris.tb, poor_long_iris.tb)
all.equal(long_iris.tb, poor_long_iris.tb)
class(long_iris.tb)
class(poor_long_iris.tb)</pre>
```

What is the difference between the values returned by the two functions? Could switching from package 'tidyr' to package 'poorman' affect code downstream of pivoting?

# 8.7 Data manipulation with 'dplyr'

The first advantage a user of the 'dplyr' functions and methods sees is the completeness of the set of operations supported and the symmetry and consistency among the different functions. A second advantage is that almost all the functions are defined not only for objects of class tibble, but also for objects of class data.table (package 'dtplyr') and for SQL databases (package 'dbplyr'), with consistent syntax (see also section 10.14 on page 400). A downside of 'dplyr' and much of the 'tidyverse' is that the syntax is not yet fully stable. Additionally, some function and method names either override those in base R or clash with names used in other packages. R itself is extremely stable and expected to remain forward and backward compatible for a long time. For code intended to remain in use for years, the fewer packages it depends on, the less maintenance it will need. When using the 'tidyverse' we need to be prepared to revise our own dependent code after any major revision to the 'tidyverse' packages we use.

## 8.7.1 Row-wise manipulations

Assuming that the data is stored in long form, row-wise operations are operations combining values from the same observation event—i.e., calculations within a single row of a data frame or tibble. Using functions mutate() and transmute() we can obtain derived quantities by combining different variables, or variables and constants, or applying a mathematical transformation. We add new variables (columns) retaining existing ones using mutate() or we assemble a new tibble containing only the columns we explicitly specify using transmute().

Different from usual R syntax, with tibble(), mutate() and transmute() we can use values passed as arguments, in the statements computing the values passed as later arguments. In many cases, this allows more concise and easier to understand code.

```
tibble(a = 1:5, b = 2 * a)
## # A tibble: 5 x 2
##
         a
               b
##
     <int> <dbl>
               2
## 1
         1
## 2
         2
               4
## 3
         3
               6
## # i 2 more rows
```

Continuing with the example from the previous section, we most likely would like to split the values in variable part into plant\_part and part\_dim. We use mutate() from 'dplyr' and str\_extract() from 'stringr'. We use regular expressions (see page ??) as arguments passed to pattern. We do not show it here, but mutate() can be used with variables of any mode, and calculations can involve values from several columns. It is even possible to operate on values applying a lag or, in other words, using rows displaced relative to the current one.

```
long_iris.tb %.>%
 mutate(.,
         plant_part = str_extract(part, "^[:alpha:]*"),
        part_dim = str_extract(part, "[:alpha:]*$")) -> long_iris.tb
long_iris.tb
## # A tibble: 600 x 5
    Species part
                          dimension plant_part part_dim
    <fct>
            <chr>
                              <dbl> <chr>
                                               <chr>
## 1 setosa Sepal.Length
                                5.1 Sepal
                                               Length
## 2 setosa Sepal.Width
                                3.5 Sepal
                                               Width
## 3 setosa Petal.Length
                                1.4 Petal
                                               Length
## # i 597 more rows
```

In the next few chunks, we print the returned values rather than saving them in variables. In normal use, one would combine these functions into a pipe using operator %.>% (see section 8.5 on page 250).

Function arrange() is used for sorting the rows—makes sorting a data frame or tibble simpler than by using sort() and order(). Here we sort the tibble long\_iris.tb based on the values in three of its columns.

Function filter() can be used to extract a subset of rows—similar to subset() but with a syntax consistent with that of other functions in the 'tidyverse'. In this case, 300 out of the original 600 rows are retained.

```
filter(long_iris.tb, plant_part == "Petal")
## # A tibble: 300 x 5
     Species part
                          dimension plant_part part_dim
##
     <fct>
             <chr>
                              <dbl> <chr>
                                                <chr>
             Petal.Length
                                1.4 Petal
                                                Length
## 1 setosa
             Petal.Width
                                0.2 Petal
                                                Width
## 2 setosa
## 3 setosa Petal.Length
                                1.4 Petal
                                                Length
## # i 297 more rows
```

Function slice() can be used to extract a subset of rows based on their positions—an operation that in base R would use positional (numeric) indexes with the [ , ] operator: long\_iris.tb[1:5, ].

```
slice(long_iris.tb, 1:5)
## # A tibble: 5 x 5
##
     Species part
                          dimension plant_part part_dim
##
     <fct>
             <chr>
                              <dbl> <chr>
                                                <chr>
## 1 setosa Sepal.Length
                                5.1 Sepal
                                                Length
## 2 setosa
            Sepal.Width
                                 3.5 Sepal
                                                width
                                1.4 Petal
## 3 setosa Petal.Length
                                                Length
## # i 2 more rows
```

Function select() can be used to extract a subset of columns-this would be done with positional (numeric) indexes with [ , ] in base R, passing them to the second argument as numeric indexes or column names in a vector. Negative indexes in base R can only be numeric, while select() accepts bare column names prepended with a minus for exclusion.

```
select(long_iris.tb, -part)
## # A tibble: 600 x 4
##
    Species dimension plant_part part_dim
##
     <fct>
                 <db1> <chr>
                                   <chr>
                   5.1 Sepal
                                   Length
## 1 setosa
## 2 setosa
                   3.5 Sepal
                                   width
## 3 setosa
                   1.4 Petal
                                   Length
## # i 597 more rows
```

In addition, select() as other functions in 'dplyr' accept "selectors" returned by functions starts\_with(), ends\_with(), contains(), and matches() to extract or retain columns. For this example we use the "wide"-shaped iris.tb instead of long\_iris.tb.

```
select(iris.tb, Species, matches("pal"))
## # A tibble: 150 x 3
     Species Sepal.Length Sepal.Width
##
     <fct>
                    <dbl>
                                 <dbl>
                                   3.5
## 1 setosa
                      5.1
## 2 setosa
                      4.9
                                   3
## 3 setosa
                      4.7
                                   3.2
## # i 147 more rows
```

Function rename() can be used to rename columns, whereas base R requires the use of both names() and names() - and *ad hoc* code to match new and old names. As shown below, the syntax for each column name to be changed is <new name> = <old name>. The two names can be given either as bare names as below or as character strings.

```
rename(long_iris.tb, dim = dimension)
## # A tibble: 600 x 5
##
    Species part
                            dim plant_part part_dim
##
     <fct>
            <chr>
                          <dbl> <chr>
                                           <chr>
## 1 setosa Sepal.Length 5.1 Sepal
                                           Length
## 2 setosa Sepal.Width
                           3.5 Sepal
                                           Width
## 3 setosa Petal.Length
                          1.4 Petal
                                           Length
## # i 597 more rows
```

## 8.7.2 Group-wise manipulations

Another important operation is to summarize quantities by groups of rows. Contrary to base R, the grammar of data manipulation as implemented in 'dplyr', makes it possible to split this operation into two steps: the setting of the grouping, and the calculation of summaries. This simplifies the code, making it more easily understandable when using pipes compared to the approach of base R aggregate(), and it also makes it easier to summarize several columns in a single operation.

The first step is to use <code>group\_by()</code> to "tag" a tibble with the grouping. We create a *tibble* and then convert it into a *grouped tibble*. Once we have a grouped tibble, function <code>summarise()</code> will recognize the grouping and use it when the summary values are calculated.

```
tibble(numbers = 1:9, letters = rep(letters[1:3], 3)) %.>%
  group_by(., letters) %.>%
  summarise(...
           mean_numbers = mean(numbers),
           median_numbers = median(numbers),
            n = n()
## # A tibble: 3 x 4
    letters mean_numbers median_numbers
                   <dbl>
##
    <chr>
                          <int> <int>
## 1 a
                        4
                                      4
                                             3
                        5
                                       5
## 2 b
## 3 c
```

How is grouping implemented for data frames and tibbles? In our case as our tibble belongs to class tibble\_df, grouping adds grouped\_df as the most derived class. It also adds several attributes with the grouping information in a format

suitable for fast selection of group members. To demonstrate this, we need to make an exception to our recommendation above and save a grouped tibble to a variable.

```
my.tb <- tibble(numbers = 1:9, letters = rep(letters[1:3], 3))</pre>
is.grouped_df(my.tb)
## [1] FALSE
class(my.tb)
## [1] "tbl_df"
                    "tbl"
                                  "data.frame"
names(attributes(my.tb))
## [1] "class"
                   "row.names" "names"
my_gr.tb <- group_by(.data = my.tb, letters)</pre>
is.grouped_df(my_gr.tb)
## [1] TRUE
class(my_gr.tb)
## [1] "grouped_df" "tbl_df"
                                  "tbl"
                                               "data.frame"
names(attributes(my_gr.tb))
## [1] "class"
                   "row.names" "names"
setdiff(attributes(my_gr.tb), attributes(my.tb))
## $class
## [1] "grouped_df" "tbl_df"
                                  "tb1"
                                               "data.frame"
##
## $groups
## # A tibble: 3 x 2
    letters
                .rows
##
    <chr> <chr>>
## 1 a
                     [3]
## 2 b
                      [3]
## 3 c
                     [3]
my_ugr.tb <- ungroup(my_gr.tb)</pre>
class(my_ugr.tb)
                    "tb1"
## [1] "tbl_df"
                                  "data.frame"
names(attributes(my_ugr.tb))
## [1] "class"
                   "row.names" "names"
all(my.tb == my_gr.tb)
## [1] TRUE
all(my.tb == my_ugr.tb)
## [1] TRUE
identical(my.tb, my_gr.tb)
## [1] FALSE
identical(my.tb, my_ugr.tb)
## [1] TRUE
```

The tests above show that members are in all cases the same as operator == tests for equality at each position in the tibble but not the attributes, while attributes, including class differ between normal tibbles and grouped ones and so they are not *identical* objects.

If we replace tibble by data.frame in the first statement, and rerun the chunk, the result of the last statement in the chunk is false instead of true. At the time of writing starting with a data.frame object, applying grouping with group\_by()

followed by ungrouping with ungroup() has the side effect of converting the data frame into a tibble. This is something to be very much aware of, as there are differences in how the extraction operator [ , ] behaves in the two cases. The safe way to write code making use of functions from 'dplyr' and 'tidyr' is to always make sure that subsequent code works correctly with both tibbles and data frames.

In early 2023, package 'dplyr' version 1.1.0 added support for per-operation grouping by adding to functions a new parameter (by or .by). This is still considered an experimental feature that may change. Anyway, it is important to keep in mind that this approach to grouping is not persistent like that described above.

### **8.7.3** Joins

Joins allow us to combine two data sources which share some variables. Variables in common are used to match the corresponding rows before "joining" variables (i.e., columns) from both sources together. There are several *join* functions in 'dplyr'. They differ mainly in how they handle rows that do not have a match between data sources.

We create here some artificial data to demonstrate the use of these functions. We will create two small tibbles, with one column in common and one mismatched row in each.

```
first.tb <- tibble(idx = c(1:4, 5), values1 = "a")
second.tb <- tibble(idx = c(1:4, 6), values2 = "b")
```

Below we apply the functions exported by 'dplyr': full\_join(), left\_join(), right\_join() and inner\_join(). These functions always retain all columns, and in case of multiple matches, keep a row for each matching combination of rows. We repeat each example with the arguments passed to x and y swapped to more clearly show their different behavior.

A full join retains all unmatched rows filling missing values with NA. By default the match is done on columns with the same name in x and y, but this can be changed by passing an argument to parameter by. Using by one can base the match on columns that have different names in x and y, or prevent matching of columns with the same name in x and y (example at end of the section).

```
full_join(x = first.tb, y = second.tb)
## Joining with `by = join_by(idx)`
## # A tibble: 6 x 3
##
       idx values1 values2
##
     <dbl> <chr>
                    <chr>
## 1
         1 a
                    b
## 2
         2 a
                    b
## 3
         3 a
                    h
## 4
         4 a
                    h
         5 a
## 5
                    <NA>
         6 <NA>
                    b
full_join(x = second.tb, y = first.tb)
## Joining with `by = join_by(idx)`
```

```
## # A tibble: 6 x 3
##
       idx values2 values1
     <dbl> <chr>
                  <chr>
## 1
         1 b
                    a
## 2
         2 b
                    a
## 3
         3 b
                    a
## 4
         4 b
                    a
## 5
         6 b
                    <NA>
## 6
         5 <NA>
```

Left and right joins retain rows not matched from only one of the two data sources, x and y, respectively.

```
left_join(x = first.tb, y = second.tb)
## Joining with `by = join_by(idx)`
## # A tibble: 5 x 3
##
      idx values1 values2
##
     <dbl> <chr>
                   <chr>
## 1
         1 a
                   b
## 2
         2 a
                   b
## 3
         3 a
                   b
## 4
         4 a
                   b
## 5
         5 a
                   <NA>
left_join(x = second.tb, y = first.tb)
## Joining with `by = join_by(idx)`
## # A tibble: 5 x 3
##
       idx values2 values1
##
     <db1> <chr>
                   <chr>
## 1
         1 b
                   a
## 2
         2 b
                   a
         3 b
## 3
                   a
## 4
         4 b
## 5
         6 b
                   <NA>
right_join(x = first.tb, y = second.tb)
## Joining with `by = join_by(idx)`
## # A tibble: 5 x 3
##
       idx values1 values2
##
     <dbl> <chr>
                   <chr>
## 1
         1 a
                   b
## 2
         2 a
                   b
         3 a
                   b
## 4
         4 a
         6 <NA>
right_join(x = second.tb, y = first.tb)
## Joining with `by = join_by(idx)`
## # A tibble: 5 x 3
       idx values2 values1
##
     <dbl> <chr>
                   <chr>
## 1
         1 b
                   a
## 2
         2 b
                   a
## 3
         3 b
                   а
## 4
         4 b
                   а
         5 <NA>
## 5
```

An inner join discards all rows in x that do not have a matching row in y and *vice versa*.

```
inner_join(x = first.tb, y = second.tb)
## Joining with `by = join_by(idx)`
## # A tibble: 4 x 3
##
       idx values1 values2
##
     <dbl> <chr>
                   <chr>
## 1
         1 a
                   b
## 2
         2 a
                   b
## 3
         3 a
                   b
## 4
         4 a
                   b
inner_join(x = second.tb, y = first.tb)
## Joining with `by = join_by(idx)`
## # A tibble: 4 x 3
##
       idx values2 values1
##
     <dbl> <chr>
                   <chr>
## 1
         1 b
                   а
## 2
         2 b
                   а
## 3
         3 b
                   а
## 4
         4 b
```

Next we apply the *filtering join* functions exported by 'dplyr': semi\_join() and anti\_join(). These functions only return a tibble that always contains only the columns from x, but retains rows based on their match to rows in y.

A semi join retains rows from x that have a match in y.

```
semi_join(x = first.tb, y = second.tb)
## Joining with `by = join_by(idx)`
## # A tibble: 4 x 2
##
       idx values1
##
     <dbl> <chr>
## 1
         1 a
## 2
         2 a
## 3
         3 a
## 4
         4 a
semi_join(x = second.tb, y = first.tb)
## Joining with `by = join_by(idx)`
## # A tibble: 4 x 2
##
       idx values2
##
     <db1> <chr>
## 1
         1 b
## 2
         2 b
         3 b
## 3
         4 b
## 4
```

A anti-join retains rows from x that do not have a match in y.

```
anti_join(x = first.tb, y = second.tb)
## Joining with `by = join_by(idx)`
## # A tibble: 1 x 2
## idx values1
## <dbl> <chr>
## 1 5 a
```

```
anti_join(x = second.tb, y = first.tb)
## Joining with `by = join_by(idx)`
## # A tibble: 1 x 2
## idx values2
## <dbl> <chr>
## 1 6 b
```

We here rename column idx in first.tb to demonstrate the use of by to specify which columns should be searched for matches.

```
first2.tb <- rename(first.tb. idx2 = idx)</pre>
full_join(x = first2.tb, y = second.tb, by = c("idx2" = "idx"))
## # A tibble: 6 x 3
##
     idx2 values1 values2
##
     <db1> <chr>
                  <chr>
## 1
                   b
         1 a
## 2
         2 a
                   b
         3 a
## 3
                   b
## 4
         4 a
                   b
## 5
         5 a
                   <NA>
## 6
         6 <NA>
                   b
```

# 8.8 Further reading

An in-depth discussion of the 'tidyverse' is outside the scope of this book. Several books describe in detail the use of these packages. As several of them are under active development, recent editions of books such as *R for Data Science* (Wickham et al. 2023) and *R Programming for Data Science* (Peng 2022) are the most useful.

# R Extensions: Grammar of Graphics

The commonality between science and art is in trying to see profoundly—to develop strategies of seeing and showing.

Edward Tufte's answer to Charlotte Thralls *An Interview with Edward R. Tufte*, 2004

# 9.1 Aims of this chapter

Three main data plotting systems are available to R users: base R, package 'lattice' (Sarkar 2008) and package 'ggplot2' (Wickham and Sievert 2016), the last one being the most recent and currently most popular system available in R for plotting data. Even two different sets of graphics primitives (i.e., those used to produce the simplest graphical elements such as lines and symbols) are available in R, those in base R and a newer one in the 'grid' package (Murrell 2011).

In this chapter you will learn the concepts of the layered grammar of graphics, on which package 'ggplot2' is based. You will also learn how to build several types of data plots with package 'ggplot2'. As a consequence of the popularity and flexibility of 'ggplot2', many contributed packages extending its functionality have been developed and deposited in public repositories. However, I will focus mainly on package 'ggplot2' only briefly describing a few of these extensions.

## 9.2 Packages used in this chapter

If the packages used in this chapter are not yet installed in your computer, you can install them as shown below, as long as package 'learnrbook' is already installed. install.packages(learnrbook::pkgs\_ch\_ggplot)

To run the examples included in this chapter, you need first to load some pack-

ages from the library (see section 6.4 on page 178 for details on the use of packages).

library(learnrbook)
library(wrapr)
library(scales)
library(ggplot2)
library(ggrepel)
library(gginnards)
library(broom)
library(ggpmisc)
library(ggbeeswarm)
library(ggforce)
library(tikzDevice)
library(lubridate)
library(tidyverse)
library(patchwork)

# 9.3 The components of a plot

I start by briefly presenting concepts central to data visualisation, following the *Data visualization handbook* (Koponen and Hildén 2019). Plots are a medium used to convey information, like text. It is worthwhile keeping this in mind. As with text, the design of plots needs to consider what we want to highlight, what is the take home message we want to convey. The style of the plot should match the expectations and the plot-reading abilities of the expected audience. One needs to be careful to avoid ambiguities and most importantly of all not to miss-inform. Data visualisations like text need to be planned, revised, commented upon, revised again until the best way of expressing our message is found. As we will see through this chapter, the flexibility of the grammar of graphics supports very well this approach to designing and producing high quality data visualizations for different audiences.

Of course, when exploring data we do not need fancy details of graphical design, but we still need the flexibility that allows looking at the same data from many differing angles, highlighting different aspects of them. In the same way as boiler-plate text and text templates have specific but limited uses, all-in-one functions for producing plots do not support well the design of original data visualizations. They tend to get the job done, but lack the flexibility needed to do the best job of communicating with readers. Being this a book about languages, the focus of this chapter is in the layered grammar of graphics.

The plots we will describe in this chapter are classified as *statistical graphics* within the larger field of data visualisation which is broader. Plots such as scatter plots include points (geometric objects) that by their position, shape, colour or some other property directly convey information. If we consider these points their location in the plot "canvas" or "plotting area" is given by the values of their coordinates and any alteration to these coordinates is wrong. Such alterations would break the correspondence between coordinates and observed values thus convey-

ing wrong/false information to the audience. A *data label* is connected to an observation but its position can be displaced as long as its link to the corresponding observation can be inferred, e.g., by the direction of an arrow or even simple proximity. Annotations, are additions to a plot that have no connection to individual observations, but rather with all observations taken together, e.g., a text like n =200 indicating the number of observations included in a corner of a plot. These three elements convey information about observations. The axis labels, legends and keys included in the visualisation make it possible for the reader to retrieve the original values represented in the plot by graphical elements. Other elements in a visualisation even when not carrying additional information still affect the easy with which a plot can be read. These include the size of text and symbols, thickness of lines, font face, the choice of colour palette, etc. In general plots designed to be included in books and journals are unsuitable for oral presentations, and vice versa, mainly because of the different length of time available for the audience to read them. It is important to be aware of the roles played by different plot components when designing a data visualisation and when implementing it using the grammar of graphics.

# 9.4 The grammar of graphics

What separates 'ggplot2' from base R and trellis/lattice plotting functions is the use of a layered grammar of graphics (the reason behind 'gg' in the name of package 'ggplot2'). What is meant by grammar in this case is that plots are assembled piece by piece using different "nouns" and "verbs" (Cleveland 1985). Instead of using a single function with many arguments, plots are assembled by combining different elements with operators + and %+%. Furthermore, the construction is mostly semantics-based and to a large extent, how plots look when printed, displayed, or exported to a bitmap or vector-graphics file is controlled by themes.

We can think of plotting as translating or mapping the observations or data into a graphical language. We use properties of graphical (or geometrical) objects to represent different aspects of our data. An observation can consist of multiple recorded values. Say an observation of air temperature may be defined by a position in 3-dimensional space and a point in time, in addition to the temperature itself. An observation for the size and shape of a plant can consist of height, stem diameter, number of leaves, size of individual leaves, length of roots, fresh mass, dry mass, etc. If we are interested in the relationship between height and stem diameter, we may want to use cartesian coordinates, mapping stem diameter to the x dimension of the plot and the height to the y dimension. The observations could be represented on the plot by points.

The grammar of graphics allows us to design plots by combining various elements in ways that are nearly orthogonal. In other words, the majority of the possible combinations of "words" yield valid plots as long as we assemble them respecting the rules of the grammar. This flexibility makes 'ggplot2' extremely

powerful as we can build plots and even types of plots which were not even considered while designing the 'ggplot2' package.

When a plot is built, the whole plot and its components are created as R objects that can be saved in the workspace or written to a file as objects. The graphical representation is generated when the object is printed, explicitly or automatically. The same "gg" plot object can be rendered into different bitmap and vector graphic formats for display or printing.

The transformation of a set of data or observations into a rendered graphic with package 'ggplot2' can be represented as a flow of information, but also as a sequence of actions. However, what avoids that the flexibility becomes a burden is that if we do not explicitly mention all steps in our code, in most cases adequate defaults for them will be used instead. The recipe to build a plot needs to specify a) the data to use, b) which variable to map to which graphical property (or aesthetic), c) which layers to add and which geometric representation to use, d) the scales that establish the link between data values and aesthetic values, e) a coordinate system (affecting only aesthetics x, y and possibly z), f) a theme to use. The result from constructing a plot with the grammar of graphics is an R object containing a "recipe for a plot", including the data. This R object, behaves like other R objects: can be assigned a name, saved to a file or printed into a rendered plot, either to a physical printer or into vector or bitmap graphics formats. The recipe includes indeed many elements, but as mentioned above, we do not need to be explicit about all of them. Obviously step a) has no default, b) has defaults only in special cases, and c) has no defaults. The layered grammar of graphics implemented in 'qqplot2' allows plots to contain multiple layers, each layer possibly created with a different geometric representation of data.

### 9.4.1 The words of the grammar

Before building a plot step by step, I introduce next the different components of a ggplot recipe, or the words in the grammar.

### Data

The data to be plotted must be available as a data.frame or tibble, with data stored so that each row represents a single observation event, and the columns are different values observed in that single event. In other words, in long form (so-called "tidy data") as described in chapter 8. The variables to be plotted can be numeric, factor, character, and time or date stored as POSIXCt. (Some extensions to 'ggplot2' add support for other types of data such as time series).

#### Mapping

When we design a plot, we need to map data variables to aesthetics (or graphic properties). Most plots will have an x dimension, which is considered an *aesthetic*, and a variable containing numbers (or categories) mapped to it. The position on a 2D plot of, say, a point, will be determined by x and y aesthetics, while in a 3D plot, three aesthetics need to be mapped x, y and z. Many aesthetics are not

related to coordinates, they are properties, like color, size, shape, line type, or even rotation angle, which add an additional dimension on which to represent the values of variables and/or constants.

#### Geometries

Geometries are "words" that describe the graphics representation of the data: for example, <code>geom\_point()</code>, plots a point or symbol for each observation or summary value, while <code>geom\_line()</code>, draws line segments between observations. Some geometries rely by default on statistics, but most "geoms" default to the identity statistics. Each time a <code>geometry</code> is used to add a graphical representation of data to a plot, we say that a new <code>layer</code> has been added. The name <code>layer</code> reflects the fact that each new layer added is plotted on top of the layers already present in the plot, or rather when a plot is printed the layers will be generated in the order they were added to the plot object. For example, one layer in a plot can display the observations, another layer a regression line fitted to them, and a third one may contain annotations such an equation or a text label.

### **Positions**

Positions are "words" that determine the displacement or not of graphical plot elements relative to their original x and y coordinates. They are one of the arguments accepted by *geometries*. Position position\_identity() introduces no displacement, and for example, position\_stack() makes it possible to create stacked bar plots and stacked area plots. Positions will be discussed together with geometries as they are always subordinate to them.

### **Statistics**

Statistics are "words" that represent calculation of summaries or some other operation on the values in the data. When *statistics* are used for a computation, the returned value is passed to a *geometry*, and consequently adding a *statistics* also adds a layer to the plot. For example, stat\_smooth() fits a smoother, and stat\_summary() applies a summary function such as mean((). Most statistics are applied automatically by group when data have been grouped by mapping additional aesthetics such as color to a factor.

### Scales

Scales give the "translation" or mapping between data values and the aesthetic values to be actually plotted. Mapping a variable to the "color" aesthetic (also recognized when spelled as "colour") only tells that different values stored in the mapped variable will be represented by different colors. A scale, such as  $scale_color_continuous()$ , will determine which color in the plot corresponds to which value in the variable. Scales can also define transformations on the data, which are used when mapping data values to aesthetic values. All continuous scales support transformations—e.g., in the case of x and y aesthetics, positions on the plotting region or graphic viewport will be affected by the transformation, while the original values will be used for tick labels along the axes. Scales are used for all

aesthetics, including continuous variables, such as numbers, and categorical ones such as factors. The grammar of graphics allows only one scale per *aesthetic* and plot. This restriction is imposed by design to avoid ambiguity (e.g., it ensures that the red color will have the same "meaning" in all plot layers where the color *aesthetic* is mapped to data). Scales have limits with observations falling outside these limits being ignored by default (replaced by NA) rather than passed to statistics or geometries—it is easy to unintentionally drop observations when setting scale limits manually, consequently warning messages reporting that NA values have been omitted from a plot should not be ignored.

### Coordinate systems

The most frequently used coordinate system when plotting data, the cartesian system, is the default for most *geometries*. In the cartesian system, x and y are represented as distances on two orthogonal (at  $90^{\circ}$ ) axes. Additional coordinate systems are available in 'ggplot2' and through extensions. For example, in the polar system of coordinates, the x values are mapped to angles around a central point and y values to the radius. Another example is the ternary system of coordinates, an extension of the grammar implemented in package 'ggtern', that allows the construction of ternary plots. Setting limits to a coordinate system changes the region of the plotting space visible in the plot, but does not discard observations. In other words, when using *statistics*, observations located outside the coordinate limits, i.e., not visible in the rendered plot, will still be included in computations if excluded by coordinate limits but will be ignored if excluded by scale limits.

### Themes

How the plots look when displayed or printed can be altered by means of themes. A plot can be saved without adding a theme and then printed or displayed using different themes. Also, individual theme elements can be changed, and whole new themes defined. This adds a lot of flexibility and helps in the separation of the data representation aspects from those related to the graphical design.

### **Operators**

To assemble the elements described above into a ggplot object we normally use operator + and exceptionally %+%. This choice makes sense, as we build ggplot objects by sequentially adding members to them.

The functions corresponding to the different elements of the grammar of graphics have distinctive names with the first few letters hinting at their roles: aesthetics mappings (aes), geometric elements (geom\_...), statistics (stat\_...), scales (scale\_...), coordinate systems (coord\_...), and themes (theme\_...).

### 9.4.2 The workings of the grammar

A "gg" plot object is an R object of mode "list" containing the recipe and data to construct a plot. It is self contained in the sense that the only requirement for rendering it into a graphical representation is the availability of package 'ggplot2'. A

"gg" object contains the data in one or more data frames and instructions encoded as functions and parameters, but not yet a rendering of the plot into graphical objects. Both data transformations and rendering of the plot into drawing instructions (encoded as graphical objects or *grobs*) take place at the time of printing or exporting the plot, e.g., when saving a bitmap to a file.

To understand ggplots we should first think in terms of the graphical organization of the plot: there is a background layer onto which layers composed by different graphical objects are laid. Each layer contains related graphical objects originating from the same data. The last layer added is the topmost and the first one added the lowermost. Graphical objects in upper layers occlude those in the layers below them if their locations overlap. Although usually the layers in a ggplot share the same data and mappings to aesthetics, this is not necessarily so. It is possible to build a ggplot where the layers are fully independent of each other, although the scales and plotting area are always shared among them.

A second perspective on ggplots is that of the process of converting the data into a graphical representation that can be printed on paper or viewed on a computer screen. The transformations applied to the data to achieve this can be thought as a dynamic data flow process divided in stages. We consider first a single self-contained layer in a plot. During this process the information contained in the data supplied by the user is transformed into instructions to draw a graphical representation. In 'ggplot2' graphical features of a plot are described as *aesthetics*, and the correspondence between values in the data and values of the aesthetic is controlled by *scales*. The values in the data are not necessarily directly mapped to aesthetics, they may be summarized by a *statistic*. *Geometries* generate graphical objects from the mapped data.



Plot layers always include a statistic and a geometry. Function <code>aes()</code> is used to define mappings to aesthetics. The default for <code>aes()</code> is for the mapping to take place at the <code>start</code> (left circle in the diagram above), mapping names in the user data to aesthetics such as x, y, colour, shape, etc. However, the data mapped at <code>start</code> can be mapped again at two later stages <code>after stat</code> and <code>after scale</code>. Many statistics return the summarized data through the same mappings (e.g., input received through <code>y</code> aesthetics is summarised and output through the same <code>y</code> aesthetics). This is the most common case and the "transfer" of the mapping is automatic, and can be safely ignored by the user. An even simpler case is when the statistic is <code>stat\_indentity()</code>, which is a placeholder that copies its input to its output.

Some statistics change the default mapping into something different to the mapped variables at their input, in which case the automatic mapping at **after stat** differs from that at **start**. Many statistics return multiple variables in their output, some of them mapped to aesthetics and some not mapped to facilitate variations on a given type of data summary. This is a case where users need to be aware of the different stages of mapping of aesthetics if they want to modify the default mapping. (See section 9.4.5 on page 281 for details.)

As mentioned above all ggplot layers include a statistic and a geometry. Both statistics are layer constructor functions, and while statistics take a geometry as one of its arguments, geometries take a statistic as one of its arguments. The default statistic of many geometries is stat\_identity() and thus behave by default as if the layer they create had no statistics. There are some statistics in 'ggplot2' that have companion geometries that can be used (almost) interchangeably. This' tends to lead into confusion, and in this book, only geometries that have as default stat\_identity() are described as geometries in section 9.5. In the case of those that by default use other statistics, like geom\_smooth() only the companion statistic, stat\_smooth() for this example, are described in section 9.6.

A ggplot can have a single layer or many layers, but when ggplots have more than one layer, the data flow, computations and generation of graphical objects takes place independently for each layer. As mentioned above, most ggplots do not have fully independent layers, but the layers share the same data and aesthetic mappings at the **start**. Ahead of this point computations in layers are always independent of those in other layers, except that for a given aesthetic only one scale is allowed per plot. This is intentional, and makes it nearly impossible for one aesthetic to be assigned different meanings in different layers of the same plot.

### 9.4.3 Plot construction

As the use of the grammar is easier to demonstrate by example than to explain with words, I will show how to build plots of increasing complexity, starting from the simplest possible. All elements of a plot have defaults, although in some cases these defaults result in empty plots. Defaults make it possible to create a plot very succinctly. When building a plot step by step, we can consider the different aspects described in the previous section: the structure of the object, the graphic output, and the transformations applied to the data in the route between the recipe stored in an object and graphic output. In this section I emphasize the syntax of the grammar and how it translated into a plot.

9.1 When reading this section, possibly a second time, use summary() and str() as described in the previous section to explore how "gg" plot objects gain new member components as the *recipe* for the plot evolves in complexity.

We start by using function ggplot() to create the skeleton for a plot, which can be enhanced, but also printed as is. *A plot with no data or layers.* 

ggplot()

ggplot(data = mtcars)

The plot above is of little use without any data, so we next pass a data frame object, in this case mtcars—mtcars is a data set included in R; to learn more about this data set, type help("mtcars") at the R command prompt. Having no layers or scale, the result is also an empty grey plotting area. (data  $\rightarrow$  *ggplot object*)

Once the data are available, we need to select a graphical or geometric representation for the quantities to plot. The overall kind of representation is determined by the geometry, such as  $geom\_point()$  and  $geom\_line()$ , drawing separate points for the observations or connecting them with lines, respectively. A mapping indicates which property of the geometric elements will be used to represent the values stored in a given variable in the user's data. For most geometries we need to provide mappings for both x and y aesthetics, to establish the position of the geometrical shapes like points or lines in the plotting area. Additional aesthetics like colour (applicable to both points and lines) or shape and linetype, applicable to points and lines, respectively have default mappings. Defaults can be overridden by including a mapping explicitly in the call to aes().

Here we map at the **start** stage two variables in the data, disp to x and and mpg to y aesthetics. This mapping can be seen in the chunk below by its effect on the plotting area ranges that now match the ranges of the mapped variables, expanded by a small margin. The axis labels also reflect the names of the mapped variables, however, there is no graphical element yet displayed for the individual observations. (data  $\rightarrow$  aes  $\rightarrow$  *ggplot object*)

```
ggplot(data = mtcars,
    aes(x = disp, y = mpg))

35-
30-
25-
20-
15-
10-
100
200
300
400
disp
```

To make observations visible we need to add a suitable *geometry* or geom to the plot recipe. Here we display the observations as points using geom\_point(), i.e, we add a *plot layer*. (data  $\rightarrow$  aes  $\rightarrow$  geom  $\rightarrow$  *ggplot object*)

```
ggplot(data = mtcars,
    aes(x = disp, y = mpg)) +
geom_point()

25
20
15-
10-
100
200
300
400
disp
```

In the examples above, the plots were printed automatically, which is the default at the R console. However, as with other R objects, ggplots can be assigned to a variable as first shown in section 9.4.2 on page 270.

and printed at a later time, and saved to and read from files on disk.

print(p)

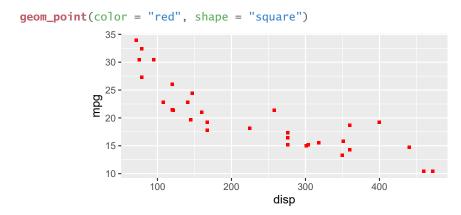
Layers and other elements can be also added to a saved ggplot as the saved objects are not the graphical representation of the plots themselves but instead a *recipe* plus data needed to build them.

9.2 Above we have seen how to build a plot and we also had a glimpse of the structure of a simple "gg" plot object. We have also saved a ggplot under the name p.

We can view the structure of any R object, including "gg" plot objects, with str(). Package 'ggplot2' provides a summary() for "gg" plot object. Package 'gginnards' provides methods str(), num\_layers(), top\_layer(), bottom\_layer(), and mapped\_vars(). As you make progress through the chapter, use these methods to explore "gg" plot objects with different numbers of layers or mappings. You will be able to see how the plot components are stored as members of the "gg" plot objects.

Although *aesthetics* are usually mapped to variables in the data, they can also be set to constant values, as many of them are by default. While variables in data can be both mapped using aes() as whole-plot defaults, as shown above, or within individual layers, constant values for aesthetics can be set, as shown here, only for individual layers and directly rather than using aes().

```
ggplot(data = mtcars,
    aes(x = disp, y = mpg)) +
```

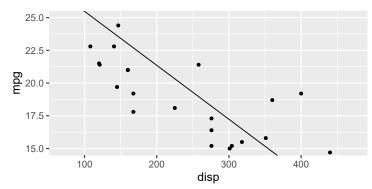


While a geometry directly constructs during rendering a graphical representation of the observations or summaries in the data it receives as input, a *statistics* or stat "sits" in-between the data and a geom, applying some computation, usually but not always, to produce a statistical summary of the data. Here we add a fitted line using  $stat_smooth()$  with its output added to the plot using  $geom_line()$  passed by name with "line" as an argument to  $stat_smooth()$ . We fit a linear regression, using lm() as the method. This plot has two layers, from geometries  $geom_point()$  and  $geom_line()$ . (data  $\rightarrow$  aes  $\rightarrow$  stat  $\rightarrow$  geom  $\rightarrow$  ggplot object)

We haven't yet added some of the elements of the grammar described above: scales, coordinates and themes. The plots were rendered anyway because these elements have defaults which are used when we do not set them explicitly. We next will see examples in which they are explicitly set. We start with a scale using a logarithmic transformation. This works like plotting by hand using graph paper with rulings spaced according to a logarithmic scale. Tick marks continue to be expressed in the original units, but statistics are applied to the transformed data. In other words, a transformed scale affects the values before they are passed to statistics, and the linear regression will be fitted to log10() transformed y values and the original x values. (data  $\rightarrow$  aes  $\rightarrow$  stat  $\rightarrow$  geom  $\rightarrow$  scale  $\rightarrow$  ggplot object)

The range limits of a scale can be set manually, instead of automatically as by default. These limits create a virtual *window into the data*: out-of-bounds (oob) observations, those outside the scale limits remain hidden and are not mapped to aesthetics—i.e., these observations are not included in the graphical representation or used in calculations. Crucially, when using *statistics* the computations are only applied to observations that fall within the limits of all scales in use. These limits *indirectly* affect the plotting area when the plotting area is automatically set based on the range of the (within limits) data—even the mapping to values of a different aesthetics may change when a subset of the data are selected by manually setting the limits of a scale.

In contrast to *scale limits*, *coordinates* function as a *zoomed view* into the plotting area, and do not affect which observations are visible to *statistics*. The coordinate system, as expected, is also determined by this grammar element—here we use cartesian coordinates which are the default, but we manually set y limits. (data  $\rightarrow$  aes  $\rightarrow$  stat  $\rightarrow$  geom  $\rightarrow$  coordinate  $\rightarrow$  theme  $\rightarrow$  *gaplot object*)



The next example uses a coordinate system transformation. When the trans-

formation is applied to the coordinate system, it affects only the plotting—it sits between the geom and the rendering of the plot. The transformation is applied to the values returned by any *statistics*. The straight line fitted is plotted on the transformed coordinates as a curve, because the model was fitted to the untransformed data and this fitted model is automatically used to obtain the predicted values, which are then plotted after the transformation is applied to them. We have here described only cartesian coordinate systems while other coordinate systems are described in sections 9.5.6 and 9.11 on pages 298 and 348, respectively.

Themes affect the rendering of plots at the time of printing—they can be thought of as style sheets defining the graphic design. A complete theme can override the default gray theme. The plot is the same, the observations are represented in the same way, the limits of the axes are the same and all text is the same. On the other, hand how these elements are rendered by different themes can be drastically different. (data  $\rightarrow$  aes  $\rightarrow$   $\rightarrow$  geom  $\rightarrow$  theme  $\rightarrow$  *gaplot object* 

We can also override the base font size and font family. This affects the size of all text elements, as their size is defined relative to the base size. Here we add the

same theme as used in the previous example, but with a different base point size for text.

```
ggplot(data = mtcars,
    aes(x = disp, y = mpg)) +
geom_point() +
theme_classic(base_size = 20, base_family = "serif")

35
30
400
disp
```

The details of how to set axis labels, tick positions and tick labels will be discussed in depth in section 9.9. Meanwhile, we will use function labs() which is *a convenience function* allowing us to easily set the title and subtitle of a plot and to replace the default name of scales, in this case, those used for axis labels—by default the name of scales is set to the name of the mapped variable. When setting the name of scales with labs(), we use as parameter names in the function call the names of aesthetics and pass as an argument a character string, or an R expression. Here we use x and y, the names of the two *aesthetics* to which we have mapped two variables in data, disp and mpg.

```
ggplot(data = mtcars,
        aes(x = disp, y = mpg)) +
  geom_point() +
  labs(x = "Engine displacement (cubic inches)",
        y = "Fuel use efficiency\n(miles per gallon)",
        title = "Motor Trend Car Road Tests",
        subtitle = "Source: 1974 Motor Trend US magazine")
                      Motor Trend Car Road Tests
                      Source: 1974 Motor Trend US magazine
                   35
              Fuel use efficiency
                (miles per gallon)
                   10 -
                                       200
                                                   300
                          100
                                                               400
                                 Engine displacement (cubic inches)
```

As elsewhere in R, when a value is expected, either a value stored in a variable or a more complex statement returning a suitable value can be passed as an argument to be mapped to an *aesthetic*. In other words, the values to be plotted do not need to be stored as variables (or columns) in the data frame passed as an argument

to parameter data, they can also be computed from these variables. Here we plot miles-per-gallon, mpg on the engine displacement per cylinder by dividing disp by cyl within the call to aes().

```
ggplot(data = mtcars, aes(x = disp / cyl, y = mpg)) +
geom_point()

35-
30-
25-
20-
15-
10-
20 30 40 50 60
```

We can summarize the data transformation steps described above as a linear chain: data  $\rightarrow$  aes  $\rightarrow$  stat  $\rightarrow$  aes  $\rightarrow$  geom  $\rightarrow$  scale  $\rightarrow$  aes  $\rightarrow$  coordinate  $\rightarrow$  theme  $\rightarrow$  *ggplot object* 

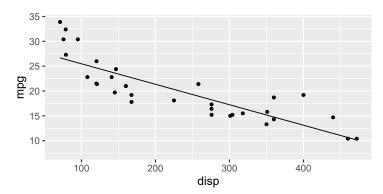
Each of the elements of the grammar exemplified above has several different member functions, and many of the individual *geometries* and *statistics* accept arguments that can be used to modify their behavior. There are also more *aesthetics* than those shown above. Multiple data objects as well as multiple mappings can coexist within a single "gg" plot object. Packages and user code can define new *geometries*, *statistics*, *coordinates* and even implement new *aesthetics*. Being ggplot() an S3 method, specializations for objects of classes different from data.frame exist. Individual elements in a theme can also be modified and new complete themes created, re-used and shared. We will describe in the remaining sections of this chapter how to use the grammar of graphics to construct other types of graphical presentations including more complex plots than those in the examples above.

## 9.4.4 Plots as R objects

We can manipulate "gg" plot objects and their components in the same way as other R objects. We can operate on them using the operators and methods defined for the "gg" class they belong to. We start by saving a ggplot into a variable.

When we used in the previous section operator + to assemble the plots, we were operating on "anonymous" R objects. In the same way, we can operate on saved or "named" objects.

```
p +
   stat_smooth(geom = "line", method = "lm", formula = y ~ x)
```



9.3 Reproduce the examples in the previous section, using p defined above as a basis instead of building each plot from scratch.

In the examples above we have been adding elements one by one, using the + operator. It is also possible to add multiple components in a single operation using a list. This is useful, when we want to save sets of components in a variable so as to reuse them in multiple plots. This saves typing, ensures consistency and can make alterations to a set of similar plots much easier.

```
my.layer <- list(
    stat_smooth(geom = "line", method = "lm", formula = y ~ x),
    scale_x_log10())

p + my.layer

35
20
15
100
disp</pre>
```

The separation of plot construction and rendering is possible, because "gg" objects are self-contained. A copy of the data object passed as argument is saved within the plot object, similarly as in model-fit objects. In the example above, p by itself could be saved to a file on disk and loaded into a clean R session, even on another computer, and rendered as long as package 'ggplot2' and its dependencies are available. Another consequence of storing a copy of the data in the plot object, is later changes to the data object used to create a "gg" object are *not* reflected in newly rendered plots from this object: we must create a new "gg" object.

We can look in more detail at how the *recipe* to make a plot is stored in a "gg" plot object. Objects of class "gg" are of mode "list". In R, lists can contain heterogeneous members. They contain data, function definitions, and unevaluated expressions. In other words the data plus instructions to transform the data, to

map them into graphic objects, and various aspects of the rendering from scale limits to type faces to use. (R lists are described in section 4.3 on page 86.)

As an example we show the top level members of a "gg" plot object for a simple plot. Method summary() shows the components without making explicit the structure of the object.

```
summary(p)
## data: mpg, cyl, disp, hp, drat, wt, qsec, vs, am, gear, carb [32x11]
## mapping: x = \sim disp, y = \sim mpg
## faceting: <ggproto object: Class FacetNull, Facet, gg>
       compute_layout: function
##
       draw_back: function
##
       draw front: function
##
##
       draw_labels: function
##
       draw_panels: function
##
       finish_data: function
       init_scales: function
##
##
       map_data: function
##
       params: list
##
       setup_data: function
##
       setup_params: function
##
       shrink: TRUE
##
       train_scales: function
##
       vars: function
##
       super: <ggproto object: Class FacetNull, Facet, gg>
## -
## geom_point: na.rm = FALSE
## stat_identity: na.rm = FALSE
## position_identity
```

Method str() shows the structure of objects and can be also used to advantage with ggplots. Alternatively we can use names() for a list of the names of members.

9.4 Explore in more detail the different members of object p. For example for the "layers" member of object p one can use.

```
str(p$layers, max.level = 1)
```

How many layers are present in this case?

You can use summary() and str() to develop an understanding of how simple as well as complex plots are stored.

# 9.4.5 Mappings in detail

In the case of simple plots, based on data contained in a single data frame, the usual style is to code a plot as described above, passing an argument, mtcars in these examples, to the data parameter of ggplot(). Data passed in this way becomes the default for all layers in the plot. The same applies to the argument passed to mapping.

```
geom_point()
```

However, the grammar of graphics contemplates the possibility of data and mappings restricted to individual layers, passed to statistics or geometries through their mapping formal parameter. In this case, those mappings set in the call to ggplot(), if present, are overridden by arguments passed to individual layers, making it possible to code the same plot as follows.

The two examples show the two most commonly used styles when working at the console or writing simple scripts. There are other possibilities which are most useful when writing complex scripts, or in function definitions. We gui The default mapping can also be added directly with the + operator, instead of being passed as an argument to ggplot().

```
ggplot(data = mtcars) +
  aes(x = disp, y = mpg) +
  geom_point()
```

It is also possible to have a default mapping for the whole plot, but no default data.

```
ggplot() +
  aes(x = disp, y = mpg) +
  geom_point(data = mtcars)
```

We can save the mapping to a variable and add the variable instead of the call to aes() in each of the examples above, of which we show only the first one.

In all these examples, the plot remains unchanged (not shown). However, this flexibility in the grammar allows, as discussed in section 9.4.2 on 270 makes it possible for layers to remain independent of each other when needed.

The argument passed to parameter data of a layer function, can be a function instead of a data frame if the plot contains default data. In this case, the function is applied to the default data and must return a data frame containing data to be used in the layer. Here I use an anonymous function defined in-line, but a function can also be passed as argument by name.

The plot's default data can also be operated upon using the 'magrittr' pipe operator, but not the pipe operator native to R (|>) or the dot-pipe operator from 'wrapr' (see section 8.5 on page 250). Using a function as above is simpler and clearer.

Late mapping of variables to aesthetics has been possible in 'ggplot2' for a long time using as notation enclosure of the name of a variable returned by a statistic between .., but this notation has been deprecated some time ago and replaced by stat(). In both cases, this imposed a limitation: it was impossible to map a computed variable to the same aesthetic as input to the statistic and to the geometry in the same layer. There were also some other quirks that prevented passing some arguments to the geometry through the dots ... parameter of a statistic.

Since version 3.3.0 of 'ggplot2' the syntax used for mapping variables to aesthetics is based on functions stage(), after\_stat() and after\_scale(). Function after\_stat() replaces stat() and the .. notation. As shown in the diagram from section 9.4 on page 267, reproduced here, aesthetic appears in three places:

```
data \rightarrow aes \rightarrow stat \rightarrow aes \rightarrow geom \rightarrow scale \rightarrow aes \rightarrow coordinate \rightarrow theme \rightarrow ggplot object
```

Variables in the data frame passed as argument to data are mapped to aesthetics before they are received as input by a statistic (possibly stat\_identity()). The mappings of variables in the data frame returned by statistics are the input to the geometry. Those statistics that operate on *x* and/or y return a transformed version of these variables, by default also mapped to these aesthetics. However, in most cases other variables in addition to *x* and/or y are included in the data returned by a *statistic*. Although their default mapping is coded in the statistic functions' definitions, the user can modify this default mapping explicitly within a call to aes() using after\_stat(), which lets us differentiate between the data frame supplied by the user and that returned by the statistic. The third stage was not accessible in earlier versions of 'ggplot2', but lack of access was usually not insurmountable. Now this third stage can be accessed with after\_scale() making coding simpler.

User-coded transformations of the data are best handled at the third stage using scale transformations. However, when the intention is to jointly display or combine different computed variables returned by a statistic we need to set the desired mapping of original and computed variables to aesthetics at more than one stage.

The documentation of 'ggplot2' gives several good examples of cases when the new syntax is useful. I give here a different example. We fit a polynomial using rlm(). RLM is a procedure that automatically assigns before computing the residual sums of squares, weights to the individual residuals in an attempt to protect the estimated fit from the influence of extreme observations or outliers. When using this and similar methods it is of interest to plot the residuals together with the weights. A frequent approach is to map weights to a gradient between two colours. We start by generating some artificial data containing outliers.

```
# we use capital letters X and Y as variable names to distinguish
# them from the x and y aesthetics
set.seed(4321)
X <- 0:10
Y <- (X + X^2 + X^3) + rnorm(length(X), mean = 0, sd = mean(X^3) / 4)
my.data <- data.frame(X, Y)</pre>
```

```
my.data.outlier <- my.data
my.data.outlier[6, "Y"] <- my.data.outlier[6, "Y"] * 10</pre>
```

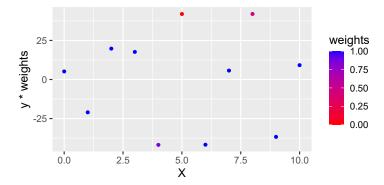
As it will be used in multiple examples, we give a name to the model formula. We do this just for convenience but also to ensure consistency in the model fits.

```
my.formula \leftarrow y \sim poly(x, 3, raw = TRUE)
```

For the first plot it is enough to use after\_stat() to map a variable weights computed by the statistic to the colour aesthetic. In the case of stat\_fit\_residuals(), geom\_point() is used by default. This figure shows the residuals before weights are applied, with the computed weights (with range 0 to 1) encoded by colours ranging between red and blue.

```
qqplot(my.data.outlier, aes(x = X, y = Y)) +
  stat_fit_residuals(formula = my.formula, method = "rlm",
                       mapping = aes(colour = after_stat(weights)),
                       show.legend = TRUE) +
  scale_color_gradient(low = "red", high = "blue", limits = c(0, 1),
                         guide = "colourbar")
                2500 -
                2000 -
                                                                 weights
                                                                     1.00
                1500 -
                                                                     0.75
                1000 -
                                                                     0.50
                                                                     0.25
                 500 -
                                                                     0.00
                   0 -
                     0.0
                                        5.0
                                                           10.0
```

In the second plot we plot the weighted residuals, again with colour for weights. In this case we need to use stage() to be able to distinguish the mapping ahead of the statistic (start) from that after the statistic, i.e., ahead of the geometry. We use as above, the default geometry, geom\_point(). The mapping in this example can be read as: the variable x from the data frame my.data.outlier is mapped to the x aesthetic at all stages. Variable y from the data frame my.data.outlier is mapped to the y aesthetic ahead of the computations in stat\_fit\_residuals(). After the computations, variables y and weights in the data frame returned by stat\_fit\_residuals() are multiplied and mapped to the y ahead of geom\_point().



In LM fits, the sum of squares of the un-weighted residuals is minimized to estimate the value of parameters for the best fitting model, while in RLM, the sum of squares of the weighted residuals is minimized instead.

### 9.5 Geometries

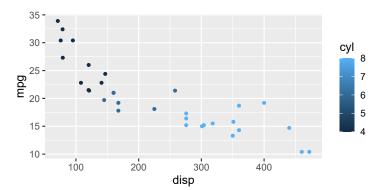
Different geometries support different *aesthetics*. While <code>geom\_point()</code> supports <code>shape</code>, and <code>geom\_line()</code> supports <code>linetype</code>, both support <code>x</code>, <code>y</code>, <code>color</code> and <code>size</code>. In this section we will describe the different <code>geometries</code> available in package '<code>ggplot2</code>' and some examples from packages that extend '<code>ggplot2</code>'. The graphic output from most code examples will not be shown, with the expectation that readers will run them to see the plots.

Mainly for historical reasons, *geometries* accept a *statistic* as an argument, in the same way as *statistics* accept a *geometry* as an argument. In this section we will only describe *geometries* which have as a default *statistic* stat\_identity which passes values directly as mapped. The *geometries* that have other *statistics* as default are described in section 9.6.2 together with the corresponding *statistics*.

### 9.5.1 Point

As shown earlier in this chapter, <code>geom\_point()</code>, can be used to add a layer with observations represented by "points" or symbols. Variable <code>cyl</code> describes the numbers of cylinders in the engines of the cars. It is a numeric variable, and when mapped to color, a continuous color scale is used to represent this variable.

The first examples build scatter plots, because numeric variables are mapped to both x and y. Some scales, like those for color, exist in two "flavors," one suitable for numeric variables (continuous) and another for factors (discrete).



If we convert cyl into a factor, a discrete color scale is used instead of a continuous one.

If we convert cyl into an ordered factor, a different discrete color scale is used by default.

9.5 Try a different mapping:  $disp \rightarrow color$ ,  $cyl \rightarrow x$ . Continue by using help(mtcars) and/or names(mtcars) to see what variables are available, and then try the combinations that trigger your curiosity—i.e., explore the data.

The mapping between data values and aesthetic values is controlled by scales. Different color scales, and even palettes within a given scale, provide different mappings between data values and rendered colours.

The data, aesthetics mappings, and geometries are the same as in earlier code; to alter how the plot looks, we have changed only the scale and palette used for the color aesthetic. Conceptually it is still exactly the same plot we created earlier, except for the colours used. This is a very important point to understand, because it allows us to separate two different concerns: the semantic structure and the graphic design.

9.6 Try the different palettes available through the brewer scale. You can play directly with the palettes using function brewer\_pal() from package 'scales' together with show\_col()).

```
show_col(brewer_pal()(3))
show_col(brewer_pal(type = "qual", palette = 2, direction = 1)(3))
```

Once you have found a suitable palette for these data, redo the plot above with the chosen palette.

When not relying on colors, the most common way of distinguishing groups

of observations in scatter plots is to use the shape of the points as an *aesthetic*. We need to change a single "word" in the code statement to achieve this different mapping.

```
ggplot(data = mtcars, aes(x = disp, y = mpg, shape = factor(cyl))) +
  geom_point()
```

We can use scale\_shape\_manual to choose each shape to be used. We set three "open" shapes that we will see later are very useful as they obey both color and fill aesthetics.

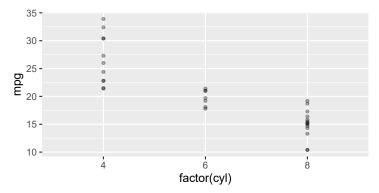
```
ggplot(data = mtcars, aes(x = disp, y = mpg, shape = factor(cyl))) +
  geom_point() +
  scale_shape_manual(values = c(21, 22, 23))
```

It is also possible to use characters as shapes. The character is centered on the position of the observation. As the numbers used as symbols are self-explanatory, we suppress the default guide or key.

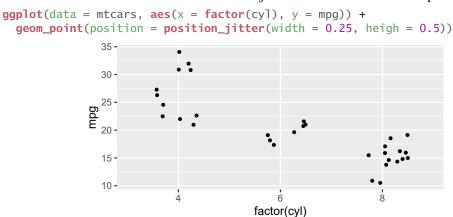
One variable in the data can be mapped to more than one aesthetic, allowing redundant aesthetics. This may seem wasteful, but it is extremely useful as it allows one to produce figures that, even when produced in color, can still be read if reproduced as black-and-white images.

Dot plots are similar to scatter plots but a factor is mapped to either the x or y *aesthetic*. Dot plots are prone to have overlapping observations, and one way of making these points visible is to make them partly transparent by setting a constant value smaller than one for the alpha *aesthetic*.

```
ggplot(data = mtcars, aes(x = factor(cyl), y = mpg)) +
   geom_point(alpha = 1/3)
```

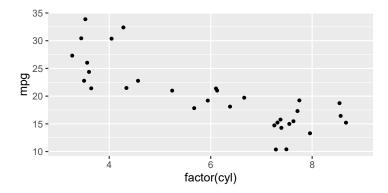


Function position\_identity(), which is the default for geom\_point(), does not alter the coordinates or position of observations, as shown in all examples above. To make overlapping observations visible, instead of making the points semitransparent as above, we can randomly displace them. This is called *jitter*, and can be added using position\_jitter() as argument to formal parameter position. The amount of jitter is set by nemeric arguments passed to width and/or height, given as a fraction of the distance between adjacent factor levels in the plot.



The name as a character string can be also used when no arguments need to be passed to the *position* function, and for some positions by passing numerical arguments to specific parameters of geometries. However, the default width of  $\pm 0.5$  tends to be rarely optimal.

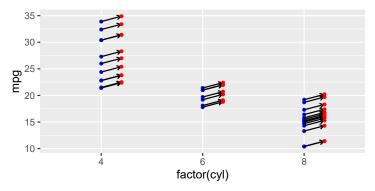
```
ggplot(data = mtcars, aes(x = factor(cyl), y = mpg), colour = factor(cyl)) +
  geom_point(position = "jitter")
```



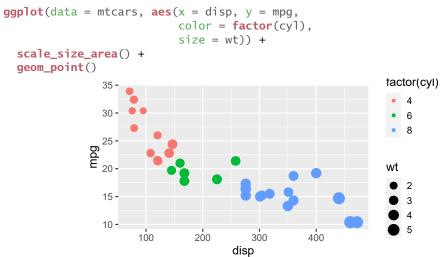
The displacement introduced by jitter and nudge differ in that jitter is random, and nudge deterministic. In each case the displacement can be separately adjusted vertically and horizontally. Jitter, as shown above is useful when we desire to make visible overlapping points. Nudge is most frequently used with data labels to avoid occluding points or other graphical features.

Layer function <code>geom\_point\_s()</code> from package 'ggpp' is used below to make the displacement visible by drawing an arrow connecting original and displaced positions for each observation. We need to use the <code>\_keep</code> flavor of the position functions for arrows to be drawn.

The amount of nudging is set by a distance expressed in data units through parameters x and y. (Factors have mode numeric and each level is represented by an integer, thus distance between levels of a factor is 1.)



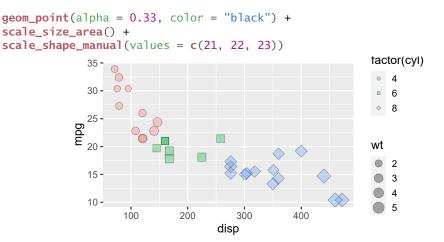
We can create a "bubble" plot by mapping the size *aesthetic* to a continuous variable. In this case, one has to think what is visually more meaningful. Although the radius of the shape is frequently mapped, due to how human perception works, mapping a variable to the area of the shape is more useful by being perceptually closer to a linear mapping. For this example we add a new variable to the plot. The weight of the car in tons and map it to the area of the points.



9.7 If we use a radius-based scale the "impression" is different.

Make the plot, look at it carefully. Check the numerical values of some of the weights, and assess if your perception of the plot matches the numbers behind it.

As a final example summarizing the use of <code>geom\_point()</code>, we combine different *aesthetics* and *scales* in the same scatter plot.

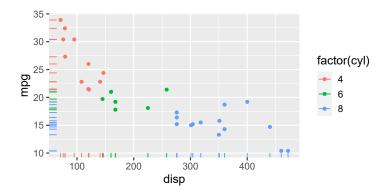


9.8 Play with the code in the chunk above. Remove or change each of the mappings and the scale, display the new plot, and compare it to the one above. Continue playing with the code until you are sure you understand what graphical element in the plot is added or modified by each individual argument or "word" in the code statement.

It is common to draw error bars together with points representing means or medians of observations and <code>geom\_pointrange()</code> achieves this task based on the values mapped to the x, y, ymin and ymax, using y for the position of the point and ymin and ymax for the positions of the ends of the line segment representing a range. Two other <code>geometries</code>, <code>geom\_range()</code> and <code>geom\_errorbar()</code> draw only a segment or a segment with capped ends. They are frequently used together with <code>statistics</code> when summaries are calculated on the fly, but can also be used directly when the data summaries are stored in a data frame passed as an argument to data.

### 9.5.2 Rug

Rarely, rug plots are used by themselves. Instead they are usually an addition to scatter plots. An example of the use of  $geom_rug()$  follows. They make it easier to see the distribution of observations along the x- and y-axes.



Rug plots are most useful when the local density of observations is not too high, otherwise rugs become too cluttered and the "rug threads" may overlap. When overlap is moderate, making the segments semitransparent by setting the alpha aesthetic to a constant value smaller than one, can make the variation in density easier to appreciate. When the number of observations is large, marginal density plots should be preferred.

#### 9.5.3 Line and area

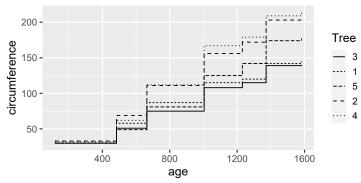
For line plots we use <code>geom\_line()</code>. The <code>size</code> of a line is its thickness, and as we had <code>shape</code> for points, we have <code>linetype</code> for lines. In a line plot, observations in successive rows of the data frame, or the subset corresponding to a group, are joined by straight lines. We use a different data set included in R, <code>Orange</code>, with data on the growth of five orange trees. See the help page for <code>Orange</code> for details.

```
ggplot(data = Orange,
                           = circumference, linetype = Tree)) +
        aes(x = age, y)
  geom_line()
                  200
                                                                            Tree
               circumference
                  150
                                                                               1
                                                                               5
                  100
                                                                               2
                   50 -
                                400
                                            800
                                                        1200
                                                                     1600
                                             age
```

Instead of drawing a line joining the successive observations, we may want to draw a disconnected straight-line segment for each observation or row in the data. In this case, we use <code>geom\_segment()</code> which accepts x, xend, y and yend as mapped aesthetics. <code>geom\_curve()</code> draws curved lines, and the curvature, control points, and angles can be controlled through additional *aesthetics*. These two *geometries* support arrow heads at their ends. Other *geometries* useful for drawing lines or segments are <code>geom\_path()</code>, which is similar to <code>geom\_line()</code>, but instead of joining ob-

servations according to the values mapped to x, it joins them according to their row-order in data, and geom\_spoke(), which is similar to geom\_segment() but using a polar parametrization, based on x, y for origin, and angle and radius for the segment. Finally, geom\_step() plots only vertical and horizontal lines to join the observations, creating a stepped line.

```
ggplot(data = Orange,
    aes(x = age, y = circumference, linetype = Tree)) +
    geom_step()
```



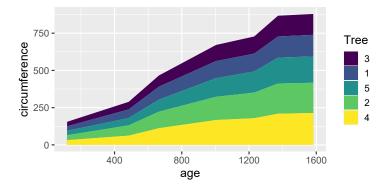
9.9 Using the following toy data, make three plots using geom\_line(), geom\_path(), and geom\_step to add a layer.

```
toy.df <- data.frame(x = c(1,3,2,4), y = c(0,1,0,1))
```

While <code>geom\_line()</code> draws a line joining observations, <code>geom\_area()</code> supports filling the area below the line according to the <code>fill</code> aesthetic. In contrast <code>geom\_ribbon()</code> draws two lines based on the <code>x</code>, <code>ymin</code> and <code>ymax</code> aesthetics, with the space between the lines filled according to the <code>fill</code> aesthetic. Finally, <code>geom\_polygon()</code> is similar to <code>geom\_path()</code> but connects the extreme observations forming a closed polygon that supports <code>fill</code>.

Much of what was described above for  $geom\_point()$  can be adapted to  $geom\_line()$ ,  $geom\_ribbon()$ ,  $geom\_area()$  and other geometries described in this section. In some cases, it is useful to stack the areas—e.g., when the values represent parts of a bigger whole. In the next, contrived, example, we stack the growth of the different trees by using position = "stack" instead of the default position = "identity". (Compare the y axis of the figure below to that drawn using  $geom\_line()$  on page 292.)

```
ggplot(data = Orange,
    aes(x = age, y = circumference, fill = Tree)) +
    geom_area(position = "stack")
```



Finally, three *geometries* for drawing lines across the whole plotting area: geom\_hline(), geom\_vline() and geom\_abline(). The first two draw horizontal and vertical lines, respectively, while the third one draws straight lines according to the *aesthetics* slope and intercept determining the position. The lines drawn with these three geoms extend to the edge of the plotting area.

geom\_hline() and geom\_vline() require a single aesthetic, yintercept and xintercept, respectively. Different from other geoms, the data for these aesthetics can also be passed as constant numeric vectors. The reason for this is that these geoms are most frequently used to annotate plots rather than plotting observations. Let's assume that we want to highlight an event at the age of 1000 days.

```
ggplot(data = Orange,
       aes(x = age, y = circumference, fill = Tree)) +
  geom_area(position = "stack") +
  geom_vline(xintercept = 1000, color = "gray75") +
  geom_vline(xintercept = 1000, linetype =
                750
                                                                    Tree
             circumference
                                                                       3
                500
                                                                       1
                                                                       5
                                                                       2
                250
                  0
                                       800
                            400
                                                  1200
                                                              1600
                                        age
```

**9.10** Change the order of the three layers in the example above. How did the figure change? What order is best? Would the same order be the best for a scatter plot? And would it be necessary to add two geom\_vline() layers?

### 9.5.4 Column

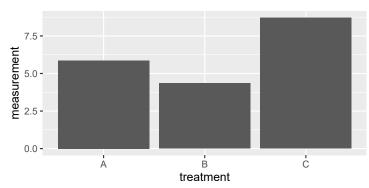
The *geometry* geom\_col() can be used to create *column plots* where each bar represents an observation or case in the data.

R users not familiar yet with 'ggplot2' are frequently surprised by the default behavior of geom\_bar() as it uses stat\_count() to produce a histogram, rather than plotting values as is (see section 9.6.4 on page 314). geom\_col() is identical to geom\_bar() but with "identity" as the default statistic.

We create artificial data that we will reuse in multiple variations of the next figure.

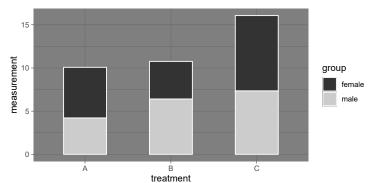
First we plot data for females only, using defaults for all *aesthetics* except x and y which we explicitly map to variables.

```
ggplot(subset(my.col.data, group == "female"),
    aes(x = treatment, y = measurement)) +
    geom_col()
```



We play with *aesthetics* to produce a plot with a semi-formal style—e.g., suitable for a science popularization article or book. See section 9.9 and section 9.12 for information on scales and themes, respectively. We set width = 0.5 to make the bars narrower. Setting color = "white" overrides the default color of the lines bordering the bars.

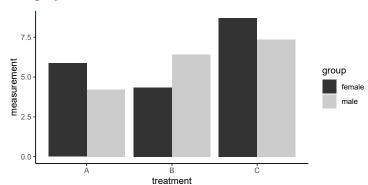
```
ggplot(my.col.data, aes(x = treatment, y = measurement, fill = group)) +
    geom_col(color = "white", width = 0.5) +
    scale_fill_grey() + theme_dark()
```



We next use a formal style, and in addition, put the bars side by side by

setting position = "dodge" to override the default position = "stack". Setting color = NA removes the lines bordering the bars.

```
ggplot(my.col.data, aes(x = treatment, y = measurement, fill = group)) +
    geom_col(color = NA, position = "dodge") +
    scale_fill_grey() + theme_classic()
```



9.11 Change the argument to position, or let the default be active, until you understand its effect on the figure. What is the difference between *positions* "identity", "dodge" and "stack"?

9.12 Use constants as arguments for *aesthetics* or map variable treatment to one or more of the *aesthetics* used by geom\_col(), such as color, fill, linetype, size, alpha and width.

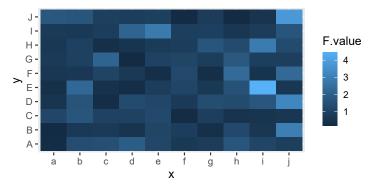
### 9.5.5 Tiles

We can draw square or rectangular tiles with <code>geom\_tile()</code> producing tile plots or simple heat maps.

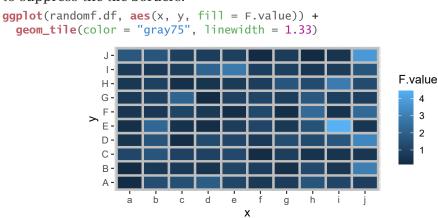
We here generate 100 random draws from the *F* distribution with degrees of freedom  $v_1 = 5$ ,  $v_2 = 20$ .

geom\_tile() requires aesthetics x and y, with no defaults, and width and height with defaults that make all tiles of equal size filling the plotting area.

```
ggplot(randomf.df, aes(x, y, fill = F.value)) +
geom_tile()
```



We can set color = "gray75" and linewidth = 1.33 to make the tile borders more visible as in the example below, or use a contrasting color, to better delineate the borders of the tiles. What to use will depend on whether the individual tiles add meaningful information. In cases like when rows of tiles correspond to individual genes and columns to discrete treatments, the use of contrasting tile borders is preferable. In contrast, in the case when the tiles are an approximation to a continuous surface such as measurements on a regular spatial grid, it is best to suppress the tile borders.



9.13 Play with the arguments passed to parameters color and size in the example above, considering what features of the data are most clearly perceived in each of the plots you create.

Any continuous fill scale can be used to control the appearance. Here we show a tile plot using a gray gradient, with missing values in red.

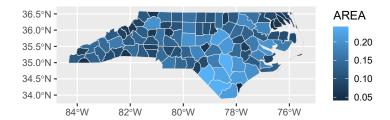
```
ggplot(randomf.df, aes(x, y, fill = F.value) +
  geom_tile(color = "white") +
  scale_fill_gradient(low = "gray15", high = "gray85", na.value = "red")
```

In contrast to geom\_tile(), geom\_rect() draws rectangular tiles based on the position of the corners, mapped to aesthetics xmin, xmax, ymin and ymax.

# 9.5.6 Simple features (sf)

'ggplot2' version 3.0.0 or later supports the plotting of shape data similar to the plotting in geographic information systems (GIS) through <code>geom\_sf()</code> and its companions, <code>geom\_sf\_text()</code>, <code>geom\_sf\_label()</code>, and <code>stat\_sf()</code>. This makes it possible to display data on maps, for example, using different fill values for different regions. Special *coordinate* <code>coord\_sf()</code> can be used to select different projections for maps. The <code>aesthetic</code> used is called <code>geometry</code> and contrary to all the other aesthetics we have seen until now, the values to be mapped are of class <code>sfc</code> containing <code>simple</code> <code>features</code> data with multiple components. Manipulation of simple features data is supported by package 'sf'. This subject exceeds the scope of this book, so a single and very simple example follows.

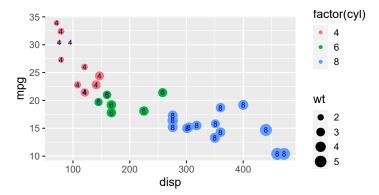
```
nc <- sf::st_read(system.file("shape/nc.shp", package = "sf"), quiet = TRUE)
ggplot(nc) +
  geom_sf(aes(fill = AREA), color = "gray90")</pre>
```



### 9.5.7 Text

We can use geom\_text() or geom\_label() to add text labels to observations. For geom\_text() and geom\_label(), the aesthetic label provides the text to be plotted and the usual aesthetics x and y, the location of the labels. As one would expect, the color and size aesthetics can also be used for the text.

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In addition, angle and vjust and hjust can be used to rotate the text and adjust its position. The default value of 0.5 for both hjust and vjust sets the center of the text at the supplied x and y coordinates. "Vertical" and "horizontal" for justification refer to the text, not the plot. This is important when angle is different from zero. Values larger than 0.5 shift the label left or down, and values smaller than 0.5, right or up with respect to its x and y coordinates. A value of 1 or 0 sets the text so that its edge is at the supplied coordinate. Values outside the range 0... 1 shift the text even farther away, however, still using units based on the length or height of the text label. Recent versions of 'ggplot2' make possible justification using character constants for alignment: "left", "middle", "right", "bottom", "center" and "top", and two special alignments, "inward" and "outward", that automatically vary based on the position in the plotting area.

In the case of geom\_label() the text is enclosed in a box, which obeys the fill *aesthetic* and takes additional parameters (described starting at page 301) allowing control of the shape and size of the box. However, geom\_label() does not support rotation with the angle aesthetic.

You should be aware that R and 'qqplot2' support the use of UNICODE, such as UTF8 character encodings in strings. If your editor or IDE supports their use, then you can type Greek letters and simple maths symbols directly, and they may show correctly in labels if a suitable font is loaded and an extended encoding like UTF8 is in use by the operating system. Even if UTF8 is in use, text is not fully portable unless the same font is available, as even if the character positions are standardized for many languages, most UNICODE fonts support at most a small number of languages. In principle one can use this mechanism to have labels both using other alphabets and languages like Chinese with their numerous symbols mixed in the same figure. Furthermore, the support for fonts and consequently character sets in R is output-device dependent. The font encoding used by R by default depends on the default locale settings of the operating system, which can also lead to garbage printed to the console or wrong characters being plotted running the same code on a different computer from the one where a script was created. Not all is lost, though, as R can be coerced to use system fonts and Google fonts with functions provided by packages 'showtext' and 'extrafont'. Encodingrelated problems, especially in MS-Windows, are common.

In the remaining examples, with output not shown, we use geom\_text() or

geom\_label() together with geom\_point() as this is how they may be used to label observations.

9.14 Modify the example above to use geom\_label() instead of geom\_text() using, in addition, the fill aesthetic.

In the next example we select a different font family, using the same characters in the Roman alphabet. The names "sans" (the default), "serif" and "mono" are recognized by all graphics devices on all operating systems. Additional fonts are available for specific graphic devices, such as the 35 "PDF" fonts by the pdf() device. In this case, their names can be queried with names(pdfFonts()).

```
ggplot(my.data, aes(x, y, label = label)) +
  geom_text(angle = 45, hjust = 1.5, size = 8, family = "serif") +
  geom_point()
```

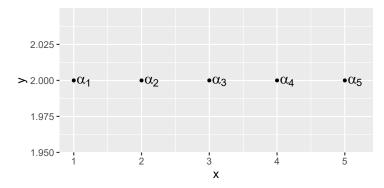
9.15 In the examples above the character strings were all of the same length, containing a single character. Redo the plots above with longer character strings of various lengths mapped to the label *aesthetic*. Do also play with justification of these labels.

Plotting (mathematical) expressions involves mapping to the label aesthetic character strings that can be parsed as expressions, and setting parse = TRUE (see section 9.14 on page 357). Here, we build the character strings using paste() but, of course, they could also have been entered one by one. This use of paste() provides an example of recycling of shorter vectors (see section 3.10 on page 64).

```
my.data <-
   data.frame(x = 1:5, y = rep(2, 5), label = paste("alpha[", 1:5, "]", sep = ""))
my.data$label
## [1] "alpha[1]" "alpha[2]" "alpha[3]" "alpha[4]" "alpha[5]"</pre>
```

Text and labels do not automatically expand the plotting area past their anchoring coordinates. In the example above, we need to use expand\_limits() to ensure that the text is not clipped at the edge of the plotting area.

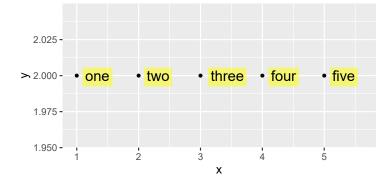
```
ggplot(my.data, aes(x, y, label = label)) +
  geom_text(hjust = -0.2, parse = TRUE, size = 6) +
  geom_point() +
  expand_limits(x = 5.2)
```



In the example above, we mapped to label the text to be parsed. It is also possible, and usually preferable, to build suitable labels on the fly within aes() when setting the mapping for label. Here we use geom\_text() with strings to be parsed into expressions created on the fly within the call to aes(). The same approach can be used for regular character strings not requiring parsing.

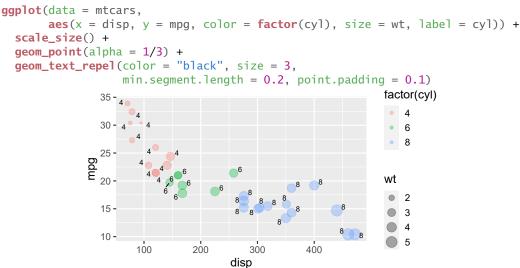
```
ggplot(my.data, aes(x, y, label = paste("alpha[", x, "]", sep = ""))) +
  geom_text(hjust = -0.2, parse = TRUE, size = 6) +
  geom_point()
```

As geom\_label() obeys the same parameters as geom\_text() except for angle, we briefly describe below only the additional parameters compared to geom\_text(). We may want to alter the default width of the border line or the color used to fill the rectangle, or to change the "roundness" of the corners. To suppress the border line, use label.size = 0. Corner roundness is controlled by parameter label.r and the size of the margin around the text by label.padding.



9.16 Play with the arguments to the different parameters and with the *aesthetics* to get an idea of what can be done with them. For example, use thicker border lines and increase the padding so that a visually well-balanced margin is retained. You may also try mapping the fill and color *aesthetics* to factors in the data.

If the parameter check\_overlap of geom\_text() is set to TRUE, text overlap will be avoided by suppressing the text that would otherwise overlap other text. *Repulsive* versions of geom\_text() and geom\_label(), geom\_text\_repel() and geom\_label\_repel(), are available in package 'ggrepel'. These *geometries* avoid overlaps by automatically repositioning the text or labels. Please read the package documentation for details of how to control the repulsion strength and direction, and the properties of the segments linking the labels to the position of their data coordinates. Nearly all aesthetics supported by geom\_text() and geom\_label() are supported by the repulsive versions. However, given that a segment connects the label or text to its anchor point, several properties of these segments can also be controlled with aesthetics or arguments.



### 9.5.8 Plot insets

The support for insets in 'ggplot2' is confined to annotation\_custom() which was designed to be used for static annotations expected to be the same in each panel of a plot (the use of annotations is described in section 9.10). Package 'ggpmisc' provides geoms that mimic geom\_text() in relation to the *aesthetics* used, but that similarly to geom\_sf(), expect that the column in data mapped to the label aesthetics are lists of objects containing multiple pieces of information, rather than atomic vectors. Three geometries are currently available: geom\_table(), geom\_plot() and geom\_grob().

Given that geom\_table(), geom\_plot() and geom\_grob() will rarely use a mapping inherited from the whole plot, by default they do not inherit it. Either the

mapping should be supplied as an argument to these functions or their parameter inherit.aes explicitly set to TRUE.

The plotting of tables by mapping a list of data frames to the label *aesthetic* is done with <code>geom\_table()</code>. Positioning, justification, and angle work as for <code>geom\_text()</code> and are applied to the whole table. Only <code>tibble</code> objects (see documentation of package 'tibble') can contain, as variables, lists of data frames, so this *geometry* requires the use of <code>tibble</code> objects to store the data. The table(s) are created as 'grid' <code>grob</code> objects, collected in a tree and added to the <code>ggplot</code> object as a new layer.

We first generate a tibble containing summaries from the data, formatted as character strings, wrap this tibble in a list, and store this list as a column in another tibble. To accomplish this, we use functions from the 'tidyverse' described in chapter 8.

```
mtcars %.>%
  group_by(., cyl) %.>%
  summarize(.,
             "mean wt" = format(mean(wt), digits = 3),
             "mean disp" = format(mean(disp), digits = 2),
             "mean mpg" = format(mean(mpg), digits = 2)) -> my.table
table.tb \leftarrow tibble(x = 500, y = 35, table.inset = list(my.table))
ggplot(data = mtcars, aes(x = disp, y = mpg,
                             color = factor(cyl),
                             size = wt,
                             label = cyl)) +
  scale_size() +
  geom_point() +
  geom_table(data = table.tb,
              aes(x = x, y = y, label = table.inset),
              color = "black", size = 3)
                                                               tactor(cyl)
                35
                                                                  4
                                       2.29
                                                                  6
                30 -
                                       3.12
                                              183
                                                      20
                                                                  8
                                              353
              6du 25
                20 -
                15 -
                                                                  4
                10 -
                                       300
                      100
                               200
                                                400
                                                         500
                                      disp
```

The color and size aesthetics control the text in the table(s) as a whole. It is also possible to rotate the table(s) using angle. As with text labels, justification is interpreted in relation to table-text orientation. We set the y=0 in data.tb and then use vjust=1 to position the top of the table at this coordinate value.

```
hjust = 1, vjust = 0, angle = 90)
```

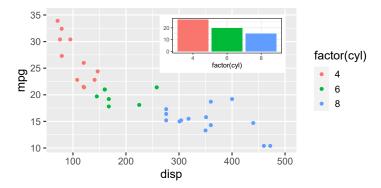
Parsed text, using R's *plotmath* syntax is supported in the table, with fallback to plain text in case of parsing errors, on a cell-by-cell basis. We end this section with a simple example, which even if not very useful, demonstrates that <code>geom\_table()</code> behaves like a "normal" ggplot *geometry* and that a table can be the only layer in a ggplot if desired. The addition of multiple tables with a single call to <code>geom\_table()</code> by passing a <code>tibble</code> with multiple rows as an argument for <code>data</code> is also possible.

The *geometry* geom\_table() uses functions from package 'gridExtra' to build a graphical object for the table. The use of table themes was not yet supported by this geometry at the time of writing.

Geometry geom\_plot() works much like geom\_table(), but instead of expecting a list of data frames or tibbles to be mapped to the label aesthetics, it expects a list of ggplots (objects of class gg). This allows adding as an inset to a ggplot, another ggplot. In the times when plots were hand drafted with India ink on paper, the use of inset plots was more frequent than nowadays. Inset plots can be very useful for zooming-in on parts of a main plot where observations are crowded and for displaying summaries based on the observations shown in the main plot. The inset plots are nested in viewports which control the dimensions of the inset plot, and aesthetics vp.height and vp.width control their sizes—with defaults of 1/3 of the height and width of the plotting area of the main plot. Themes can be applied separately to the main and inset plots.

In the first example of inset plots, we include one of the summaries shown above as an inset table. We first create a tibble containing the plot to be inset.

```
mtcars %.>%
  group_by(., cyl) %.>%
  summarize(., mean.mpg = mean(mpg)) %.>%
  ggplot(data = .,
         aes(factor(cyl), mean.mpg, fill = factor(cyl))) +
  scale_fill_discrete(guide = "none") +
  scale_y_continuous(name = NULL) +
    geom_col() +
    theme_bw(8) -> my.plot
plot.tb <- tibble(x = 500, y = 35, plot.inset = list(my.plot))</pre>
ggplot(data = mtcars, aes(x = disp, y = mpg,
                          color = factor(cyl))) +
  geom_point() +
  geom_plot(data = plot.tb,
            aes(x = x, y = y, label = plot.inset),
            vp.width = 1/2,
            hjust = "inward", vjust = "inward")
```



In the second example we add the zoomed version of the same plot as an inset. 1) Manually set limits to the coordinates to zoom into a region of the main plot, 2) set the *theme* of the inset, 3) remove axis labels as they are the same as in the main plot, 4) and 5) highlight the zoomed-in region in the main plot. This fairly complex example shows how a new extension to 'ggplot2' can integrate well into the grammar of graphics paradigm. In this example, to show an alternative approach, instead of collecting all the data into a data frame, we map constant values directly to the various aesthetics within annotate() (see section 9.10 on page 345).

```
p.main <- ggplot(data = mtcars, aes(x = disp, y = mpg, color = factor(cyl))) +</pre>
  geom_point()
p.inset <- p.main +
  coord_cartesian(xlim = c(270, 330), ylim = c(14, 19)) +
  labs(x = NULL, y = NULL) +
  scale_color_discrete(guide = "none") +
  theme_bw(8) + theme(aspect.ratio = 1)
p.main +
  geom_plot(x = 480, y = 34, label = list(p.inset), vp.height = 1/2,
            hjust = "inward", vjust = "inward") +
  annotate(geom = "rect", fill = NA, color = "black",
           xmin = 270, xmax = 330, ymin = 14, ymax = 19,
           linetype = "dotted")
               30 -
                                                             factor(cyl)
               25
                                                                4
                                                                6
               20 -
               15 -
               10 -
                              200
                     100
                                       300
                                                400
                                    disp
```

Geometry geom\_grob() works much like geom\_table() and geom\_plot() but expects a list of 'grid' graphical objects, called grob for short. This adds generality at the expense of having to separately create the grobs either using 'grid' or by converting other objects into grobs. This geometry is as flexible as annotation\_custom() with respect to the grobs, but behaves as a *geometry*. We

show an example that adds two bitmaps to the plot. The bitmaps are read from PNG files, converted into grobs, and added to the plot as a new layer. The PNG bitmaps used have a transparent background.

```
file1.name <-
    system.file("extdata", "Isoquercitin.png", package =
                                                                "ggpmisc",
Work = TRUE)
Isoquercitin <- magick::image_read(file1.name)</pre>
file2.name <-
  system.file("extdata", "Robinin.png", package = "ggpmisc", mustWork = TRUE)
Robinin <- magick::image_read(file2.name)</pre>
grob.tb <- tibble(x = c(0, 100), y = c(10, 20), height = 1/3, width = c(1/2),
                   grobs = list(grid::rasterGrob(image = Isoquercitin),
                                grid::rasterGrob(image = Robinin)))
ggplot() +
  geom_grob(data = grob.tb,
          aes(x = x, y = y, label = grobs, vp.height = height, vp.width = width),
                hjust = "inward", vjust = "inward")
               20.0 -
               175
             > 15.0 ⋅
               12.5
               10.0
                                                       75
                                                                  100
                     Ò
                                           50
                                           х
```

Grid graphics provide the low-level functions that both 'ggplot2' and 'lattice' use under the hood. Grid supports different types of units for expressing the coordinates of positions within the plotting area. All examples outside this text box use "native" data coordinates, however, coordinates can be also given in physical units like "mm". More useful when working with scalable plots is to use "npc" normalized parent coordinates, which are expressed as numbers in the range 0 to 1, relative to the dimensions of the sides of the current viewport, with origin at the lower left corner.

Package 'ggplot2' interprets x and y coordinates in "native" data coordinates, and trickery seems to be needed to get around this limitation. A rather general solution is provided by package 'ggpmisc' through *aesthetics* npcx and npcy and *geometries* that support them. At the time of writing, geom\_text\_npc(), geom\_label\_npc(), geom\_table\_npc(), geom\_plot\_npc() and geom\_grob\_npc(). These *geometries* are useful for annotating plots and adding insets at positions relative to the plotting area that remain always consistent across different plots, or across panels when using facets with free axis limits. Being geometries they provide freedom in the elements added to different panels and their positions.

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# 9.6 Statistics

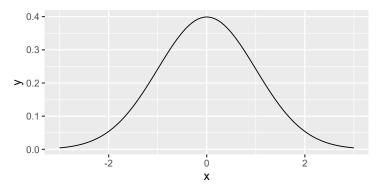
Before learning about 'ggplot2' *statistics*, it is important to have clear how the mapping of factors to *aesthetics* works. When a factor, for example, is mapped to color, it creates a new grouping, with the observations matching a given level of the factor, corresponding to a group. Most *statistics* operate on the data for each of these groups separately, returning a summary for each group, for example, the mean of the observations in a group.

### 9.6.1 Functions

In addition to plotting data from a data frame with variables to map to x and y aesthetics, it is possible to have only a variable mapped to x and use  $stat_function()$  to compute the values to be mapped to y using an R function. This avoids the need to generate data beforehand as even the number of data points to be generated can be set in  $geom_function()$ . Any R function, user defined or not, can be used as long as it is vectorized, with the length of the returned vector equal to the length of the vector passed as first argument to it. The variable mapped to x determines the range, and the argument to parameter x of x of x determines the range and the argument to parameter x of x determines to x determines the values to napped to x. These are the x and y values passed to the x determines the values to napped to x.

We start with the Normal distribution function. We rely on the defaults n = 101 and geom = "path".

```
ggplot(data.frame(x = -3:3), aes(x = x)) +
stat_function(fun = dnorm)
```



Using a list we can even pass by name additional arguments to use when the function is called.

```
ggplot(data.frame(x = -3:3), aes(x = x)) +
    stat_function(fun = dnorm, args = list(mean = 1, sd = .5))
```

9.17 Edit the code above so as to plot in the same figure three curves, either for three different values for mean or for three different values for sd.

Named user-defined functions (not shown), and anonymous functions (below) can also be used.

9.18 Edit the code above to use a different function, such as  $e^{x+k}$ , adjusting the argument(s) passed through args accordingly. Do this by means of an anonymous function, and by means of an equivalent named function defined by your code.

### 9.6.2 Summaries

The summaries discussed in this section can be superimposed on raw data plots, or plotted on their own. Beware, that if scale limits are manually set, the summaries will be calculated from the subset of observations within these limits. Scale limits can be altered when explicitly defining a scale or by means of functions xlim() and ylim(). See section 9.11 on page 348 for an explanation of how coordinate limits can be used to zoom into a plot without excluding of x and y values from the data.

It is possible to summarize data on the fly when plotting. We describe in the same section the calculation of measures of central tendency and of variation, as stat\_summary() allows them to be calculated simultaneously and added together with a single layer.

For use in the examples, we generate some normally distributed artificial data.

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We will reuse a "base" scatter plot in a series of examples, so that the differences are easier to appreciate. We first add just the mean. In this case, we need to pass as an argument to stat\_summary(), the geom to use, as the default one, geom\_pointrange(), expects data for plotting error bars in addition to the mean. This example uses a hyphen character as the constant value of shape (see the example for geom\_point() on page 287 on the use of digits as shape). Instead of passing "mean" as an argument to parameter fun (earlier called fun.y), we can pass, if desired, other summary functions like "median". In the case of these functions that return a single computed value, we pass them, or character strings with their names, as an argument to parameter fun.

To pass as an argument a function that returns a central value like the mean plus confidence or other limits, we use parameter fun.data instead of fun. In the next example we add means and confidence intervals for p=0.95 (the default) assuming normality.

```
stat_summary(fun.data = "mean_cl_normal", color = "red", size = 1, alpha = 0.7)
```

We can override the default of p=0.95 for confidence intervals by setting, for example, conf.int = 0.90 in the list of arguments passed to the function. The intervals can also be computed without assuming normality, using the empirical distribution estimated from the data by bootstrap. To achieve this we pass to fun.data the argument "mean\_cl\_boot" instead of "mean\_cl\_normal".

```
 \begin{array}{lll} \textbf{stat\_summary}(\texttt{fun.data} = \texttt{"mean\_cl\_boot"}, \\ & \texttt{fun.args} = \textbf{list}(\texttt{conf.int} = 0.90), \\ & \texttt{color} = \texttt{"red"}, \texttt{ size} = 1, \texttt{ alpha} = 0.7) \\ & \textbf{For } \bar{x} \pm \texttt{s.e.} \text{ we should pass "mean\_se" and for } \bar{x} \pm \texttt{s.d. "mean\_sdl"}. \\ & \textbf{stat\_summary}(\texttt{fun.data} = \texttt{"mean\_se"}, \\ & \texttt{color} = \texttt{"red"}, \texttt{ size} = 1, \texttt{ alpha} = 0.7) \\ \end{array}
```

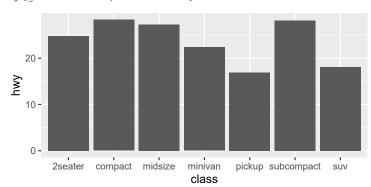
We do not give an example here, but it is possible to use user-defined functions instead of the functions exported by package 'ggplot2' (based on those in package 'Hmisc'). Because arguments to the function used, except for the first one containing the variable in data mapped to the *y* aesthetic, are supplied as a named

list through parameter fun.args, the names used for parameters in the function definition need only match the names in this list.

Finally, we plot the means in a scatter plot, with the observations superimposed on the error bars as a result of the order in which the layers are added to the plot. In this case, we set fill, color and alpha (transparency) to constants, but in more complex data sets, mapping them to factors in data can be used for grouping of observations. Here, adding two plot layers with stat\_summary() allows us to plot the mean and the error bars using different colors.

We can plot means, or other summaries, by group mapped to x (class in this example) as columns by passing "col" as an argument to geom. In this way we avoid the need to compute the summaries in advance.

```
ggplot(mpg, aes(class, hwy)) +
    stat_summary(geom = "col", fun = mean)
```



We can easily add error bars to the column plot. We use size to make the lines of the error bars thicker. The default *geometry* in stat\_summary() is geom\_pointrange(), so we can pass "linerange" as an argument for geom to eliminate the point.

Passing "errorbar" instead of "linerange" to geom results in traditional "capped" error bars. However, this type of error bar has been criticized as adding unnecessary clutter to plots (Tufte 1983). We can use width to reduce the width of the caps at the ends of the error bars.

If we have already calculated values for the summaries, we can still obtain the same plots by mapping variables to the *aesthetics* required by geom\_errorbar() and geom\_linerange(): x, y, ymax and ymin.

The "reverse" syntax is also valid, as we can add the *geometry* to the plot object and pass the *statistics* as an argument to it. In general in this book we avoid this alternative syntax for the sake of consistency.

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```
ggplot(mpg, aes(class, hwy)) +
  geom_col(stat = "summary", fun = mean)
```

### 9.6.3 Smoothers and models

For describing or highlighting relationships between pairs of continuous variables, using a line, straight or curved, in a plot is very effective. To draw lines that provide a meaningful and accurate description of the relationship, we fit models to observations and base the plotted line on model predictions. Being this a statistical procedure and observations subject to uncontrolled variation, we can also assess the reliability of the estimation. See section 7.8 on page 197 for a description of the model fitting procedures underlying the plotting described in the current section.

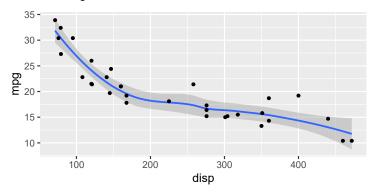
The statistic stat\_smooth() fits a smooth curve to observations in the case when the scales for x and y are continuous—the corresponding geometry  $geom_smooth$ () uses this statistic, and differs only in how arguments are passed to formal parameters. For the first example, we use  $stat_smooth$ () with the default smoother, a spline. The type of smoother is automatically chosen based on the number of observations and informed by a message. The formula must be stated using the names of the x and y aesthetics, rather than the original names of the mapped variables in the mtcars data frame. Splines are described in section 7.12 on page 221.

```
ggplot(data = mtcars, aes(x = disp, y = mpg)) +
    stat_smooth(formula = y ~ x)
```

In most cases we will want to plot the observations as points together with the smoother. We can plot the observation on top of the smoother, as done here, or the smoother on top of the observations.

```
ggplot(data = mtcars, aes(x = disp, y = mpg)) +
    stat_smooth(formula = y ~ x) +
    geom_point()
```

## `geom\_smooth()` using method = 'loess'

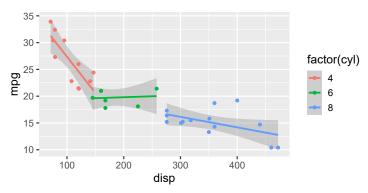


Instead of using the default spline, we can fit a different model. In this example we use a linear model as smoother, fitted by lm(). Model fitting is explained in section 7.9 on page 198.

```
stat\_smooth(method = "lm", formula = y \sim x) +
```

These data are really grouped, so we map variable cyl to the color *aesthetic*. Now we get three groups of points with different colours but also three separate smooth lines.

```
ggplot(data = mtcars, aes(x = disp, y = mpg, color = factor(cyl))) +
    stat_smooth(method = "lm", formula = y ~ x) +
    geom_point()
```

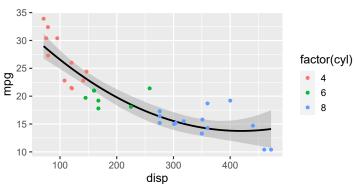


To obtain a single smoother for the three groups, we need to set the mapping of the color *aesthetic* to a constant within stat\_smooth(). This local value overrides the default color mapping set in ggplot() just for this plot layer. We use "black" but this could be replaced by any other color definition known to R.

```
ggplot(data = mtcars, aes(x = disp, y = mpg, color = factor(cyl))) +
    stat_smooth(method = "lm", formula = y ~ x, color = "black") +
    geom_point()
```

Instead of using the formula for a linear regression as smoother, we pass a different formula as an argument. In this example we use a polynomial of order 2.

```
ggplot(data = mtcars, aes(x = disp, y = mpg, color = factor(cyl))) +
    stat_smooth(method = "lm", formula = y ~ poly(x, 2), color = "black") +
    geom_point()
```



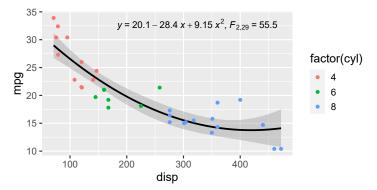
It is possible to use other types of models, including GAM and GLM, as smoothers, but we will give only two simple examples of the use of nls() to fit a model non-linear in its parameters (see section 7.11 on page 218 for details about fitting this same model with nls()). In the first one we fit a Michaelis-Menten equation to reaction rate (rate) versus reactant concentration (conc). Puromycin is a

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data set included in the R distribution. Function SSmicmen() is also from R, and is a *self-starting* implementation of the Michaelis-Menten equation. Thanks to this, even though the fit is done with an iterative algorithm, we do not need to explicitly provide starting values for the parameters to be fitted. We need to set se = FALSE because standard errors are not supported by the predict() method for nls fitted models.

In the second example we define the same model directly in the model formula, and provide the starting values explicitly. The names used for the parameters to be fitted can be chosen at will, within the restrictions of the R language, but of course the names used in formula and start must match each other.

In some cases it is desirable to annotate plots with fitted model equations or fitted parameters. One way of achieving this is by fitting the model and then extracting the parameters to manually construct text strings to use for text or label annotations. However, package 'ggpmisc' makes it possible to automate such annotations in many cases. This package also provides stat\_poly\_line() which is similar to stat\_smooth() but with method = "lm" consistently as its default irrespective of the number of observations.



This same package makes it possible to annotate plots with summary tables from a model fit.

```
my.formula \leftarrow y \sim poly(x, 2)
ggplot(data = mtcars, aes(x = disp, y = mpg, color = factor(cyl))) +
  stat_poly_line(formula = my.formula, color = "black") +
  stat_fit_tb(method.args = list(formula = my.formula),
                color = "black",
                tb.vars = c(Parameter = "term",
                              Estimate = "estimate",
                              "s.e." = "std.error",
                              "italic(t)" = "statistic",
                               "italic(P)" = "p.value").
                label.y.npc = "top", label.x.npc = "right".
                parse = TRUE) +
  geom_point()
                 35
                 30
                                (Intercept)
                                               0.501
                                                   40.1 < 0.001
                                poly(x, 2)1
                                           - 28 4
                                                2.84
                                                    - 10 < 0.001
                                                                  factor(cyl)
                                 poly(x, 2)2
                                                2.84 3.23
                                                         0.003
                                                                     4
                                                                      6
                 20 -
                                                                      8
                 15 -
                 10 -
                                 200
                                           300
                       100
                                                     400
                                        disp
```

Package 'ggpmisc' provides additional *statistics* for the annotation of plots based on fitted models supported by package 'broom' and its extensions. It also supports lines and equations for quantile regression and major axis regression. Please see the package documentation for details.

## 9.6.4 Frequencies and counts

When the number of observations is rather small, we can rely on the density of graphical elements to convey the density of the observations. For example, scatter plots using well-chosen values for alpha can give a satisfactory impression of the density. Rug plots, described in section 9.5.2 on page 291, can also satisfactorily convey the density of observations along x and/or y axes. Such approaches

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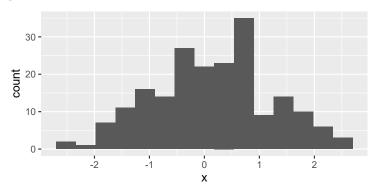
do not involve computations, while the *statistics* described in this section do. Frequencies by value-range (or bins) and empirical density functions are summaries especially useful when the number of observations is large. These summaries can be computed in one or more dimensions.

Histograms are defined by how the plotted values are calculated. Although histograms are most frequently plotted as bar plots, many bar or "column" plots are not histograms. Although rarely done in practice, a histogram could be plotted using a different *geometry* using stat\_bin(), the *statistic* used by default by geom\_histogram(). This *statistic* does binning of observations before computing frequencies, and is suitable for continuous *x* scales. When a factor is mapped to x, stat\_count() should be used, which is the default stat for geom\_bar(). These two *geometries* are described in this section about statistics, because they default to using statistics different from stat\_identity() and consequently summarize the data.

As before, we generate suitable artificial data.

We could have relied on the default number of bins automatically computed by the stat\_bin() statistic, however, we here set it to 15 with bins = 15. It is important to remember that in this case no variable in data is mapped onto the y aesthetic.

```
ggplot(my.data, aes(x)) +
  geom_histogram(bins = 15)
```



If we create a grouping by mapping a factor to an additional *aesthetic* how the bars created are positioned with respect to each other becomes relevant. We can then plot side by side with position = "dodge", stacked one above the other with position = "stack" and overlapping with position = "identity" in which case we need to make them semi-transparent with alpha = 0.5 so that they all remain visible.

```
ggplot(my.data, aes(y, fill = group)) +
  geom_histogram(bins = 15, position = "dodge")
```

The computed values are contained in the data that the *geometry* "receives" from the *statistic*. Many statistics compute additional values that are not mapped

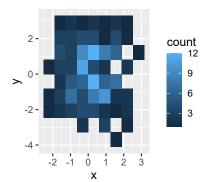
by default. These can be mapped with aes() by enclosing them in a call to stat(). From the help page we can learn that in addition to counts in variable count, density is returned in variable density by this statistic. Consequently, we can create a histogram with the counts per bin expressed as densities whose integral is one (rather than their sum, as the width of the bins is in this case different from one), as follows.

If it were not for the easier to remember name of geom\_histogram(), adding the layers with stat\_bin() or stat\_count() would be preferable as it makes clear that computations on the data are involved.

```
ggplot(my.data, aes(y, fill = group)) +
    stat_bin(bins = 15, position = "dodge")
```

The statistic  $stat_bin2d()$ , and its matching geometry  $geom_bin2d()$ , by default compute a frequency histogram in two dimensions, along the x and y aesthetics. The frequency for each rectangular tile is mapped onto a fill scale. As for  $stat_bin()$ , density is also computed and available to be mapped as shown above for  $geom_histogram$ . In this example, to compare dispersion in two dimensions, equal x and y scales are most suitable, which we achieve by adding  $coord_fixed()$ , which is a variation of the default  $coord_cartesian()$  (see section 9.11 on page 348 for details on other systems of coordinates).

```
ggplot(my.data, aes(x, y)) +
  stat_bin2d(bins = 8) +
  coord_fixed(ratio = 1)
```



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The *statistic* stat\_bin\_hex(), and its matching *geometry* geom\_hex(), differ from stat\_bin2d() in their use of hexagonal instead of square tiles. By default the frequency or count for each hexagon is mapped to the fill aesthetic, but counts expressed as density are also computed and can be mapped with aes(fill = after\_stat(density)).

# 9.6.5 Density functions

Empirical density functions are the equivalent of a histogram, but are continuous and not calculated using bins. They can be estimated in 1 or 2 dimensions (1D or 2D), for x or x and y, respectively. As with histograms it is possible to use different *geometries* to visualize them. Examples of the use of <code>geom\_density()</code> to create 1D density plots follow.

A semitransparent fill can be used instead of coloured lines.

```
ggplot(my.data, aes(y, fill = group)) +
  geom_density(alpha = 0.5)
```

Examples of 2D density plots follow. In the first example we use two *geometries* which were earlier described, <code>geom\_point()</code> and <code>geom\_rug()</code>, to plot the observations in the background. With <code>stat\_density\_2d()</code> we add a two-dimensional density "map" represented using isolines. We map <code>group</code> to the <code>color</code> aesthetic.

```
ggplot(my.data, aes(x, y, color = group)) +
geom_point() +
geom_rug() +
stat_density_2d()
group

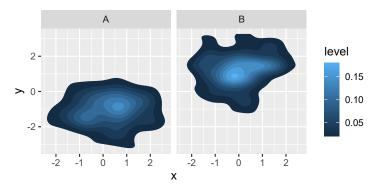
A
B
```

In this case, geom\_density\_2d() is equivalent, and we can replace it in the last line in the chunk above.

```
geom_density_2d()
```

In the next example we plot the groups in separate panels, and use a *geometry* supporting the fill *aesthetic* and we map to it the variable level, computed by stat\_density\_2d()

```
ggplot(my.data, aes(x, y)) +
stat_density_2d(aes(fill = after_stat(level)), geom = "polygon") +
facet_wrap(~group)
```

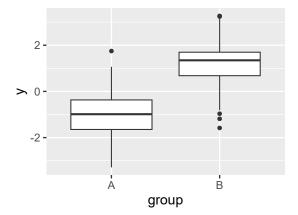


## 9.6.6 Box and whiskers plots

Box and whiskers plots, also very frequently called just box plots, are also summaries that convey some of the properties of a distribution. They are calculated and plotted by means of stat\_boxplot() or its matching geom\_boxplot(). Although they can be calculated and plotted based on just a few observations, they are not useful unless each box plot is based on more than 10 to 15 observations.

```
ggplot(my.data, aes(group, y)) +
    stat_boxplot()
```

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As with other *statistics*, their appearance obeys both the usual *aesthetics* such as color, and parameters specific to this type of visual representation: outlier.color, outlier.fill, outlier.shape, outlier.size, outlier.stroke and outlier.alpha, which affect the outliers in a way similar to the equivalent aethetics in geom\_point(). The shape and width of the "box" can be adjusted with notch, notchwidth and varwidth. Notches in a boxplot serve a similar role for comparing medians as confidence limits serve when comparing means.

## 9.6.7 Violin plots

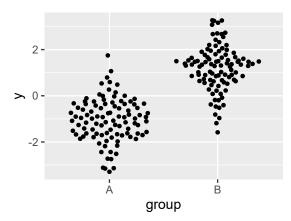
Violin plots are a more recent development than box plots, and usable with relatively large numbers of observations. They could be thought of as being a sort of hybrid between an empirical density function (see section 9.6.5 on page 317) and a box plot (see section 9.6.6 on page 318). As is the case with box plots, they are particularly useful when comparing distributions of related data, side by side. They can be created with <code>geom\_violin()</code> as shown in the examples below.

```
ggplot(my.data, aes(group, y)) +
  geom_violin()
```

As with other *geometries*, their appearance obeys both the usual *aesthetics* such as color, and others specific to these types of visual representation.

Other types of displays related to violin plots are *beeswarm* plots and *sina* plots, and can be produced with *geometries* defined in packages 'ggbeeswarm' and 'ggforce', respectively. A minimal example of a beeswarm plot is shown below. See the documentation of the packages for details about the many options in their use.

```
ggplot(my.data, aes(group, y)) +
  geom_quasirandom()
```



# 9.7 Flipped plot layers

Although it is the norm to design plots so that the independent variable is on the x axis, i.e., mapped to the x aesthetic, there are situations where swapping the roles of x and y is useful. In 'ggplot2' this is described as *flipping the orientation* of a plot. In the present section I exemplify both cases where the flipping is automatic

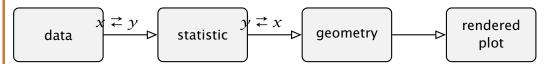
and where it requires user intervention. Some geometries like  $geom\_point()$  are symmetric on the x and y aesthetics, but others like  $geom\_line()$  operate differently on x and y. This is also the cases for almost all *statistics*.

'ggplot2' version 3.3.5, supports flipping in most geometries and statistics where it is meaningful, using a new syntax. This new approach is different to the flip of the coordinate system, and similar to that implemented by package 'ggstance'. However, instead of defining new horizontal layer functions as in 'ggstance', now the orientation of many layer functions from 'ggplot2' can be changed by the user. This has made 'ggstance' nearly redundant and the coding of flipped plots easier and more intuitive. Although 'ggplot2' has offered coord\_flip() for a long time, this affects the whole plot rather than individual layers.

When a factor is mapped to x or y flipping is automatic. A factor creates groups and summaries are computed per group, i.e., per level of the factor irrespective of the factor being mapped to the x or y aesthetic. Dodging and jitter do not need any special syntax as it was the case with package 'ggstance'.

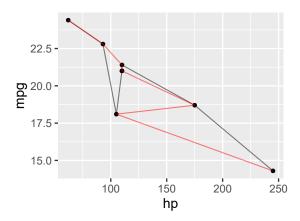
There are also cases that require user intervention. For example, flipping must be requested manually if both x and y are mapped to continuous variables. This is, for example, the case with  $\mathsf{stat\_smooth}()$  and a fit of x on y.

In ggplot statistics, passing orientation = "y" results in flipping, that is applying the calculations after swapping the mappings of the x and y aesthetics. After applying the calculations the mappings of the x and y aesthetics are swapped again (diagram below).



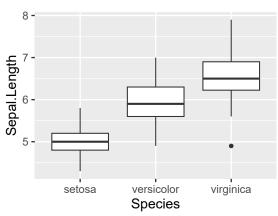
In geometries, passing orientation = "y" results in flipping of the aesthetics but with a twist. For example, in  $geom\_line()$ , flipping changes the drawing of the lines. Normally observations are sorted along the x axis for drawing the segments connecting them. If we flip this layer, observations are sorted along the y axis before drawing the connecting segments, which can make a major difference. The variables shown on each axis remain the same, as does the position of points drawn with  $geom\_point()$ . In this example only two segments are the same in the flipped plot and the not-flipped one.

```
ggplot(mtcars[1:8, ], aes(x = hp, y = mpg)) +
    geom_point() +
    geom_line(alpha = 0.5) +
    geom_line(alpha = 0.5, orientation = "y", colour = "red")
```

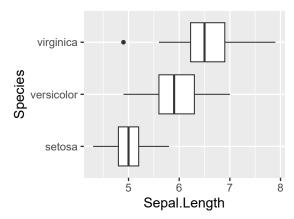


The next pair of examples exemplify automatic flipping using  $stat_boxplot()$ . Here we map the factor species first to x and then to y. In both cases boxplots have been computed and plotted for each level of the factor. Statistics  $stat_boxplot()$ ,  $stat_summary()$ ,  $stat_histogram()$  and  $stat_density()$  behave similarly with respect to flipping.

```
ggplot(iris, aes(x = Species, y = Sepal.Length)) +
    stat_boxplot()
```

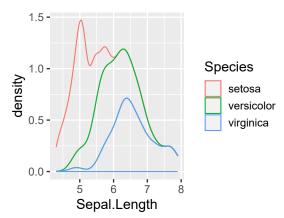


ggplot(iris, aes(x = Sepal.Length, y = Species)) +
 stat\_boxplot()

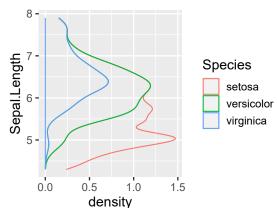


When we map a variable to only one of x or y the flip is also automatic.

```
ggplot(iris, aes(x = Sepal.Length, color = Species)) +
    stat_density(fill = NA)
```



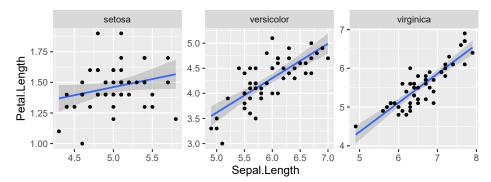
```
ggplot(iris, aes(y = Sepal.Length, color = Species)) +
    stat_density(fill = NA)
```



In the case of ordinary least squares (OLS), regressions of y on x and of x on y in most cases yield different fitted lines, even if  $R^2$  is consistent. This is due to the assumption that x values are known, either set or measured without error, i.e., not subject to random variation. All unexplained variation in the data is assumed to be in y. See Chapter ?? on page ?? or consult a Statistics book such as *Modern Statistics for Modern Biology* (Holmes and Huber 2019, pp. 168–170) for additional information.

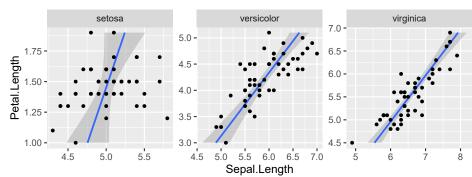
With two continuous variables mapped, the default is to take x as independent and y as dependent. This matters, of course, when computations as in model fitting treat x and y differently. In this case parameter orientation can be used to indicate which of x or y is the independent or explanatory variable.

```
ggplot(iris, aes(Sepal.Length, Petal.Length)) +
    stat_smooth(method = "lm", formula = y ~ x) +
    geom_point() +
    facet_wrap(~Species, scales = "free")
```



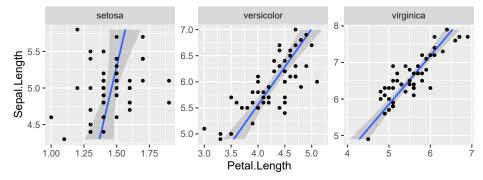
With orientation = "y" we tell that y is the independent variable. In the case of geom\_smooth() this means implicitly swapping x and y in formula.

```
ggplot(iris, aes(Sepal.Length, Petal.Length)) +
    stat_smooth(method = "lm", formula = y ~ x, orientation = "y") +
    geom_point() +
    facet_wrap(~Species, scales = "free")
```



Flipping the orientation of plot layers with orientation = "y" is not equivalent to flipping the whole plot with  $coord_flip()$ . In the first case which axis is considered independent for computation changes but not the positions of the axes in the plot, while in the second case the position of the x and y axes in the plot is swapped. So, when coordinates are flipped the x aesthetic is plotted on the vertical axis and the y aesthetic on the horizontal axis, but the role of the variable mapped to the x aesthetic remains as explanatory variable.

```
ggplot(iris, aes(Sepal.Length, Petal.Length)) +
    stat_smooth(method = "lm", formula = y ~ x) +
    geom_point() +
    coord_flip() +
    facet_wrap(~Species, scales = "free")
```

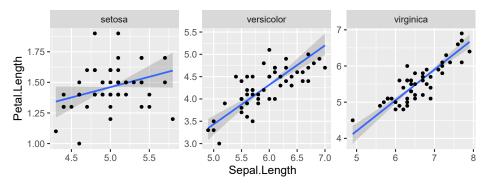


In package 'ggpmisc' (version  $\geq 0.4.1$ ) statistics related to model fitting have an orientation parameter as those from package 'ggplot2' do, but in addition they accept formulas where x is on the lhs and y on the rhs, such as formula = x ~ y providing a syntax consistent with R's model fitting functions. In the next pair of examples we use  $stat_poly_line()$ . In the first example in this pair, the default formula = y ~ x is used, while in the second example we pass explicitly formula = x ~ y to force the flipping of the fitted model. To make the difference clear, we plot both linear regressions on the same plots.

```
ggplot(iris, aes(Sepal.Length, Petal.Length)) +
    stat_poly_line() +
    stat_poly_line(formula = x ~ y, color = "red", fill = "yellow") +
    geom_point() +
    facet_wrap(~Species, scales = "free")
                     setosa
                                                versicolo
                                                                          virginica
                                    5.0 -
     Petal.Length
                                    4.5
        1.50
                                    4.0
        1.25
                                    3.5
        1.00 -
                                    3.0
                             5.5
                                      4.5
                                               5.5 6.0
                                                        6.5
                      5.0
                                           5.0
                                            Sepal.Length
```

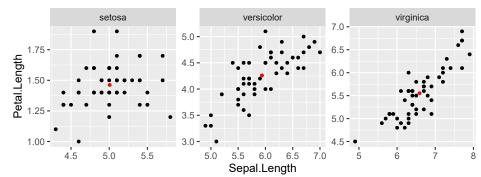
In the case of the iris data used for these examples, both approaches used above to linear regression are wrong. The variables mapped to x and y are correlated but both are measured with error and subject to biological variation. In this case the correct approach is to not assume that there is a variable that can be considered independent, and instead use a method like major axis (MA) regression, as can be seen below.

```
ggplot(iris, aes(Sepal.Length, Petal.Length)) +
    stat_ma_line() +
    geom_point() +
    facet_wrap(~Species, scales = "free")
```

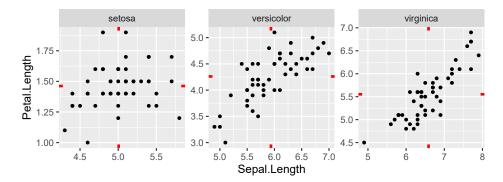


A related problem is when we need to summarize in the same plot layer x and y values. A simple example is adding a point with coordinates given by the means along the x and y axes as we need to pass these computed means simultaneously to  $geom_point()$ . Package 'ggplot2' provides  $stat_density_2d()$  and  $stat_summary_2d()$ . However,  $stat_summary_2d()$  uses bins, and is similar to  $stat_density_2d()$  in how the computed values are returned. Package 'ggpmisc' provides two dimensional equivalents of  $stat_summary()$ :  $stat_centroid()$ , which applies the same summary function along x and y, and  $stat_summary_xy()$ , which accepts one function for x and one for y.

```
ggplot(iris, aes(Sepal.Length, Petal.Length)) +
    geom_point() +
    stat_centroid(color = "red") +
    facet_wrap(~Species, scales = "free")
```



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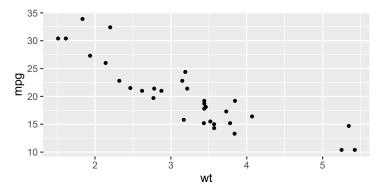
9.19 Which of the plots in the last two chunks above can be created by adding two layers with stat\_summary()? Recreate this plot using stat\_summary().

# 9.8 Facets

Facets are used in a special kind of plots containing multiple panels in which the panels share some properties. These sets of coordinated panels are a useful tool for visualizing complex data. These plots became popular through the trellis graphs in S, and the 'lattice' package in R. The basic idea is to have rows and/or columns of plots with common scales, all plots showing values for the same response variable. This is useful when there are multiple classification factors in a data set. Similar-looking plots, but with free scales or with the same scale but a 'floating' intercept, are sometimes also useful. In 'ggplot2' there are two possible types of facets: facets organized in a grid, and facets along a single 'axis' of variation but, possibly, wrapped into two or more rows. These are produced by adding facet\_grid() or facet\_wrap(), respectively. In the examples below we use geom\_point() but faceting can be used with ggplot objects containing diverse kinds of layers, displaying either observations or summaries from data.

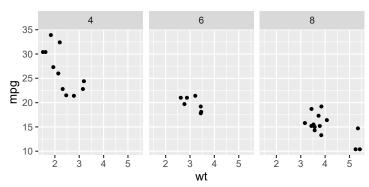
We start by creating and saving a single-panel plot that we will use through this section to demonstrate how the same plot changes when we add facets.

```
p <- ggplot(data = mtcars, aes(wt, mpg)) +
   geom_point()
n</pre>
```



A grid of panels has two dimensions, rows and cols. These dimensions in the grid of plot panels can be "mapped" to factors. Until recently a formula syntax was the only available one. Although this notation has been retained, the preferred syntax is currently to use the parameters rows and cols. We use cols in this example. Note that we need to use vars() to enclose the names of the variables in the data. The "headings" of the panels or *strip labels* are by default the levels of the factors.

```
p + facet_grid(cols = vars(cyl))
```



In the "historical notation" the same plot would have been coded as follows.

```
p + facet_grid(. ~ cyl)
```

By default, all panels share the same scale limits and share the plotting space evenly, but these defaults can be overridden.

```
p + facet_grid(cols = vars(cyl), scales = "free")
p + facet_grid(cols = vars(cyl), scales = "free", space = "free")
```

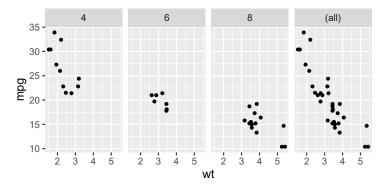
To obtain a 2D grid we need to specify both rows and cols.

```
p + facet_grid(rows = vars(vs), cols = vars(am))
```

Margins display an additional column or row of panels with the combined data.

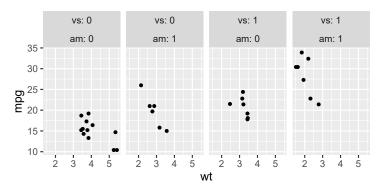
```
p + facet_grid(cols = vars(cyl), margins = TRUE)
```

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We can represent more than one variable per dimension of the grid of plot panels. For this example, we also override the default labeller used for the panels with one that includes the name of the variable in addition to factor levels in the *strip labels*.

```
p + facet_grid(cols = vars(vs, am), labeller = label_both)
```



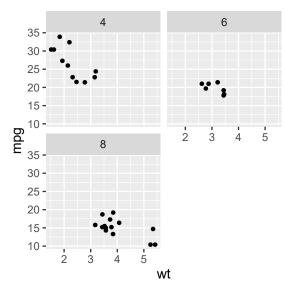
Sometimes we may want to have mathematical expressions or Greek letters in the panel headings. The next example shows a way of achieving this. The key is to use as labeller a function that parses character strings into R expressions.

More frequently we may need to include the levels of the factor used in the faceting as part of the labels. Here we use as labeller, function label\_bquote() with a special syntax that allows us to use an expression where replacement based on the facet (panel) data takes place. See section 9.14 for an example of the use of bquote(), the R function on which label\_bquote(), is built.

In the next example we create a plot with wrapped facets. In this case the number of levels is small, and no wrapping takes place by default. In cases when more panels are present, wrapping into two or more continuation rows is the default.

Here, we force wrapping with nrow = 2. When using facet\_wrap() there is only one dimension, and the parameter is called facets, instead of rows or cols.

p + facet\_wrap(facets = vars(cyl), nrow = 2)



The example below (plot not shown), is similar to the earlier one for facet\_grid, but faceting according to two factors with facet\_wrap() along a single wrapped row of panels.

```
p + facet_wrap(facets = vars(vs, am), nrow = 2, labeller = label_both)
```

## 9.9 Scales

In earlier sections of this chapter, examples have used the default *scales* or we have set them with convenience functions. In the present section we describe in more detail the use of *scales*. There are *scales* available for different *aesthetics* ( $\approx$  attributes) of the plotted geometrical objects, such as position (x, y, z), size, shape, linetype, color, fill, alpha or transparency, angle. Scales determine how values in data are mapped to values of an *aesthetics*, and how these values are labeled.

Depending on the characteristics of the data being mapped, *scales* can be continuous or discrete, for numeric or factor variables in data, respectively. On the other hand, some *aesthetics*, like size, can vary continuously but others like linetype are inherently discrete. In addition to discrete scales for inherently discrete *aesthetics*, discrete scales are available for those *aesthetics* that are inherently continuous, like x, y, size, color, etc.

The scales used by default set the mapping automatically (e.g., which color value corresponds to x = 0 and which one to x = 1). However, for each *aesthetic* such

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as color, there are multiple scales to choose from when creating a plot, both continuous and discrete (e.g., 20 different color scales in 'qqplot2' 3.2.0).

Aesthetics in a plot layer, in addition to being determined by mappings, can also be set to constant values (e.g., plotting all points in a layer in red instead of the default black). Aesthetics set to constant values, are not mapped to data, and are consequently independent of scales. In other words, properties of plot elements can be either set to a single constant value of an aesthetic affecting all observations present in the layer data, or mapped to a variable in data in which case the value of the aesthetic, such as color, will depend on the values of the mapped variable.

The most direct mapping to data is identity, which means that the data is taken at its face value. In a color scale, say scale\_color\_identity(), the variable in the data would be encoded with values such as "red", "blue"—i.e., valid R colours. In a simple mapping using scale\_color\_discrete() levels of a factor, such as "treatment" and "control" would be represented as distinct colours with the correspondence of individual factor levels to individual colours selected automatically by default. In contrast with scale\_color\_manual() the user needs to explicitly provide the mapping between factor levels and colours by passing arguments to the scale functions' parameters breaks and values.

A continuous data variable needs to be mapped to an *aesthetic* through a continuous scale such as scale\_color\_continuous() or one its various variants. Values in a numeric variable will be mapped into a continuous range of colours, determined either automatically through a palette or manually by giving the colours at the extremes, and optionally at multiple intermediate values, within the range of variation of the mapped variable (e.g., scale settings so that the color varies gradually between "red" and "gray50"). Handling of missing values is such that mapping a value in a variable to an NA value for an aesthetic such as color makes the mapped values invisible. The reverse, mapping NA values in the data to a specific value of an aesthetic is also possible (e.g., displaying NA values in the mapped variable in red, while other values are mapped to shades of blue).

## 9.9.1 Axis and key labels

First we describe a feature common to all scales, their name. The default name of all scales is the name of the variable or the expression mapped to it. In the case of the x, y and z *aesthetics* the name given to the scale is used for the axis labels. For other *aesthetics* the name of the scale becomes the "heading" or *key title* of the guide or key. All scales have a name parameter to which a character string or R expression (see section 9.14) can be passed as an argument to override the default.

Whole-plot title, subtitle and caption are not connected to *scales* or data. A title (label) and subtitle can be added least confusingly with function ggtitle() by passing either character strings or R expressions as arguments.

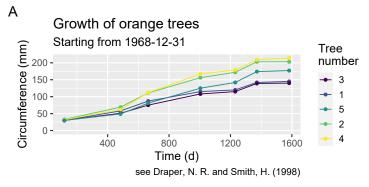
```
ggplot(data = Orange,
    aes(x = age, y = circumference, color = Tree)) +
  geom_line() +
  geom_point() +
```

```
expand_limits(y = 0) +
scale_x_continuous(name = "Time (d)") +
scale_y_continuous(name = "Circumference (mm)") +
ggtitle(label = "Growth of orange trees",
         subtitle = "Starting from 1968-12-31")
                  Growth of orange trees
                  Starting from 1968-12-31
            Circumference (mm)
              200 -
                                                                    Tree
                                                                        3
              150 -
               100 -
                                                                        4
                0 -
                                       800
                                                              1600
                           400
                                                  1200
                                      Time (d)
```

Convenience functions xlab() and ylab() can be used to set the axis labels to match those in the previous chunk.

```
xlab("Time (d)") +
ylab("Circumference (mm)") +
```

Convenience function labs() is useful when we use default scales for all the *aesthetics* in a plot but want to manually set axis labels and/or key titles—i.e., the name of these scales. labs() accepts arguments for these names using, as parameter names, the names of the *aesthetics*. It also allows us to set title, subtitle, caption and tag, of which the first two can also be set with ggtitle().



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9.20 Make an empty plot (ggplot()) and add to it as title an R expression producing  $y = b_0 + b_1 x + b_2 x^2$ . (Hint: have a look at the examples for the use of expressions in the plotmath demo in R by typing demo(plotmath) at the R console.

#### 9.9.2 Continuous scales

We start by listing the most frequently used arguments to the continuous scale functions: name, breaks, minor\_breaks, labels, limits, expand, na.value, trans, guide, and position. The value of name is used for axis labels or the key title (see previous section). The arguments to breaks and minor\_breaks override the default locations of major and minor ticks and grid lines. Setting them to NULL suppresses the ticks. By default the tick labels are generated from the value of breaks but an argument to labels of the same length as breaks will replace these defaults. The values of limits determine both the range of values in the data included and the plotting area as described above—by default the out-of-bounds (oob) observations are replaced by NA but it is possible to instead "squish" these observations towards the edge of the plotting area. The argument to expand determines the size of the margins or padding added to the area delimited by 1ims when setting the "visual" plotting area. The value passed to na.value is used as a replacement for NA valued observations—most useful for color and fill aesthetics. The transformation object passed as an argument to trans determines the transformation used—the transformation affects the rendering, but breaks and tick labels remain expressed in the original data units. The argument to quide determines the type of key or removes the default key. Depending on the scale in question not all these parameters are available.

We generate new fake data.

## Limits

Limits are relevant to all kinds of *scales*. Limits are set through parameter limits of the different scale functions. They can also be set with convenience functions xlim() and ylim() in the case of the x and y *aesthetics*, and more generally with function lims() which like labs(), takes arguments named according to the name of the *aesthetics*. The limits argument of scales accepts vectors, factors or a function computing them from data. In contrast, the convenience functions do not accept functions as their arguments.

In the next example we set "hard" limits, which will exclude some observations from the plot and from any computation of summaries or fitting of smoothers. More exactly, the off-limits observations are converted to NA values before they are passed as data to *qeometries*.

```
ggplot(fake2.data, aes(z, y)) + geom_point() +
scale_y_continuous(limits = c(0, 100))
```

To set only one limit leaving the other free, we can use NA as a boundary.

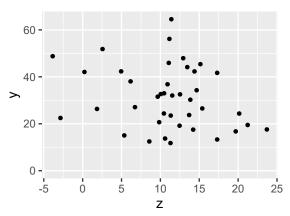
```
scale_y_continuous(limits = c(50, NA))
```

Convenience functions ylim() and xlim() can be used to set the limits to the default x and y scales in use. We here use ylim(), but xlim() is identical except for the *scale* it affects.

```
ylim(50, NA)
```

In general, setting hard limits should be avoided, even though a warning is issued about NA values being omitted, as it is easy to unwillingly subset the data being plotted. It is preferable to use function <code>expand\_limits()</code> as it safely <code>expands</code> the dynamically computed default limits of a scale—the scale limits will grow past the requested expanded limits when needed to accommodate all observations. The arguments to x and y are numeric vectors of length one or two each, matching how the limits of the x and y continuous scales are defined. Here we expand the limits to include the origin.

```
ggplot(fake2.data, aes(z, y)) +
  geom_point() +
  expand_limits(y = 0, x = 0)
```



The expand parameter of the scales plays a different role than expand\_limits(). It controls how much larger the "visual" plotting area is compared to the limits of the actual plotting area. In other words, it adds a "margin" or padding to the plotting area outside the limits set either dynamically or manually. Very rarely plots are drawn so that observations are plotted on top of the axes, avoiding this is a key role of expand. Rug plots and marginal annotations will also require the plotting area to be expanded. In 'ggplot2' the default is to always apply some expansion.

We here set the upper limit of the plotting area to be expanded by adding padding to the top and remove the default padding from the bottom of the plotting area.

```
ggplot(fake2.data,
  aes(fill = group, color = group, x = y)) +
  stat_density(alpha = 0.3) +
  scale_y_continuous(expand = expand_scale(add = c(0, 0.02)))
```

Here we instead use a multiplier to a similar effect as above; we add 10% compared to the range of the limits.

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```
scale_y_continuous(expand = expand_scale(mult = c(0, 0.1)))
```

In the case of scales, we cannot reverse their direction through the setting of limits. We need instead to use a transformation as described in section 9.9.2 on page 337. But, inconsistently, xlim() and ylim() do implicitly allow this transformation through the numeric values passed as limits.

9.21 Test what the result is when the first limit is larger than the second one. Is it the same as when setting these same values as limits with ylim()?

```
ggplot(fake2.data, aes(z, y)) + geom_point() +
scale_y_continuous(limits = c(100, 0))
```

### Ticks and their labels

Parameter breaks is used to set the location of ticks along the axis. Parameter labels is used to set the tick labels. Both parameters can be passed either a vector or a function as an argument. The default is to compute "good" breaks based on the limits and format the numbers as strings.

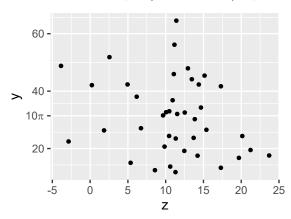
When manually setting breaks, we can keep the default computed labels for the breaks.

```
ggplot(fake2.data, aes(z, y)) +
  geom_point() +
  scale_y_continuous(breaks = c(20, pi * 10, 40, 60))
```

The default breaks are computed by function pretty\_breaks() from 'scales'. The argument passed to its parameter n determines the target number ticks to be generated automatically, but the actual number of ticks computed may be slightly different depending on the range of the data.

```
scale_y_continuous(breaks = pretty_breaks(n = 7))
```

We can set tick labels manually, in parallel to the setting of breaks by passing as arguments two vectors of equal length. In the next example we use an expression to obtain a Greek letter.



20

15

z

25

Package 'scales' provides several functions for the automatic generation of tick labels. For example, to display tick labels as percentages for data available as decimal fractions, we can use function percent().

```
ggplot(fake2.data, aes(z, y / max(y))) +
geom_point() +
scale_y_continuous(labels = percent)
100% -

$\times 50\% -
25\% -
$\times 50\% -
$\times
```

-5

For currency, we can use dollar(), to include commas separating thousands, millions, so on, we can use comma(), and for numbers formatted using exponents of 10—useful for logarithmic-transformed scales—we can use scientific\_format(), label\_number(scale\_cut = cut\_short\_scale()), label\_log(), or label\_number(scale\_cut = cut\_si("g"). As shown below, some of these functions can be useful with untransformed continuous scales.

```
ggplot(fake2.data, aes(z, y * 1000)) +
  geom_point() +
                                                   "Mass",
            scale_y_continuous(name
                                                                 labels
                                                                                     la-
bel_number(scale_cut = cut_si("q")))
                        60 kg
                        50 kg
                     Mass
                        40 kg
                        30 kg
                        20 kg
                        10 kg -
                                   Ö
                                                     15
                                                                 25
                                               10
                                                           20
                                               Z
```

With date values mapped to x or y, tick labels are created with functions label\_date() or label\_date\_short(). In the case of time, tick labels are created with function label\_time().

```
## ADD EXAMPLES USING FORMATS for dates and times
```

It is also possible to use user-defined functions both for breaks and labels.

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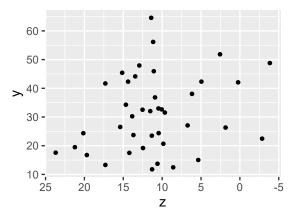
#### Transformed scales

The default scales used by the x and y aesthetics, scale\_x\_continuous() and scale\_y\_continuous(), accept a user-supplied transformation function as an argument to trans with default codetrans = "identity" (no transformation). In addition, there are predefined convenience scale functions for log10, sqrt and reverse.

Similar to the maths functions of R, the name of the scales are scale\_x\_log10() and scale\_y\_log10() rather than scale\_y\_log() because in R, the function log returns the natural logarithm.

We can use scale\_x\_reverse() to reverse the direction of a continuous scale,

```
ggplot(fake2.data, aes(z, y)) +
  geom_point() +
  scale_x_reverse()
```



Axis tick-labels display the original values before applying the transformation. The "breaks" need to be given in the original scale as well. We use  $scale_y_log10()$  to apply a  $log_{10}$  transformation to the y values.

```
scale_y_log10(breaks=c(10,20,50,100))
```

Using a transformation in a scale is not equivalent to applying the same transformation on the fly when mapping a variable to the x (or y) *aesthetic* as this results in tick-labels expressed in transformed values.

```
ggplot(fake2.data, aes(z, log10(y))) +
  geom_point()
```

We show next how to specify a transformation to a continuous scale, using a predefined "transformation" object.

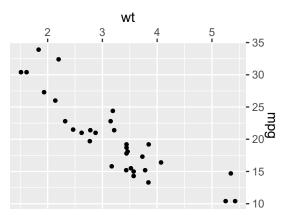
```
scale_y_continuous(trans = "reciprocal")
```

Natural logarithms are important in growth analysis as the slope against time gives the relative growth rate. We show this with the **orange** data set.

## Position of x and y axes

The default position of axes can be changed through parameter position, using character constants "bottom", "top", "left" and "right".

```
ggplot(data = mtcars, aes(wt, mpg)) +
  geom_point() +
  scale_x_continuous(position = "top") +
  scale_y_continuous(position = "right")
```



## Secondary axes

It is also possible to add secondary axes with ticks displayed in a transformed scale.

```
ggplot(data = mtcars, aes(wt, mpg)) +
  geom_point() +
  scale_y_continuous(sec.axis = sec_axis(~ . ^-1, name = "1/y") )
                         35
                                                              -0.03
                         30 -
                         25 -
                                                              - <sub>0.05</sub>
                         20 -
                         15 -
                                                               - 0.07
                                                              -0.09
                         10 -
                                 2
                                         3
                                                         5
                                            wt
```

It is also possible to use different breaks and labels than for the main axes, and to provide a different name to be used as a secondary axis label.

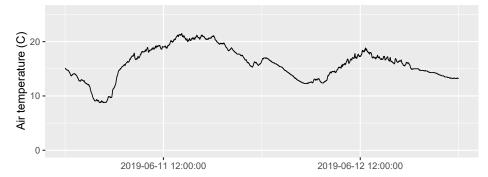
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## 9.9.3 Time and date scales for x and y

In R and many other computing languages, time values are stored as integer or numeric values subject to special interpretation. Times stored as objects of class POSIXct can be mapped to continuous *aesthetics* such as x and y. Special scales are available for these quantities.

We can set limits and breaks using constants as time or dates. These are most easily input with the functions in packages 'lubridate' or 'anytime'.

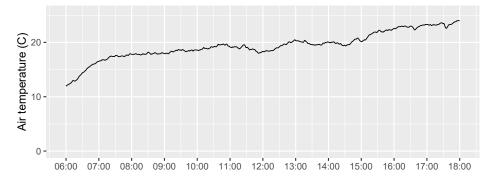
Warnings are issued in the next two chunks as we are using scale limits to subset a part of the observations present in data.



By default the tick labels produced and their formatting are automatically selected based on the extent of the time data. For example, if we have all data collected within a single day, then the tick labels will show hours and minutes. If we plot data for several years, the labels will show the date portion of the time instant. The default is frequently good enough, but it is possible, as for numbers, to use different formatter functions to generate the tick labels.

## Warning: Removed 9359 rows containing missing values or values outside the

```
scale range
## (`geom_line()`).
```



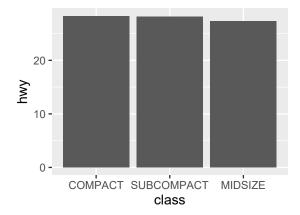
9.22 The formatting strings used are those supported by strptime() and help(strptime) lists them. Change, in the two examples above, the *y*-axis labels used and the limits—e.g., include a single hour or a whole week of data, check which tick labels are produced by default and then pass as an argument to date\_labels different format strings, taking into account that in addition to the *conversion specification* codes, format strings can include additional text.

# 9.9.4 Discrete scales for x and y

In the case of ordered or unordered factors, the tick labels are by default the names of the factor levels. Consequently, one roundabout way of obtaining the desired tick labels is to set them as factor levels. This approach is not recommended as in many cases the text of the desired tick labels may not be recognized as a valid name making the code using them more difficult to type in scripts or at the command prompt. It is best to use simple mnemonic short names for factor levels and variables, and to set suitable labels through *scales* when plotting, as we will show here.

We can use scale\_x\_discrete() to reorder and select the columns without altering the data. If we use this approach to subset the data, then to avoid warnings we need to add na.rm = TRUE. We additionally use scale\_x\_discrete to convert level names to uppercase.

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If, as in the previous example, only the case of character strings needs to be changed, passing function toupper() or tolower() allows a more general and less error-prone approach. In fact any function, user defined or not, which converts the values of limits into the desired values can be passed as an argument to labels.

Alternatively, we can change the order of the columns in the plot by reordering the levels of factor mpg\$class. This approach makes sense if the ordering needs to be done programmatically based on values in data. See section 3.12 on page 79 for details. The example below shows how to reorder the columns, corresponding to the levels of class based on the mean() of hwy.

```
ggplot(mpg, aes(reorder(x = factor(class), X = hwy, FUN = mean), hwy)) +
    stat_summary(geom = "col", fun = mean)
```

### 9.9.5 Size

For the size *aesthetic*, several scales are available, both discrete and continuous. They do not differ much from those already described above. *Geometries* geom\_point(), geom\_line(), geom\_hline(), geom\_vline(), geom\_text(), geom\_label() obey size as expected. In the case of geom\_bar(), geom\_col(), geom\_area() and all other geometric elements bordered by lines, size is obeyed by these border lines. In fact, other aesthetics natural for lines such as linetype also apply to these borders.

When using size scales, breaks and labels affect the key or guide. In scales that produce a key passing guide = "none" removes the key corresponding to the scale.

### 9.9.6 Color and fill

color and fill scales are similar, but they affect different elements of the plot. All visual elements in a plot obey the color *aesthetic*, but only elements that have an inner region and a boundary, obey both color and fill *aesthetics*. There are separate but equivalent sets of scales available for these two *aesthetics*. We will

describe in more detail the color *aesthetic* and give only some examples for fill. We will, however, start by reviewing how colors are defined and used in R.

#### Color definitions in R

Colors can be specified in R not only through character strings with the names of previously defined colors, but also directly as strings describing the RGB (red, green and blue) components as hexadecimal numbers (on base 16 expressed using 0, 1, 2, 3, 4, 6, 7, 8, 9, A, B, C, D, E, and F as "digits") such as "#FFFFFF" for white or "#000000" for black, or "#FF0000" for the brightest available pure red.

The list of color names known to R can be obtained be typing colors() at the R console. Given the number of colors available, we may want to subset them based on their names. Function colors() returns a character vector. We can use grep() to find the names containing a given character substring, in this example "dark".

```
length(colors())
## [1] 657
grep("dark",colors(), value = TRUE)
                           "darkcyan"
    [1] "darkblue"
                                              "darkgoldenrod"
                                                                 "darkgoldenrod1"
        "darkgoldenrod2"
                           "darkgoldenrod3"
                                                                 "darkgray"
                                              "darkgoldenrod4"
##
        "darkgreen"
                           "darkgrey"
                                              "darkkhaki"
                                                                 "darkmagenta"
##
    [9]
        "darkolivegreen"
                          "darkolivegreen1"
                                             "darkolivegreen2"
                                                                "darkolivegreen3"
## [13]
        "darkolivegreen4" "darkorange"
                                              "darkorange1"
                                                                 "darkorange2"
##
  [17]
                           "darkorange4"
                                              "darkorchid"
                                                                 "darkorchid1"
        "darkorange3"
##
  [21]
        "darkorchid2"
                           "darkorchid3"
                                              "darkorchid4"
                                                                 "darkred"
  [25]
##
        "darksalmon"
                           "darkseagreen"
                                              "darkseagreen1"
                                                                 "darkseagreen2"
  [29]
        "darkseagreen3"
                           "darkseagreen4"
  [33]
                                              "darkslateblue"
                                                                 "darkslategray"
## [37] "darkslategray1"
                           "darkslategray2"
                                              "darkslategray3"
                                                                 "darkslategray4"
## [41] "darkslategrey"
                           "darkturquoise"
                                              "darkviolet"
```

To retrieve the RGB values for a color definition we use:

```
col2rgb("purple")
##
          [,1]
## red
           160
## green
            32
## blue
           240
col2rqb("#FF0000")
##
          Γ.17
## red
           255
## areen
             0
## blue
```

Color definitions in R can contain a *transparency* described by an alpha value, which by default is not returned.

```
col2rgb("purple", alpha = TRUE)
## [,1]
## red 160
## green 32
## blue 240
## alpha 255
```

With function rgb() we can define new colors. Enter help(rgb) for more details.

```
rgb(1, 1, 0)
## [1] "#FFFF00"
```

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```
rgb(1, 1, 0, names = "my.color")
## my.color
## "#FFFF00"
rgb(255, 255, 0, names = "my.color", maxColorValue = 255)
## my.color
## "#FFFF00"
```

As described above, colors can be defined in the RGB *color space*, however, other color models such as HSV (hue, saturation, value) can be also used to define colours.

```
hsv(c(0,0.25,0.5,0.75,1), 0.5, 0.5)
## [1] "#804040" "#608040" "#408080" "#604080" "#804040"
```

Probably a more useful flavor of HSV colors for use in scales are those returned by function hc1() for hue, chroma and luminance. While the "value" and "saturation" in HSV are based on physical values, the "chroma" and "luminance" values in HCL are based on human visual perception. Colours with equal luminance will be seen as equally bright by an "average" human. In a scale based on different hues but equal chroma and luminance values, as used by package 'ggplot2', all colours are perceived as equally bright. The hues need to be expressed as angles in degrees, with values between zero and 360.

```
hcl(c(0,0.25,0.5,0.75,1) * 360)
## [1] "#FFC5D0" "#D4D8A7" "#99E2D8" "#D5D0FC" "#FFC5D0"
```

It is also important to remember that humans can only distinguish a limited set of colours, and even smaller color gamuts can be reproduced by screens and printers. Furthermore, variation from individual to individual exists in color perception, including different types of color blindness. It is important to take this into account when choosing the colors used in illustrations.

### 9.9.7 Continuous color-related scales

Continuous color scales scale\_color\_continuous(), scale\_color\_gradient(), scale\_color\_gradient2(), scale\_color\_gradientn(), scale\_color\_date() and scale\_color\_datetime(), give a smooth continuous gradient between two or more colours. They are used with numeric, date and datetime data. A corresponding set of fill scales is also available. Other scales like scale\_color\_viridis\_c() and scale\_color\_distiller() are based on the use of ready-made palettes of sets of color gradients chosen to work well together under multiple conditions or for human vision including different types of color blindness.

### 9.9.8 Discrete color-related scales

Color scales scale\_color\_discrete(), scale\_color\_hue(), scale\_color\_gray() are used with categorical data stored as factors. Other scales like scale\_color\_viridis\_d() and scale\_color\_brewer() provide discrete sets of colours based on palettes.

### 9.9.9 Binned scales

Before version 3.3.0 of 'ggplot2' only two types of scales were available, continuous and discrete. A third type of scales (implemented for all the aesthetics where relevant) was added in version 3.3.0 called *binned*. They are to be used with continuous variables, but they discretize the continuous values into bins or classes, each for a range of values, and then represent them in the plot using a discrete set of values. We re-do the figure shown on page 284 but replacing scale\_color\_gradient() by scale\_color\_binned().

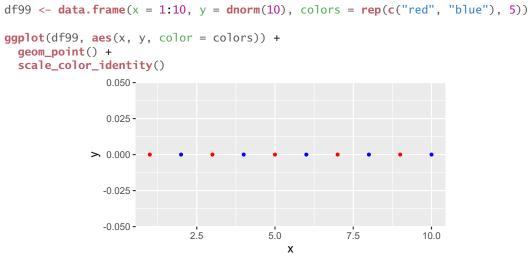
```
# we use capital letters X and Y as variable names to distinguish
# them from the x and y aesthetics
set.seed(4321)
X < -0:10
Y < -(X + X^2 + X^3) + rnorm(length(X), mean = 0, sd = mean(X^3) / 4)
my.data <- data.frame(X, Y)</pre>
my.data.outlier <- my.data
my.data.outlier[6, "Y"] <- my.data.outlier[6, "Y"] * 10
my.formula \leftarrow y \sim poly(x, 3, raw = TRUE)
ggplot(my.data.outlier) +
  stat_fit_residuals(formula = my.formula,
                       method = "rlm",
                       mapping = aes(x = X,
                                      y = stage(start = Y,
                                                 after_stat = y * weights),
                                      colour = after_stat(weights)),
                       show.legend = TRUE) +
  scale_color_binned(low = "red", high = "blue", limits = c(0, 1),
                       guide = "colourbar", n.breaks = 5)
                25
                                                                weights
             y * weights
                                                                   0.75
                 0
                                                                   0.50
                                                                   0.25
                -25
                                                                   0.00
                   0.0
                             2.5
                                       5.0
                                                7.5
                                                         10.0
```

The advantage of binned scales is that they facilitate the fast reading of the plot while their disadvantage is the decreased resolution of the scale. The choice of a binned vs. continuous scale, and the number and boundaries of bins, set by the argument passed to parameter n.breaks or to breaks need to be chosen carefully, taking into account the audience, the length of time available to the viewer to peruse the plot vs. the density of observations. Transformations are also allowed in these scales as in others.

## 9.9.10 Identity scales

In the case of identity scales, the mapping is one to-one to the data. For example, if we map the color or fill *aesthetic* to a variable using scale\_color\_identity() or scale\_fill\_identity(), the mapped variable must already contain valid color definitions. In the case of mapping alpha, the variable must contain numeric values in the range 0 to 1.

We create a data frame containing a variable colors containing character strings interpretable as the names of color definitions known to R. We then use them directly in the plot.



9.23 How does the plot look, if the identity scale is deleted from the example above? Edit and re-run the example code.

While using the identity scale, how would you need to change the code example above, to produce a plot with green and purple points?

# 9.10 Adding annotations

The idea of annotations is that they add plot elements that are not directly connected with data, which we could call "decorations" such as arrows used to highlight some feature of the data, specific points along an axis, etc. They are referenced to the "natural" coordinates used to plot the observations, but are elements that do not represent observations or summaries computed from the observations. Annotations are added to a ggplot with annotate() as plot layers (each call to annotate() creates a new layer). To achieve the behavior expected of annotations, annotate() does not inherit the default data or mapping of variables to *aesthetics*. Annotations frequently make use of "text" or "label" *geometries* with character strings as data, possibly to be parsed as expressions. However, for example, the "segment" geometry can be used to add arrows.

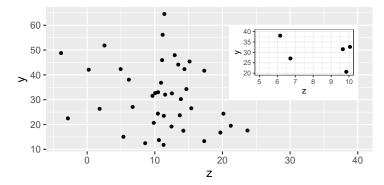
While layers added to a plot directly using *geometries* and *statistics* respect faceting, annotation layers added with annotate() are replicated unchanged in every panel of a faceted plot. The reason is that annotation layers accept *aesthetics* only as constant values which are the same for every panel as no grouping is possible without a mapping to data.

We show a simple example using "text" as geometry.

```
ggplot(fake2.data, aes(z, y)) +
  geom_point() +
  annotate(geom = "text"
             label = "origin",
            x = 0, y = 0,
            color = "blue"
            size=4)
                60 -
                40
                 20 -
                 0 -
                           origin
                                                        15
                   -5
                                               10
                                                                 20
                                                                          25
```

9.24 Play with the values of the arguments to annotate() to vary the position, size, color, font family, font face, rotation angle and justification of the annotation.

It is relatively common to use inset tables, plots, bitmaps or vector plots as annotations. With annotation\_custom(), grobs ('grid' graphical object) can be added to a ggplot. To add another or the same plot as an inset, we first need to convert it into a grob. In the case of a ggplot we use ggplotGrob(). In this example the inset is a zoomed-in window into the main plot. In addition to the grob, we need to provide the coordinates expressed in "natural" data units of the main plot for the location of the grob.



This approach has the limitation that if used together with faceting, the inset will be the same for each plot panel. See section 9.5.8 on page 302 for *geometries* that can be used to add insets.

In the next example, in addition to adding expressions as annotations, we also pass expressions as tick labels through the scale. Do notice that we use recycling for setting the breaks, as c(0, 0.5, 1, 1.5, 2) \* pi is equivalent to c(0, 0.5 \* pi, pi, 1.5 \* pi, 2 \* pi. Annotations are plotted at their own position, unrelated to any observation in the data, but using the same coordinates and units as for plotting the data.

```
ggplot(data.frame(x = c(0, 2 * pi)), aes(x = x)) +
  stat_function(fun = sin) +
  scale_x_continuous(
    breaks = c(0, 0.5, 1, 1.5, 2) * pi,
    labels = c("0", expression(0.5~pi), expression(pi),
             expression(1.5~pi), expression(2~pi))) +
  labs(y = "sin(x)") +
  annotate(geom = "text"
            label = c("+", "-"),
           x = c(0.5, 1.5) * pi, y = c(0.5, -0.5),
           size = 20) +
  annotate(geom = "point",
           color = "red",
           shape = 21,
           fill = "white",
           x = c(0, 1, 2) * pi, y = 0,
           size = 6)
                1.0 -
                0.5 -
               0.0 -
               -0.5
               -1.0 -
                               0.5 π
                                                      1.5 π
                                                                  2π
```

Χ

9.25 Modify the plot above to show the cosine instead of the sine function, replacing sin with cos. This is easy, but the catch is that you will need to relocate the annotations.

We cannot use annotate() with geom = "vline" or geom = "hline" as we can use geom = "line" or geom = "segment". Instead, geom\_vline() and/or geom\_hline() can be used directly passing constant arguments to them. See section 9.5.3 on page 294.

## 9.11 Coordinates and circular plots

Circular plots can be thought of as plots equivalent to those described earlier in this chapter but drawn using a different system of coordinates. This is a key insight, that the grammar of graphics as implemented in 'ggplot2' makes use of. To obtain circular plots we use the same *geometries*, *statistics* and *scales* we have been using with the default system of cartesian coordinates. The only thing that we need to do is to add coord\_polar() to override the default. Of course only some observed quantities can be better perceived in circular plots than in cartesian plots. Here we add a new "word" to the grammar of graphics, *coordinates*, such as coord\_polar(). When using polar coordinates, the x and y *aesthetics* correspond to the angle and radial distance, respectively.

## 9.11.1 Wind-rose plots

Some types of data are more naturally expressed on polar coordinates than on cartesian coordinates. The clearest example is wind direction, from which the name derives. In some cases of time series data with a strong periodic variation, polar coordinates can be used to highlight any phase shifts or changes in frequency. A more mundane application is to plot variation in a response variable through the day with a clock-face-like representation of time of day.

Wind rose plots are frequently histograms or density plots drawn on a polar system of coordinates (see sections 9.6.4 and 9.6.5 on pages 314 and 317, respectively for a description of the use of these *statistics* and *geometries*). We will use them for examples where we plot wind speed and direction data, measured once per minute during 24 h (from package 'learnrbook').

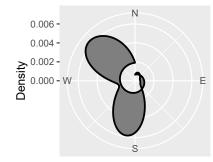
Here we plot a circular histogram of wind directions with 30-degree-wide bins. We use stat\_bin(). The counts represent the number of minutes during 24 h when the wind direction was within each bin.

```
p + stat_bin(color = "black", fill = "gray50", geom = "bar", binwidth = 30, na.rm = TRUE) + labs(y = "Frequency")

300-
200-
0-W
```

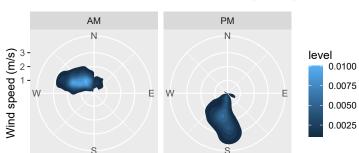
Wind direction

For an equivalent plot, using an empirical density, we have to use stat\_density() instead of stat\_bin(), geom\_polygon() instead of geom\_bar() and change the name of the y scale.



Wind direction

As the final wind-rose plot example, we do 2D density plot with facets added with facet\_wrap() to have separate panels for AM and PM. This plot uses fill to describe the density of observations for different combinations wind directions and speeds, the radius (y aesthetic) to represent wind speeds and the angle (x aesthetic) to represent wind direction.



facet\_wrap(~factor(ifelse(hour(solar\_time) < 12, "AM", "PM")))</pre>

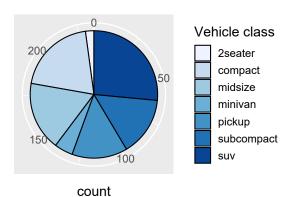
Wind direction

#### **9.11.2** Pie charts

Pie charts are more difficult to read than bar charts because our brain is better at comparing lengths than angles. If used, pie charts should only be used to show composition, or fractional components that add up to a total. In this case, used only if the number of "pie slices" is small (rule of thumb: seven at most), however in general, they are best avoided.

As we use geom\_bar() which defaults to use stat\_count(). We use the brewer scale for nice colors.

```
ggplot(data = mpg, aes(x = factor(1), fill = factor(class))) +
  geom_bar(width = 1, color = "black") +
  coord_polar(theta = "y") +
  scale_fill_brewer() +
  scale_x_discrete(breaks = NULL) +
  labs(x = NULL, fill = "Vehicle class")
```



9.26 Edit the code for the pie chart above to obtain a bar chart. Which one of the two plots is easier to read?

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#### 9.12 Themes

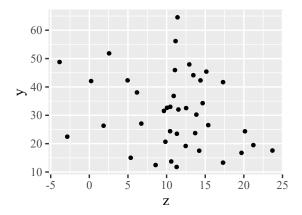
In 'ggplot2', themes are the equivalent of style sheets. They determine how the different elements of a plot are rendered when displayed, printed or saved to a file. Themes do not alter what aesthetics or scales are used to plot the observations or summaries, but instead how text-labels, titles, axes, grids, plotting-area background and grid, etc., are formatted and if displayed or not. Package 'ggplot2' includes several predefined theme constructors (usually described as themes), and independently developed extension packages define additional ones. These constructors return complete themes, which when added to a plot, replace any theme already present in whole. In addition to choosing among these already available complete themes, users can modify the ones already present by adding incomplete themes to a plot. When used in this way, incomplete themes usually are created on the fly. It is also possible to create new theme constructors that return complete themes, similar to theme\_gray() from 'ggplot2'.

## 9.12.1 Complete themes

The theme used by default is theme\_gray() with default arguments. In 'ggplot2', predefined themes are defined as constructor functions, with parameters. These parameters allow changing some "base" properties. The base\_size for text elements controlled is given in points, and affects all text elements in the returned theme object as the size of these elements is by default defined relative to the base size. Another parameter, base\_family, allows the font family to be set. These functions return complete themes.

Themes have no effect on layers produced by *geometries* as themes have no effect on *mappings*, *scales* or *aesthetics*. In the name theme\_bw() black-and- white refers to the color of the background of the plotting area and labels. If the *color* or fill *aesthetics* are mapped or set to a constant in the figure, these will be respected irrespective of the theme. We cannot convert a color figure into a black-and-white one by adding a *theme*, we need to change the *aesthetics* used, for example, use shape instead of color for a layer added with geom\_point().

Even the default theme\_gray() can be added to a plot, to modify it, if arguments different to the defaults are passed when called. In this example we override the default base size with a larger one and the default sans-serif font with one with serifs.



9.27 Change the code in the previous chunk to use, one at a time, each of the predefined themes from 'ggplot2': theme\_bw(), theme\_classic(), theme\_minimal(), theme\_linedraw(), theme\_light(), theme\_dark() and theme\_void().

Predefined "themes" like theme\_gray() are, in reality, not themes but instead are constructors of theme objects. The *themes* they return when called depend on the arguments passed to their parameters. In other words, theme\_gray(base\_size = 15), creates a different theme than theme\_gray(base\_size = 11). In this case, as sizes of different text elements are defined relative to the base size, the size of all text elements changes in coordination. Font size changes by *themes* do not affect the size of text or labels in plot layers created with geometries, as their size is controlled by the size *aesthetic*.

A frequent idiom is to create a plot without specifying a theme, and then adding the theme when printing or saving it. This can save work, for example, when producing different versions of the same plot for a publication and a talk.

```
p <- ggplot(fake2.data, aes(z, y)) +
          geom_point()
print(p + theme_bw())</pre>
```

It is also possible to change the theme used by default in the current R session with theme\_set().

```
old_theme <- theme_set(theme_bw(15))</pre>
```

Similar to other functions used to change options in R, theme\_set() returns the previous setting. By saving this value to a variable, here old\_theme, we are able to restore the previous default, or undo the change.

```
theme_set(old_theme)
```

The use of a grey background as default for plots is unusual. This graphic design decision originates in the typesetters desire to maintain a uniform luminosity throughout the text and plots in a page. Many scientific journals require or at least prefer a more traditional graphic design. Theme theme\_bw() is the most versatile of the traditional designs supported as it works well both for individual plots as for plots with facets as it includes a box. Theme theme\_classic() lacking

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a box and grid works well for individual plots as is, but needs changes to the facet bars when used with facets.

## 9.12.2 Incomplete themes

If we want to extensively modify a theme, and/or reuse it in multiple plots, it is best to create a new constructor, or a modified complete theme as described in the next section. In other cases we may need to tweak some theme settings for a single figure, in which case we can most effectively do this when creating a plot. We exemplify this approach by solving the problem of overlapping x-axis tick labels. In practice this problem is most frequent when factor levels have long names or the labels are dates. Rotating the tick labels is the most elegant solution from the graphics design point of view.

```
ggplot(fake2.data, aes(z + 1000, y)) +
geom_point() +
scale_x_continuous(breaks = scales::pretty_breaks(n = 8)) +
theme(axis.text.x = element_text(angle = 90, hjust = 1, vjust = 0.5))
```

When tick labels are rotated, one usually needs to set both the horizontal and vertical justification, hjust and vjust, as the default values stop being suitable. This is due to the fact that justification settings are referenced to the text itself rather than to the plot, i.e., **vertical** justification of x-axis tick labels rotated 90 degrees shifts their alignment with respect to tick marks along the (**horizontal**) x axis.

9.28 Play with the code in the last chunk above, modifying the values used for angle, hjust and vjust. (Angles are expressed in degrees, and justification with values between 0 and 1).

A less elegant approach is to use a smaller font size. Within theme(), function rel() can be used to set size relative to the base size. In this example, we use axis.text.x so as to change the size of tick labels only for the x axis.

```
theme(axis.text.x = element_text(size = rel(0.6)))
```

Theme definitions follow a hierarchy, allowing us to modify the formatting of groups of similar elements, as well as of individual elements. In the chunk above,

had we used axis.text instead of axis.text.x, the change would have affected the tick labels in both x and y axes.

9.29 Modify the example above, so that the tick labels on the *x*-axis are blue and those on the *y*-axis red, and the font size is the same for both axes, but changed from the default. Consult the documentation for theme() to find out the names of the elements that need to be given new values. For examples, see *ggplot2: Elegant Graphics for Data Analysis* (Wickham and Sievert 2016) and *R Graphics Cookbook* (Chang 2018).

Formatting of other text elements can be adjusted in a similar way, as well as thickness of axes, length of tick marks, grid lines, etc. However, in most cases these are graphic design elements that are best kept consistent throughout sets of plots and best handled by creating a new *theme* that can be easily reused.

If you both add a *complete theme* and want to modify some of its elements, you should add the whole theme before modifying it with + theme(...). This may seem obvious once one has a good grasp of the grammar of graphics, but can be at first disconcerting.

It is also possible to modify the default theme used for rendering all subsequent plots.

```
old_theme <- theme_update(text = element_text(color = "darkred"))</pre>
```

#### 9.12.3 Defining a new theme

Themes can be defined both from scratch, or by modifying existing saved themes, and saving the modified version. As discussed above, it is also possible to define a new, parameterized theme constructor function.

Unless we plan to widely reuse the new theme, there is usually no need to define a new function. We can simply save the modified theme to a variable and add it to different plots as needed. As we will be adding a "ready-build" theme object rather than a function, we do not use parentheses.

```
my_theme <- theme_bw() + theme(text = element_text(color = "darkred"))
p + my_theme</pre>
```



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9.30 It is always good to learn to recognize error messages. One way of doing this is by generating errors on purpose. So do add parentheses to the statement in the code chunk above and study the error message.

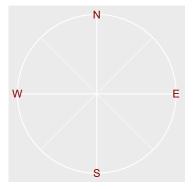
How to create a new theme constructor similar to those in package 'ggplot2' can be fairly simple if the changes are few. As the implementation details of theme objects may change in future versions of 'ggplot2', the safest approach is to rely only on the public interface of the package. We can "wrap" the functions exported by package 'ggplot2' inside a new function. For this we need to find out what are the parameters and their order and duplicate these in our wrapper. Looking at the "usage" section of the help page for theme\_gray() is enough. In this case, we retain compatibility, but add a new base parameter, base\_color, and set a different default for base\_family. The key detail is passing complete = TRUE to theme(), as this tags the returned theme as being usable by itself, resulting in replacement of any theme already in a plot when it is added.

In the chunk above we have created our own theme constructor, without too much effort, and using an approach that is very likely to continue working with future versions of 'ggplot2'. The saved theme is a function with parameters and defaults for them. In this example we have kept the function parameters the same as those used in 'ggplot2', only adding an additional parameter after the existing ones to maximize compatibility and avoid surprising users. To avoid surprising users, we may want additionally to make my\_theme\_grey() a synonym of my\_theme\_gray() following 'ggplot2' practice.

```
my_theme_grey <- my_theme_gray</pre>
```

Finally, we use the new theme constructor in the same way as those defined in 'ggplot2'.

```
p + my_theme_gray(15, base_color = "darkred")
```



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## 9.13 Composing plots

In section 9.8 on page 327, we described how facets can be used to create coordinated sets of panels, based on a single data set. Rather frequently, we need to assemble a composite plot from individually created plots. If one wishes to have correctly aligned axis labels and plotting areas, similar to when using facets, then the task is not easy to achieve without the help of especial tools.

Package 'patchwork' defines a simple grammar for composing plots created with 'ggplot2'. We briefly describe here the use of operators +, | and /, although 'patchwork' provides additional tools for defining complex layouts of panels. While + allows different layouts, | composes panels side by side, and / composes panels on top of each other. The plots to be used as panels can be grouped using parentheses.

We start by creating and saving three plots.

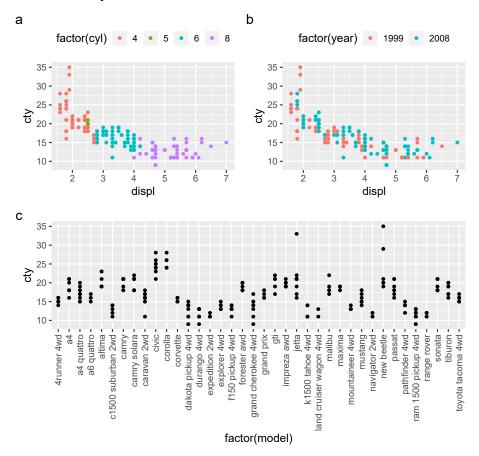
Next, we compose a plot using as panels the three plots created above (plot not shown).

```
(p1 | p2) / p3
```

We add a title and tag the panels with a letter. In this, and similar cases, parentheses may be needed to alter the default precedence of the R operators.

```
((p1 | p2) / p3) +
   plot_annotation(title = "Fuel use in city traffic:", tag_levels = 'a')
```





Package 'patchwork' has in recent versions tools for the creation of complex layouts, addition of insets and combining in the same layout plots and other graphic objects such as bitmaps such as photographs and even tables.

## 9.14 Using plotmath expressions

In sections 9.6.1 and 9.5.7 we gave some simple examples of the use of R expressions in plots. The plotmath demo and help in R provide enough information to start using expressions in plots. However, composing syntactically correct expressions can be challenging because their syntax is rather unusual. Although expressions are shown here in the context of plotting, they are also used in other contexts in R code.

In general it is possible to create *expressions* explicitly with function expression(), or by parsing a character string. In the case of 'ggplot2' for some plot elements, layers created with geom\_text() and geom\_label(), and the strip labels of facets the parsing is delayed and applied to mapped character variables

in data. In contrast, for titles, subtitles, captions, axis-labels, etc. (anything that is defined within labs()) the expressions have to be entered explicitly, or saved as such into a variable, and the variable passed as an argument.

When plotting expressions using <code>geom\_text()</code>, that character strings are to be parsed is signaled with <code>parse = TRUE</code>. In the case of facets' strip labels, parsing or not depends on the *labeller* function used. An additional twist is in this case the possibility of combining static character strings with values taken from data.

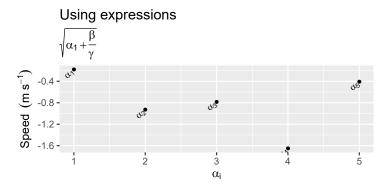
The most difficult thing to remember when writing expressions is how to connect the different parts. A tilde (~) adds space in between symbols. Asterisk (\*) can be also used as a connector, and is needed usually when dealing with numbers. Using space is allowed in some situations, but not in others. To include bits of text within an expression we need to use quotation marks. For a long list of examples have a look at the output and code displayed by demo(plotmath) at the R command prompt.

We will use a couple of complex examples to show how to use expressions for different elements of a plot. We first create a data frame, using paste() to assemble a vector of subscripted  $\alpha$  values as character strings suitable for parsing into expressions.

We use as x-axis label, a Greek  $\alpha$  character with i as subscript, and in the y-axis label, we have a superscript in the units. For the title we use a character string but for the subtitle a rather complex expression. We create these expressions with function expression().

We label each observation with a subscripted *alpha*. We cannot pass expressions to *geometries* by simply mapping them to the label aesthetic. Instead, we pass character strings that can be parsed into expressions. In other words, character strings, that are written using the syntax of expressions. We need to set parse = TRUE in the call to the *geometry* so that the strings, instead of being plotted as is, are parsed into expressions before the plot is rendered.

```
ggplot(my.data, aes(x, y, label = greek.label)) +
    geom_point() +
    geom_text(angle = 45, hjust = 1.2, parse = TRUE) +
    labs(x = expression(alpha[i]),
        y = expression(Speed~~(m~s^{-1})),
        title = "Using expressions",
        subtitle = expression(sqrt(alpha[1] + frac(beta, gamma))))
```



We can also use a character string stored in a variable, and use function parse() to parse it in cases where an expression is required as we do here for subtitle. In this example we also set tick labels to expressions, taking advantage that expression() accepts multiple arguments separated by commas returning a vector of expressions.

A different approach (no example shown) would be to use parse() explicitly for each individual label, something that might be needed if the tick labels need to be "assembled" programmatically instead of set as constants.

Differences between parse() and expression(). Function parse() takes as an argument a character string. This is very useful as the character string can be created programmatically. When using expression() this is not possible, except for substitution at execution time of the value of variables into the expression. See the help pages for both functions.

Function expression() accepts its arguments without any delimiters. Function parse() takes a single character string as an argument to be parsed, in which case quotation marks within the string need to be *escaped* (using \" where a literal " is desired). We can, also in both cases, embed a character string by means of one of the functions plain(), italic(), bold() or bolditalic() which also affect the font

used. The argument to these functions needs to be a character string delimited by quotation marks if it is not to be parsed.

When using expression(), bare quotation marks can be embedded,

```
ggplot(cars, aes(speed, dist)) +
    geom_point() +
    xlab(expression(x[1]*" test"))
    while in the case of parse() they need to be escaped,
ggplot(cars, aes(speed, dist)) +
    geom_point() +
    xlab(parse(text = "x[1]*\" test\""))
    and in some cases will be enclosed within a format function.
ggplot(cars, aes(speed, dist)) +
    geom_point() +
    xlab(parse(text = "x[1]*italic(\" test\")"))
```

Some additional remarks. If expression() is passed multiple arguments, it returns a vector of expressions. Where ggplot() expects a single value as an argument, as in the case of axis labels, only the first member of the vector will be used.

```
ggplot(cars, aes(speed, dist)) +
  geom_point() +
  xlab(expression(x[1], " test"))
```

Depending on the location within a expression, spaces maybe ignored, or illegal. To juxtapose elements without adding space use \*, to explicitly insert white space, use ~. As shown above, spaces are accepted within quoted text. Consequently, the following alternatives can also be used.

```
xlab(parse(text = "x[1]~~~\"test\""))
xlab(parse(text = "x[1]~~~plain(test)"))
However, unquoted white space is discarded.
xlab(parse(text = "x[1]*plain( test)"))
```

Finally, it can be surprising that trailing zeros in numeric values appearing within an expression or text to be parsed are dropped. To force the trailing zeros to be retained we need to enclose the number in quotation marks so that it is interpreted as a character string.

Above we used paste() to insert values stored in a variable; functions format(), sprintf(), and strftime() allow the conversion into character strings of other values. These functions can be used when creating plots to generate suitable character strings for the label *aesthetic* out of numeric, logical, date, time, and even character values. They can be, for example, used to create labels within a call to aes().

```
sprintf("log(%.3f) = %.3f", 5, log(5))
## [1] "log(5.000) = 1.609"
sprintf("log(%.3g) = %.3g", 5, log(5))
```

```
## [1] "log(5) = 1.61"
```

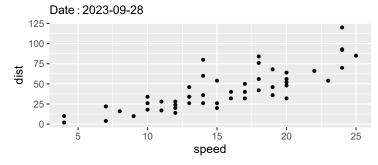
9.31 Study the chunck above. If you are familiar with C or C++ function sprintf() will already be familiar to you, otherwise study its help page.

Play with functions format(), sprintf(), and strftime(), formatting different types of data, into character strings of different widths, with different numbers of digits, etc.

It is also possible to substitute the value of variables or, in fact, the result of evaluation, into a new expression, allowing on the fly construction of expressions. Such expressions are frequently used as labels in plots. This is achieved through use of *quoting* and *substitution*.

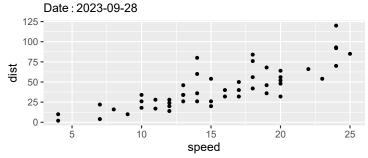
We use bquote() to substitute variables or expressions enclosed in .( ) by their value. Be aware that the argument to bquote() needs to be written as an expression; in this example we need to use a tilde, ~, to insert a space between words. Furthermore, if the expressions include variables, these will be searched for in the environment rather than in data, except within a call to aes().

## Time zone: Europe/Helsinki



In the case of substitute() we supply what is to be used for substitution through a named list.





For example, substitution can be used to assemble an expression within a function based on the arguments passed. One case of interest is to retrieve the name of the object passed as an argument, from within a function.

```
deparse_test <- function(x) {
    print(deparse(substitute(x)))
}

a <- "saved in variable"

deparse_test("constant")
## [1] "\"constant\""

deparse_test(1 + 2)
## [1] "1 + 2"

deparse_test(a)
## [1] "a"</pre>
```

Package 'ggtext' provides rich-text (basic HTML and Markdown) support for 'ggplot2', both for annotations and for data visualization. This is an alternative to the use of R expressions.

# 9.15 Creating complex data displays

The grammar of graphics allows one to build and test plots incrementally. In daily use, when creating a completely new plot, it is best to start with a simple design for a plot, print() this plot, checking that the output is as expected and the code error-free. Afterwards, one can map additional *aesthetics* and add *geometries* and *statistics* gradually. The final steps are then to add *annotations* and the text or expressions used for titles, and axis and key labels. Another approach is to start with an existing plot and modify it, e.g., by using the same plotting code with different data or mapping different variables. When reusing code for a different data set, scale limits and names are likely to need to be edited.

9.32 Build a graphically complex data plot of your interest, step by step. By step by step, I do not refer to using the grammar in the construction of the plot as earlier, but of taking advantage of this modularity to test intermediate versions in an iterative design process, first by building up the complex plot in stages as

a tool in debugging, and later using iteration in the processes of improving the graphic design of the plot and improving its readability and effectiveness.

## 9.16 Creating sets of plots

Plots to be presented at a given occasion or published as part of the same work need to be consistent in various respects: themes, scales and palettes, annotations, titles and captions. To guarantee this consistency we need to build plots modularly and avoid repetition by assigning names to the "modules" that need to be used multiple times.

## 9.16.1 Saving plot layers and scales in variables

When creating plots with 'ggplot2', objects are composed using operator + to assemble together the individual components. The functions that create plot layers, scales, etc. are constructors of objects and the objects they return can be stored in variables, and once saved, added to multiple plots at a later time.

We create a plot and save it to variable myplot and we separately save the values returned by a call to function labs().

We assemble the final plot from the two parts we saved into variables. This is useful when we need to create several plots ensuring that scale name arguments are used consistently. In the example above, we saved these names, but the approach can be used for other plot components or lists of components.

When composing plots with the + operator, the left-hand-side operand must be a "gg" object. The left operand is added to the "gg" object and the result returned.

```
myplot
myplot + mylabs + theme_bw(16)
myplot + mylabs + theme_bw(16) + ylim(0, NA)

We can also save intermediate results.
mylogplot <- myplot + scale_y_log10(limits=c(8,55))
mylogplot + mylabs + theme_bw(16)</pre>
```

#### 9.16.2 Saving plot layers and scales in lists

If the pieces to be put together do not include a "gg" object, we can group them into an R list and save it. When we later add the saved list to a "gg" object, the members of the list are added one by one to the plot respecting their order.

```
myparts <- list(mylabs, theme_bw(16))
mylogplot + myparts</pre>
```

9.33 Revise the code you wrote for the "playground" exercise in section 9.15, but this time, pre-building and saving groups of elements that you expect to be useful unchanged when composing a different plot of the same type, or a plot of a different type from the same data.

## 9.16.3 Using functions as building blocks

When the blocks we assemble need to accept arguments when used, we have to define functions instead of saving plot components to variables. The functions we define, have to return a "gg" object, a list of plot components, or a single plot component. The simplest use is to alter some defaults in existing constructor functions returning "gg" objects or layers. The ellipsis (...) allows passing named arguments to a nested function. In this case, every single argument passed by name to bw\_ggplot() will be copied as argument to the nested call to ggplot(). Be aware, that supplying arguments by position, is possible only for parameters explicitly included in the definition of the wrapper function,

## 9.17 Generating output files

It is possible, when using RStudio, to directly export the displayed plot to a file using a menu. However, if the file will have to be generated again at a later time, or a series of plots need to be produced with consistent format, it is best to include the commands to export the plot in the script.

In R, files are created by printing to different devices. Printing is directed to a currently open device such a window in RStudio. Some devices produce screen output, others files. Devices depend on drivers. There are both devices that are part of R and additional ones defined in contributed packages.

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Creating a file involves opening a device, printing and closing the device in sequence. In most cases the file remains locked until the device is close.

For example when rendering a plot to PDF, Encapsulated Postcript, SVG or other vector graphics formats, arguments passed to width and height are expressed in inches.

```
fig1 <- ggplot(data.frame(x = -3:3), aes(x = x)) +
    stat_function(fun = dnorm)
pdf(file = "fig1.pdf", width = 8, height = 6)
print(fig1)
dev.off()</pre>
```

For Encapsulated Postscript and SVG output, we only need to substitute pdf() with postscript() or svg(), respectively.

```
postscript(file = "fig1.eps", width = 8, height = 6)
print(fig1)
dev.off()
```

In the case of graphics devices for file output in BMP, JPEG, PNG and TIFF bitmap formats, arguments passed to width and height are expressed in pixels.

```
tiff(file = "fig1.tiff", width = 1000, height = 800)
print(fig1)
dev.off()
```

Some graphics devices are part of base-R, and others are implemented in contributed packages. In some cases, there are multiple graphic device available for rendering graphics in a given file format. These devices usually use different libraries, or have been designed with different aims. These alternative graphic devices can also differ in their function signature, i.e., have differences in the parameters and their names. In cases when rendering fails inexplicably, it can be worthwhile to switch to an alternative graphics device to find out if the problem is in the plot or in the rendering engine.

## 9.18 Further reading

An in-depth discussion of the many extensions to package 'ggplot2' is outside the scope of this book. Several books describe in detail the use of 'ggplot2', being *ggplot2: Elegant Graphics for Data Analysis* (Wickham and Sievert 2016) the one written by the main author of the package. For inspiration or worked out examples, the book *R Graphics Cookbook* (Chang 2018) is an excellent reference. In depth explanations of the technical aspects of R graphics are available in the book *R Graphics* (Murrell 2019).

```
## Error : package 'ggplot2' is required by 'ggpp' so will not be detached
```

# Base R and Extensions: Data Sharing

Most programmers have seen them, and most good programmers realize they've written at least one. They are huge, messy, ugly programs that should have been short, clean, beautiful programs.

John Bentley *Programming Pearls*, 1986

# 10.1 Aims of this chapter

Base R and the recommended packages (installed by default) include several functions for importing and exporting data. Contributed packages provide both replacements for some of these functions and support for several additional file formats. In the present chapter, I aim at describing both data input and output covering in detail only the most common "foreign" data formats (those not native to R).

Data file formats that are foreign to R are not always well defined, making it necessary to reverse-engineer the algorithms needed to read them. These formats, even when clearly defined, may be updated by the developers of the foreign software that writes the files. Consequently, developing software to read and write files using foreign formats can easily result in long, messy, and ugly R scripts. We can also unwillingly write code that usually works but occasionally fails with specific files, or even worse, occasionally silently corrupts the imported data. The aim of this chapter is to provide guidance for finding functions for reading data encoded using foreign formats, covering both base R, including the 'foreign' package, and independently contributed packages. Such functions are well tested or validated.

In this chapter you will familiarize yourself with how to exchange data between R and other applications. The functions save() and load(), and saveRDS() and readRDS(), all of which save and read data in R's native formats, are described in sections 4.7.2 and 4.7.3 starting on page 118.

#### 10.2 Introduction

The first step in any data analysis with R is to input or read-in the data. Available sources of data are many and data can be stored or transmitted using various formats, both based on text or binary encodings. It is crucial that data is not altered (corrupted) when read and that in the eventual case of an error, errors are clearly reported. Most dangerous are silent non-catastrophic errors.

The very welcome increase of awareness of the need for open availability of data, makes the output of data from R into well-defined data-exchange formats another crucial step. Consequently, in many cases an important step in data analysis is to export the data for submission to a repository, in addition to publication of the results of the analysis.

Faster internet access to data sources and cheaper random-access memory (RAM) has made it possible to efficiently work with relatively large data sets in R. That R keeps all data in memory (RAM), imposes limits to the size of data R functions can operate on. For data sets large enough not to fit in computer RAM, one can use selective reading of data from flat files, or from databases outside of R.

Some contributed R packages support import of data saved in the same formats already supported by base R, but using different compromises between reliability, easy of use and performance. Functions in base R tend to prioritize reliability and protection from data corruption while some contributed packages prioritize performance. Other contributed packages make it possible to import and export data stored in file formats not supported by base R functions. Some of these formats are subject-area specific while others are in widespread use. Packages supporting direct download of data sets from public repositories are becoming also common.

# 10.3 Packages used in this chapter

```
install.packages(learnrbook::pkgs_ch_data)
```

To run the examples included in this chapter, you need first to load some packages from the library (see section 6.4 on page 178 for details on the use of packages).

```
library(learnrbook)
library(tibble)
library(purrr)
library(wrapr)
library(stringr)
library(dplyr)
library(tidyr)
library(readr)
library(readxl)
library(xlsx)
library(readODS)
```

```
library(pdftools)
library(foreign)
library(haven)
library(xml2)
library(XML)
library(ncdf4)
library(tidync)
library(lubridate)
library(jsonlite)
```

Some data sets used in this and other chapters are available in package 'learnrbook'. In addition to the R data objects, the package includes files saved in *foreign* formats used in examples of importing data. The files can be either read from the R library, or from a copy in a local folder. In this chapter we assume the user has copied the folder "extdata" from the package to a working folder.

Copy the files using:

```
pkg.path <- system.file("extdata", package = "learnrbook")
file.copy(pkg.path, ".", overwrite = TRUE, recursive = TRUE)
## [1] TRUE

We also make sure the folder used to save data read from the internet, exists.
save.path = "./data"
if (!dir.exists(save.path)) {
    dir.create(save.path)
}</pre>
```

# 10.4 File names and operations

We start with the naming of files as it affects data sharing irrespective of the format used for its encoding. The main difficulty is that different operating systems have different rules governing the syntax used for file names and file paths. In many cases, like when depositing data files in a public repository, we need to ensure that file names are valid in multiple operating systems (OSs). If the script used to create the files is itself expected to be OS agnostic, we also need to be careful to query the OS for file names and paths without making assumptions on the naming rules or available OS commands. This is especially important when developing R packages.

A For maximum portability, file names should never contain white-space characters and contain at most one dot. For the widest possible portability, underscores should be avoided using dashes instead. As an example, instead of my data.2019.csv, use my-data-2019.csv.

R provides functions which help with portability, by hiding the idiosyncrasies of the different OSs from R code. In scripts these functions should be preferred over direct call to OS commands (i.e., using shell() or system()) whenever possible. As the algorithm needed to extract a file name from a file path is OS specific, R provides functions such as basename(), whose implementation is OS specific but from the side of R code behave identically—these functions hide the differences among OSs from the user of R. The chunk below can be expected to work correctly under any OS for which R is available.

```
basename("extdata/my-file.txt")
## [1] "my-file.txt"
```

While in Unix and Linux folder nesting in file paths is marked with a forward slash character (/), under MS-Windows it is marked with a backslash character (\). Backslash (\) is an escape character in R and interpreted as the start of an embedded special sequence of characters (see section 3.4 on page 41), while in R a forward slash (/) can be used for file paths under any OS, and escaped backslash (\\) is valid only under MS-Windows. Consequently, / should be always preferred to \\ to ensure portability, and is the approach used in this book.

```
basename("extdata/my-file.txt")
## [1] "my-file.txt"
basename("extdata\\my-file.txt")
## [1] "my-file.txt"
```

The complementary function to basename() is dirname() and extracts the bare path to the containing folder, from a full file path.

```
dirname("extdata/my-file.txt")
## [1] "extdata"
```

Functions getwd() and setwd() can be used to get the path to the current working directory and to set a directory as current, respectively.

```
# not run
getwd()
```

Function setwd() returns the path to the current working directory, allowing us to portably set the working directory to the previous one. Both relative paths (relative to the current working directory), as in the example, or absolute paths (given in full) are accepted as an argument. In mainstream OSs "." indicates the current directory and ".." the directory above the current one.

```
# not run
oldwd <- setwd("..")
getwd()</pre>
```

The returned value is always an absolute full path, so it remains valid even if the path to the working directory changes more than once before being restored.

```
# not run
oldwd
setwd(oldwd)
getwd()
```

We can also obtain lists of files and/or directories (= disk folders) portably across OSs.

```
head(list.files())
## [1] "abbrev.sty"
## [2] "anscombe.svg"
## [3] "aphalo-Learn-R-2ed-crc-2023-06-14.pdf"
## [4] "aphalo-learn-R-2ed-draft-2022-02-01.pdf"
## [5] "Aphalo-Learn-R-2ed-DRAFT-2023-07-04.pdf"
```

```
## [6] "aphalo-learn-r-2ed-draft.pdf"
head(list.dirs())
## [1] "." "./.git" "./.git/hooks" "./.git/info"
## [5] "./.git/logs" "./.git/logs/refs"
head(dir())
## [1] "abbrev.sty"
## [2] "anscombe.svg"
## [3] "aphalo-Learn-R-2ed-crc-2023-06-14.pdf"
## [4] "aphalo-learn-R-2ed-draft-2022-02-01.pdf"
## [5] "Aphalo-Learn-R-2ed-DRAFT-2023-07-04.pdf"
## [6] "aphalo-learn-r-2ed-draft.pdf"
```

- 10.1 The default argument for parameter path is the current working directory, under Windows, Unix, and Linux indicated by ".". Convince yourself that this is indeed the default by calling the functions with an explicit argument. After this, play with the functions trying other existing and non-existent paths in your computer.
- 10.2 Use parameter full.names with list.files() to obtain either a list of file paths or bare file names. Similarly, investigate how the returned list of files is affected by the argument passed to all.names.
- 10.3 Compare the behavior of functions dir() and list.dirs(), and try by overriding the default arguments of list.dirs(), to get the call to return the same output as dir() does by default.

Base R provides several functions for portably working with files, and they are listed in the help page for files and in individual help pages. Use help("files") to access the help for this "family" of functions.

```
if (!file.exists("xxx.txt")) {
 file.create("xxx.txt")
## [1] TRUE
file.size("xxx.txt")
## [1] 0
file.info("xxx.txt")
##
       size isdir mode
                                   mtime
##
                     atime exe
## xxx.txt 2023-09-28 00:02:34 no
file.rename("xxx.txt", "zzz.txt")
## [1] TRUE
file.exists("xxx.txt")
## [1] FALSE
file.exists("zzz.txt")
## [1] TRUE
file.remove("zzz.txt")
## [1] TRUE
```

10.4 Function file.path() can be used to construct a file path from its components in a way that is portable across OSs. Look at the help page and play with the function to assemble some paths that exist in the computer you are using.

## 10.5 Opening and closing file connections

Examples in the rest of this chapter use as an argument for the file formal parameter literal paths or URLs, and complete the reading or writing operations within the call to a function. Sometimes it is necessary to read or write a text file sequentially, one row or record at a time. In such cases it is most efficient to keep the file open between reads and close the connection only when it is no longer needed. See help(connections) for details about the various functions available and their behavior in different OSs. In the next example we open a file connection, read two lines, first the top one with column headers, then in a separate call to readLines(), the two lines or records with data, and finally close the connection.

```
f1 <- file("extdata/not-aligned-ASCII-UK.csv", open = "r") # open for reading
readLines(f1, n = 1)
## [1] "col1,col2,col3,col4"

readLines(f1, n = 2)
## [1] "1.0,24.5,346,ABC" "23.4,45.6,78,Z Y"
close(f1)</pre>
```

When R is used in batch mode, the "files" stdin, stdout and stderror can be opened, and data read from, or written to. These *standard* sources and sinks, so familiar to C programmers, allow the use of R scripts as tools in data pipes coded as shell scripts under Unix and other OSs.

#### 10.6 Plain-text files

In general, text files are the most portable approach to data storage but usually also the least efficient with respect to the size of the file. Text files are composed of encoded characters. This makes them easy to edit with text editors and easy to read from programs written in most programming languages. On the other hand, how the data encoded as characters is arranged can be based on two different approaches: positional or using a specific character as a separator. The positional approach is more concise but almost unreadable to humans as the values run into each other. Reading of data stored using a positional approach requires access to a format definition and was common in FORTRAN and COBOL at the time when punch cards were used to store data. In the case of separators, different separators are in common use. Comma-separated values (CSV) encodings use either a comma or semicolon to separate the fields or columns. Tabulator, or tab-separated values (TSV) use the tab character as a column separator. Sometimes white space is used as a separator, most commonly when all values are to be converted to numeric.

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Not all text files are born equal. When reading text files, and *foreign* binary files which may contain embedded text strings, there is potential for their misinterpretation during the import operation. One common source of problems, is that column headers are to be read as R names. As earlier discussed, there are strict rules, such as avoiding spaces or special characters if the names are to be used with the normal syntax. On import, some functions will attempt to sanitize the names, but others not. Most such names are still accessible in R statements, but a special syntax is needed to protect them from triggering syntax errors through their interpretation as something different than variable or function names—in R jargon we say that they need to be quoted.

Some of the things we need to be on the watch for are: 1) Mismatches between the character encoding expected by the function used to read the file, and the encoding used for saving the file—usually because of different locales. 2) Leading or trailing (invisible) spaces present in the character values or column names—which are almost invisible when data frames are printed. 3) Wrongly guessed column classes—a typing mistake affecting a single value in a column, e.g., the wrong kind of decimal marker, prevents the column from being recognized as numeric. 4) Mismatched decimal marker in csv files—the marker depends on the locale (language and sometimes country) settings.

If you encounter problems after import, such as failure of indexing of data frame columns by name, use function names() to get the names printed to the console as a character vector. This is useful because character vectors are always printed with each string delimited by quotation marks making leading and trailing spaces clearly visible. The same applies to use of levels() with factors created with data that might have contained mistakes.

To demonstrate some of these problems, I create a data frame with name sanitation disabled, and in the second statement with sanitation enabled. The first statement is equivalent to the default behavior of functions in package 'readr' and the second is equivalent to the behavior of base R functions. 'readr' prioritizes the integrity of the original data while R prioritizes compatibility with R's naming rules.

An even more subtle case is when characters can be easily confused by the user reading the output: zero and o (a0 vs. a0) or el and one (a1 vs. a1) can be difficult to distinguish in some fonts. When using encodings capable of storing many character shapes, such as unicode, in some cases two characters with almost identical visual shape may be encoded as different characters.

```
data.frame(al = 1, a1 = 2, a0 = 3, a0 = 4)
## al a1 a0 a0
## 1 1 2 3 4
```

Reading data from a text file can result in very odd-looking values stored in R

variables because of a mismatch in encoding, e.g., when a CSV file saved with MS-Excel is silently encoded using 16-bit unicode format, but read as an 8-bit unicode encoded file.

The hardest part of all these problems is to diagnose their origin, as function arguments and working environment options can in most cases be used to force the correct decoding of text files with diverse characteristics, origins and vintages once one knows what is required. One function in the R 'tools' package, which is not exported, can at the time of writing be used to test files for the presence on non-ASCII characters: tools:::showNonASCIIfile(). This function takes as an argument the path to a file.

#### 10.6.1 Base R and 'utils'

Text files containing data in columns can be divided into two broad groups. Those with fixed-width fields and those with delimited fields. Fixed-width fields were especially common in the early days of FORTRAN and COBOL when data storage capacity was very limited. These formats are frequently capable of encoding information using fewer characters than when delimited fields are used. The best way of understanding the differences is with examples. Although in this section we exemplify the use of functions by passing a file name as an argument, URLs, and open file descriptors are also accepted (see section 10.5 on page 372).

In the first example we will read a file with fields solely delimited by "," This is what is called comma-separated-values (CSV) format which can be read and written with read.csv() and write.csv(), respectively.

Example file not-aligned-ASCII-UK.csv contains:

```
col1, col2, col3, col4
1.0,24.5,346,ABC
23.4,45.6,78,Z Y
from_csv_a.df
               <- read.csv("extdata/not-aligned-ASCII-UK.csv", stringsAsFac-</pre>
tors = FALSE)
sapply(from_csv_a.df, class)
          col1
                      co12
                                   co13
                 "numeric"
                              "integer" "character"
##
     "numeric"
from_csv_a.df[["col4"]]
## [1] "ABC" "Z Y"
```

Wether columns containing character strings that cannot be converted into numbers are converted into factors or remain as character strings in the returned data frame depends on the value passed to parameter stringsasfactors. The default changed in R version 4.0.0 from TRUE into FALSE, so it is better to explicitly pass an argument when it is possible that code is run on both newer and older versions of R.

```
from_csv_a.df <- read.csv("extdata/not-aligned-ASCII-UK.csv", stringsAsFac-
tors = TRUE)
```

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```
sapply(from_csv_a.df, class)
## col1 col2 col3 col4
## "numeric" "numeric" "integer" "factor"
from_csv_a.df[["col4"]]
## [1] ABC Z Y
## Levels: ABC Z Y
levels(from_csv_a.df[["col4"]])
## [1] "ABC" "Z Y"
```

10.5 Read the file not-aligned-ASCII-UK.csv with function read.csv2() instead of read.csv(). Although this may look like a waste of time, the point of the exercise is for you to get familiar with R behavior in case of such a mistake. This will help you recognize similar errors when they happen accidentally, which is quite common when files are shared.

Example file aligned-ASCII-UK.csv contains comma-separated-values with added white space to align the columns, to make it easier to read by humans. These aligned fields contain leading and trailing white spaces that are included in string values when the file is read.

```
col1, col2, col3, col4
1.0, 24.5, 346, ABC
23.4, 45.6, 78, Z Y
```

Although space characters are read as part of the fields, they are ignored when conversion to numeric takes place. The remaining leading and trailing spaces in character strings are difficult to see when data frames are printed.

```
from_csv_b.df <- read.csv("extdata/aligned-ASCII-UK.csv", stringsAsFac-
tors = TRUE)</pre>
```

Using levels() we can more clearly see that the labels of the automatically created factor levels contain leading spaces.

```
sapply(from_csv_b.df, class)
## col1 col2 col3 col4
## "numeric" "numeric" "integer" "factor"
from_csv_b.df[["col4"]]
## [1] ABC Z Y
## Levels: ABC Z Y
levels(from_csv_b.df[["col4"]])
## [1] " ABC" " Z Y"
```

By default, column names are sanitized but factor levels are not. By consulting the documentation with help(read.csv) we discover that by passing an additional argument we can change this default and obtain the data read as desired. Most likely the default has been chosen so that by default data integrity is maintained.

Decimal points and exponential notation are allowed for floating point values. In English-speaking locales, the decimal mark is a point, while in many other locales it is a comma. If a comma is used as decimal marker, we can no longer use it as field separator and is usually substituted by a semicolon (;). In such a case we can use read.csv2() and write.csv2(). Furthermore, parameters dec and sep allow setting them to arbitrary characters. Function read.table() does the actual work and functions like read.csv() only differ in the default arguments for the different parameters. By default, read.table() expects fields to be separated by white space (one or more spaces, tabs, new lines, or carriage return). Strings with embedded spaces need to be quoted in the file as shown below.

```
col1 col2 col3 col4
1.0 24.5 346 ABC
23.4 45.6
           78 "Z Y"
from_txt_b.df <- read.table("extdata/aligned-ASCII.txt", header = TRUE)</pre>
sapply(from_txt_b.df, class)
          col1
                      co12
                                   col3
     "numeric"
                 "numeric"
                              "integer" "character"
##
from_txt_b.df[["col4"]]
## [1] "ABC" "Z Y"
levels(from_txt_b.df[["col4"]])
## NULL
```

With a fixed-width format, no delimiters are needed. Decoding is based solely on the position of the characters in the line or record. A file like this cannot be interpreted without a description of the format used for saving the data. Files containing data stored in *fixed width format* can be read with function read.fwf(). Records for a single observation can be stored in a single or multiple lines. In either case, each line has fields of different but fixed known widths.

Function read.fortran() is a wrapper on read.fwf() that accepts format definitions similar to those used in FORTRAN. One particularity of FORTRAN formatted data transfer is that the decimal marker can be omitted in the saved file and its position specified as part of the format definition, a trick used to make text files (or stacks of punch cards!) smaller. Modern versions of FORTRAN support reading from and writing to other formats like those using field delimiters described above.

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The file reading functions described above share with read.table() the same parameters. In addition to those described above, other frequently useful parameters are skip and n, which can be used to skip lines at the top of a file and limit the number of lines (or records) to read; header, which accepts a logical argument indicating if the fields in the first text line read should be decoded as column names rather than data; na.strings, to which can be passed a character vector with strings to be interpreted as NA; and colclasses, which provides control of the conversion of the fields to R classes and possibly skipping some columns altogether. All these parameters are described in the corresponding help pages.

10.6 In reality read.csv(), read.csv2() and read.table() are the same function with different default arguments to several of their parameters. Study the help page, and by passing suitable arguments, make read.csv() behave like read.table(), then make read.table() behave like read.csv2().

We can read a text file as character strings, without attempting to decode them. This is occasionally useful, such as when we do the decoding as part of our own script. In this case, the function to use is readLines(). The returned value is a character vector in which each member string corresponds to one line or record in the file, with the end-of-line markers stripped (see example in section 10.5 on page 372).

Next we give one example of the use of a *write* function matching one of the *read* functions described above. The *write.csv()* function takes as an argument a data frame, or an object that can be coerced into a data frame, converts it to character strings, and saves them to a text file. We first create the data frame that we will write to disk.

```
my.df \leftarrow data.frame(x = 1:5, y = 5:1 / 10, z = letters[1:5])
```

We write my.df to a CSV file suitable for an English language locale, and then display its contents.

```
write.csv(my.df, file = "my-file1.csv", row.names = FALSE)
file.show("my-file1.csv", pager = "console")

"x","y","z"
1,0.5,"a"
2,0.4,"b"
3,0.3,"c"
4,0.2,"d"
5,0.1,"e"
```

- In most cases setting, as above, row.names = FALSE when writing a CSV file will help when it is read. Of course, if row names do contain important information, such as gene tags, you cannot skip writing the row names to the file unless you first copy these data into a column in the data frame. (Row names are stored separately as an attribute in data.frame objects, see section 4.6 on page 114 for details.)
- 10.7 Write the data frame my.df into text files with functions write.csv2() and write.table() instead of read.csv() and display the files.

Function cat() takes R objects and writes them after conversion to character

strings to the console or a file, inserting one or more characters as separators, by default, a space. This separator can be set through parameter sep. In our example we set sep to a new line (entered as the escape sequence "\n").

```
my.lines <- c("abcd", "hello world", "123.45")
cat(my.lines, file = "my-file2.txt", sep = "\n")
file.show("my-file2.txt", pager = "console")
abcd
hello world
123.45</pre>
```

#### 10.6.2 'readr'

Package 'readr' is part of the 'tidyverse' suite. It defines functions that have different default behavior and that are designed to be faster under different situations than those native to R. The functions from package 'readr' can sometimes wrongly decode their input and rarely even silently do this. Base R functions do less *guessing*, e.g., the delimiters must be supplied as arguments. The 'readr' functions guess more properties of the text file format; in most cases they succeed, which is very handy, but occasionally they fail. Automatic guessing can be overridden by passing arguments and this is recommended for scripts that may be reused to read different files in the future. Another important advantage is that these functions read character strings formatted as dates or times directly into columns of class POSIXct. All write functions defined in 'readr' have an append parameter, which can be used to change the default behavior of overwriting an existing file with the same name, to appending the output at its end.

Although in this section we exemplify the use of these functions by passing a file name as an argument, as is the case with R native functions, URLs, and open file descriptors are also accepted (see section 10.5 on page 372). Furthermore, if the file name ends in a tag recognizable as indicating a compressed file format, the file will be uncompressed on the fly.

Functions "equivalent" to native R functions described in the previous section have names formed by replacing the dot with an underscore, e.g., read\_csv() ≈ read.csv(). The similarity refers to the format of the files read, but not the order, names, or roles of their formal parameters. For example, function read\_table() has a slightly different behavior than read.table(), although they both read fields separated by white space. Other aspects of the default behavior are also different, for example 'readr' functions do not convert columns of character strings into factors as R functions did by default in versions earlier than 4.2.0. Row names are not set in the returned tibble, which inherits from data.frame, but is not fully compatible (see section 8.4.2 on page 245).

Package 'readr' is under active development, and functions with the same name from different major versions are not fully compatible. Code chunks for examples from the previous edition of the book no longer work because the new implementation fails to recognize escaped special characters. In addition function read\_table2() has been renamed read\_table().

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As we can see in this first example, these functions also report to the console the specifications of the columns, which is important when these are guessed from the file contents, or even only from rows near the top of the file.

```
read_csv(file = "extdata/aligned-ASCII-UK.csv")
## Rows: 2 Columns: 4
## -- Column specification -------
## Delimiter: ","
## chr (1): col4
## dbl (3): col1, col2, col3
## i Use `spec()` to retrieve the full column specification for this data.
## i Specify the column types or set `show_col_types = FALSE` to quiet this
messaae.
## # A tibble: 2 x 4
     col1 col2 col3 col4
##
    <dbl> <dbl> <dbl> <chr>
## 1 1
          24.5
                346 ABC
## 2 23.4 45.6
                  78 Z Y
read_csv(file = "extdata/not-aligned-ASCII-UK.csv")
## Rows: 2 Columns: 4
## -- Column specification -----
## Delimiter: ","
## chr (1): col4
## dbl (3): col1, col2, col3
## i Use `spec()` to retrieve the full column specification for this data.
## i Specify the column types or set `show_col_types = FALSE` to quiet this
message.
## # A tibble: 2 x 4
##
     col1 col2 col3 col4
##
    <dbl> <dbl> <dbl> <chr>
## 1 1
           24.5
                 346 ABC
## 2 23.4 45.6
                  78 Z Y
```

Package 'readr' is under active development, and different major versions are not fully compatible with each other. Because of the misaligned fields in file "not-aligned-ASCII.txt" in the past we needed to use read\_table2(), which allowed misalignment of fields, similarly to read.table(). This function has been renamed as read\_table() and read\_table2() deprecated. However, parsing of both files fails if they are read with read\_table().

```
read_table(file = "extdata/aligned-ASCII.txt")

##

## -- Column specification ------

## cols(

## cols(

## col2 = col_double(),

## col3 = col_double(),

## col4 = col_character()

## warning: 1 parsing failure.
```

```
## row col expected actual file
## 2 -- 4 columns 5 columns 'extdata/aligned-ASCII.txt'
```

```
read_table(file = "extdata/not-aligned-ASCII.txt")
##
## -- Column specification -------
## cols(
    col1 = col_double(),
##
##
    col2 = col_double(),
##
    col3 = col_double(),
##
    col4 = col_character()
## )
## Warning: 1 parsing failure.
## row col expected
                    actual
                                                     file
    2 -- 4 columns 5 columns 'extdata/not-aligned-ASCII.txt'
## # A tibble: 2 x 4
##
     col1 col2 col3 col4
##
    <dbl> <dbl> <dbl> <chr>
               346 "ABC"
## 1 1
          24.5
                 78 "\"z"
## 2 23.4 45.6
```

Function read\_delim() with space as the delimiter needs to be used instead of read\_table().

```
read_delim(file = "extdata/not-aligned-ASCII.txt", delim = " ")
## Rows: 2 Columns: 4
## -- Column specification -------
## Delimiter: " "
## chr (1): col4
## dbl (3): col1, col2, col3
## i Use `spec()` to retrieve the full column specification for this data.
## i Specify the column types or set `show_col_types = FALSE` to quiet this
message.
## # A tibble: 2 x 4
##
     col1 col2 col3 col4
    <dbl> <dbl> <dbl> <chr>
## 1
          24.5
                 346 ABC
    1
## 2 23.4 45.6
                  78 Z Y
```

Function read\_tsv() reads files encoded with the tab character as the delimiter, and read\_fwf() reads files with fixed width fields. There is, however, no equivalent to read.fortran(), supporting implicit decimal points.

10.8 Use the "wrong" read\_ functions to read the example files used above and/or your own files. As mentioned earlier, forcing errors will help you learn how to diagnose when such errors are caused by coding or data entry mistakes. In this case, as wrongly read data are not always accompanied by error or warning messages, carefully check the returned tibbles for misread data values.

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The functions from R's package 'utils' read the whole file as text before attempting to guess the class of the columns or their alignment. This is reliable but slow for text files with many lines. The functions from 'readr' read by default only the top 1000 lines when guessing the format and class, and then rather blindly read the whole files assuming that the guessed properties also apply to the remaining lines of the file. This is more efficient in the case of such files, but somehow risky. In contrast, the functions from R's package 'utils' are much faster than those from package 'readr' at reading files with many fields (or columns) per line.

In earlier versions of 'readr', a typical failure to correctly decode fields was when numbers are in increasing order and the field widths continue increasing in the lines below those used for guessing, but this case seems to be, at the time of writing correctly, handled. A guess based on the top 1000 lines of a text file also means that in cases values in lines below <code>guess\_max</code> lines cannot be converted to numeric, instead of returning a column of character strings as functions from R's package 'utils', their values are replaced by numeric NA values with a warning. To demonstrate this we will drastically reduce <code>guess\_max</code> from its default so that we can use an for the example a file only a few lines in length.

```
read_table(file = "extdata/miss-aligned-ASCII.txt")
## -- Column specification -----
## cols(
##
     col1 = col_character(),
##
     col2 = col\_double(),
##
     col3 = col\_double(),
##
     col4 = col_character()
## )
##
  # A tibble: 4 x 4
##
    col1
            col2 col3 col4
     <chr> <dbl> <dbl> <chr>
## 1 1.0
            24.5
                   346 ABC
## 2 2.4
            45.6
                    78 XYZ
## 3 20.4
            45.6
                    78 XYZ
## 4 a
            20
                  2500 abc
```

```
read_table(file = "extdata/miss-aligned-ASCII.txt", guess_max = 3L)
##
## -- Column specification --------
## cols(
##
    col1 = col_double(),
    col2 = col\_double(),
##
##
    col3 = col\_double(),
    col4 = col_character()
##
## )
## Warning: 1 parsing failure.
## row col expected actual
                                                    file
   4 col1 a double
                        a 'extdata/miss-aligned-ASCII.txt'
## # A tibble: 4 x 4
     col1 col2 col3 col4
    <dbl> <dbl> <dbl> <chr>
      1
           24.5
                 346 ABC
      2.4 45.6
                  78 XYZ
          45.6
                  78 XYZ
## 3 20.4
## 4 NA
           20
                 2500 abc
```

The write\_functions from 'readr' are the counterpart to write. functions from 'utils'. In addition to the expected write\_csv(), write\_csv2(), write\_tsv() and write\_delim(), 'readr' provides functions that write MS-Excel-friendly CSV files. We demonstrate here the use of write\_excel\_csv() to produce a text file with comma-separated fields suitable for import into MS-Excel.

```
write_excel_csv(my.df, file = "my-file6.csv")
file.show("my-file6.csv", pager = "console")
```

That saves a file containing the following text:

```
"x","y","z"
1,0.5,"a"
2,0.4,"b"
3,0.3,"c"
4,0.2,"d"
5,0.1,"e"
```

10.9 Compare the output from write\_excel\_csv() and write\_csv(). What is the difference? Does it matter when you import the written CSV file into Excel (in the version you are using, and with the locale settings of your computer)?

The pair of functions read\_lines() and write\_lines() read and write character vectors without conversion, similarly to base R readLines() and writeLines(). Functions read\_file() and write\_file() read and write the contents of a whole text file into, and from, a single character string. Functions read\_file() and write\_file() can also be used with raw vectors to read and write binary files or text files of unknown encoding.

The contents of the whole file are returned as a character vector of length one, with the embedded new line markers. We use cat() to print it so these new line characters force the start of a new print-out line.

```
one.str <- read_file(file = "extdata/miss-aligned-ASCII.txt")
length(one.str)
## [1] 1</pre>
```

```
cat(one.str)
## col1 col2 col3 col4
## 1.0 24.5 346 ABC
## 2.4 45.6 78 XYZ
## 20.4 45.6 78 XYZ
## a 20 2500 abc
```

■ **10.10** Use write\_file() to write a file that can be read with read\_csv().

#### 10.7 XML and HTML files

XML files contain text with special markup. Several modern data exchange formats are based on the XML standard (see https://www.w3.org/TR/xml/) which uses schemas for flexibility. Schemas define specific formats, allowing reading of formats not specifically targeted during development of the read functions. Even the modern XHTML standard used for web pages is based on such schemas, while HTML only differs slightly in its syntax.

#### 10.7.1 'xml2'

Package 'xml2' provides functions for reading and parsing XTML and HTML files. This is a vast subject, of which I will only give a brief example.

We first read a web page with function read\_html(), and explore its structure.

```
web_page <- read_html("https://r.r4photobiology.info/index.html")</pre>
html_structure(web_page)
## <html [xmlns, lang, xml:lang]>
##
     <head>
##
       <meta [charset]>
##
       <meta [name, content]>
##
       <meta [name, content]>
##
       <meta [name, content]>
##
       <meta [name, content]>
##
       <title>
##
         {text}
##
       <style>
##
         {cdata}
##
       <script>
```

```
##
         {cdata}
##
       <style [type]>
##
         {cdata}
##
       <link#quarto-text-highlighting-styles [href, rel]>
##
       <script>
##
         {cdata}
##
       <style [type]>
##
         {cdata}
##
       <link#quarto-bootstrap [href, rel, data-mode]>
       link [rel, href]>
##
##
     <body.fullcontent>
##
       {text}
##
      <div#quarto-content .page-columns.page-rows-contents.page-layout-article>
##
         {text}
##
         <main#quarto-document-content .content>
##
            <header#title-block-header .quarto-title-block.default>
##
              <div.quarto-title>
##
                {text}
                <h1.title>
##
                  {text}
##
##
                {text}
##
                <p.subtitle.lead>
##
                  {text}
##
                {text}
##
              {text}
##
              <div.quarto-title-meta>
##
                {text}
                <div>
##
##
                  {text}
                  <div.quarto-title-meta-heading>
##
##
                    {text}
##
                  {text}
##
                  <div.quarto-title-meta-contents>
##
                    {text}
##
                    >
##
                      {text}
##
                    {text}
##
                  {text}
##
                {text}
##
                <div>
##
##
                  <div.quarto-title-meta-heading>
##
                    {text}
##
                  {text}
##
                  <div.quarto-title-meta-contents>
##
                    {text}
                    <p.date>
##
##
                      {text}
##
                    {text}
##
                  {text}
##
                {text}
##
              {text}
            <section#what-is-stored-in-this-repository .level2>
##
              <h2.anchored [data-anchor-id]>
##
##
                {text}
              {text}
##
##
              >
```

```
##
                {text}
##
                <br>
##
                {text}
##
                <a [href]>
                  {text}
##
##
                {text}
##
              {text}
            <section#installation .level2>
##
##
              <h2.anchored [data-anchor-id]>
##
                {text}
##
              {text}
##
              >
##
                {text}
              {text}
##
##
              ##
                {text}
##
                <a [href]>
##
                  {text}
##
                {text}
##
                <a [href]>
##
                  {text}
##
                {text}
##
              {text}
##
              >
##
                {text}
##
                <code>
##
                  {text}
##
                {text}
##
                <code>
##
                  {text}
##
                {text}
##
              {text}
##
              <div.cell>
##
                {text}
##
                <div#cb1 .sourceCode.cell-code>
##
                  <pre.sourceCode.r.code-with-copy>
##
                    <code.sourceCode.r>
##
                       <span#cb1-1>
##
                         <a [href, aria-hidden, tabindex]>
##
                         {text}
##
                         <span.ot>
##
                           {text}
##
                         {text}
##
                         <span.fu>
##
                           {text}
##
                         {text}
##
                         <span.st>
##
                           {text}
##
                         {text}
##
                       {text}
##
                       <span#cb1-2>
##
                         <a [href, aria-hidden, tabindex]>
                         <span.cf>
##
##
                           {text}
##
                         {text}
##
                         <span.fu>
##
                           {text}
```

```
##
                         {text}
                       {text}
##
##
                       <span#cb1-3>
##
                         <a [href, aria-hidden, tabindex]>
##
                         {text}
##
                         <span.st>
##
                           {text}
##
                         {text}
##
                         <span.ot>
##
                           {text}
##
                         {text}
##
                         <span.st>
##
                           {text}
##
                       {text}
                       <span#cb1-4>
##
##
                         <a [href, aria-hidden, tabindex]>
##
##
                       {text}
                       <span#cb1-5>
##
                         <a [href, aria-hidden, tabindex]>
##
##
                         {text}
##
                         <span.st>
##
                           {text}
##
                         {text}
##
                         <span.ot>
##
                           {text}
##
                         {text}
##
                         <span.st>
                           {text}
##
##
                       {text}
##
                       <span#cb1-6>
##
                         <a [href, aria-hidden, tabindex]>
##
                         <span.fu>
##
                           {text}
##
                         {text}
##
                         <span.at>
##
                           {text}
##
                         {text}
##
                     <button.code-copy-button [title]>
##
                       <i.bi>
##
                {text}
##
              {text}
##
          {comment}
##
          <script#quarto-html-after-body [type]>
##
##
        {text}
##
        {comment}
##
        {text}
```

Next we extract the text from its title attribute, using functions xml\_find\_all() and xml\_text().

```
xml_text(xml_find_all(web_page, ".//title"))
## [1] "R for photobiology repository"
```

The functions defined in this package can be used to "harvest" data from web pages, but also to read data from files using formats that are defined through XML schemas.

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#### 10.8 GPX files

GPX (GPS Exchange Format) files use an XML scheme designed for saving and exchanging data from geographic positioning systems (GPS). There is some variation on the variables saved depending on the settings of the GPS receiver. The example data used here is from a Transmeta BT747 GPS logger. The example below reads the data into a tibble as character strings. For plotting, the character values representing numbers and dates would need to be converted to numeric and datetime (POSIXct) values, respectively. In the case of plotting tracks on a map, it is preferable to use package 'sf' to import the tracks directly from the .gpx file into a layer (use of the dot pipe operator is described in section 8.5 on page 250).

```
xmlTreeParse(file = "extdata/GPSDATA.gpx", useInternalNodes = TRUE) %.>%
xmlRoot(x = .) %.>%
xmlToList(node = .)[["trk"]] %.>%
unlist(x = .[names(.) == "trkseg"], recursive = FALSE) %.>%
map_df(.x = ., .f = function(x) as_tibble(x = t(x = unlist(x = x))))
## # A tibble: 199 x 7
                           speed name
                                               type fix
    time
                                                           .attrs.lat .attrs.lon
     <chr>>
                               <chr> <chr>
                                                   <chr> <chr> <chr>
## 1 2018-12-08T23:09:02.000Z 0.0366 trkpt-2018-~ T
                                                           -34.912071 138.660595
## 2 2018-12-08T23:09:04.000Z 0.0884 trkpt-2018-~ T
                                                      3d
                                                           -34.912067 138.660543
## 3 2018-12-08T23:09:06.000Z 0.0147 trkpt-2018-~ T
                                                      3d
                                                           -34.912102 138.660554
## # i 196 more rows
```

I have passed all arguments by name to make explicit how this pipe works. See section 8.5 on page 250 for details on the use of the pipe and dot-pipe operators.

10.11 To understand what data transformation takes place in each statement of this pipe, start by executing the first statement by itself, excluding the dot-pipe operator, and continue adding one statement at a time, and at each step check the returned value and look out for what has changed from the previous step.

#### 10.9 Worksheets

Microsoft Office, Open Office and Libre Office are the most frequently used suites containing programs based on the worksheet paradigm. There is available a standardized file format for exchange of worksheet data, but it does not support all the features present in native file formats. We will start by considering MS-Excel. The file format used by MS-Excel has changed significantly over the years, and old formats tend to be less well supported by available R packages and may require the file to be updated to a more modern format with MS-Excel itself before import into R. The current format is based on XML and relatively simple to decode, whereas older binary formats are more difficult. Worksheets contain code as equations in addition to the actual data. In all cases, only values entered as such or those computed by means of the embedded equations can be imported into R rather than the equations themselves.

When directly reading from a worksheet, a column of cells with mixed type, can introduce NA values. A wrongly selected cell range from the worksheet can result in missing columns or rows, if the area is too small, or in rows or columns filled with NA values, if the range includes empty cells in the worksheet. Depending on the function used, it may be possible to ignore empty cells, by passing an argument.

Many problems related to the import of data from work sheets and work books are due to translation between two different formats that impose different restrictions on what is allowed or not. While in a worksheet it is allowed to set the "format" (as called in Excel, and roughly equivalent to mode in R) of individual cells, a variable (column) in an R data frame is expected to be vector, and thus contain members belonging the same mode or type. For the import to work as expected, the "format" must be consistent, i.e., all cells in a column to be imported are marked as one of the Number, Date, Time or Text formats, with the possible exception of a single row of column headers with the names of the variables as Text. The default format General also works but as it does not ensure consistency, it makes more difficult to see format inconsistencies at a glance in Excel.

When reading a CSV file, text representing numbers will be recognized and converted, but only if the decimal point is encoded as expected from the arguments passed to the function call. So a single number with a comma instead of a dot as decimal marker (or vice versa) will result in most cases in the column not being decoded as numbers and returned as a character vector (or column) in the data frame. In the case of package 'readr' a numeric vector containing NA values for the non-decoded text may be returned instead of a character vector depending on whether the wrong decimal marker appears near the top or near the end of the file.

When importing data from a worksheet or workbook, my recommendation is first to check it in the original software to ensure that the cells to be imported are encoded as expected. When using a CSV as an intermediate step, it is crucial to also open this file in a plain-text editor such as the editor pane in RStudio (or Notepad in Windows or Nano, Emacs, etc., in Unix and Linux). Based on what field separator, decimal mark, and possibly character encoding has been used, which depends on the locale settings in the operating system of the computer and in the worksheet program, select a suitable function to call and the necessary arguments to pass to it.

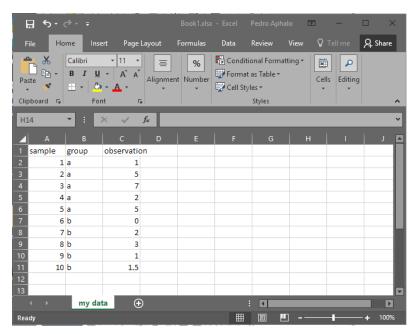
#### 10.9.1 CSV files as middlemen

If we have access to the original software used for creating a worksheet or workbook, then exporting worksheets to text files in CSV format and importing them into R using the functions described in sections 10.6 and 10.6.2 starting on pages 372 and 378 provides a broadly compatible route for importing data—with the caveat that we should take care that delimiters and decimal marks match the expectations of the functions used. This approach is not ideal from the perspective of having to create intermediate CSV formatted text files. A better approach is, when feasible, to import the data directly from the workbook or worksheets into R.

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#### 10.9.2 'readxl'

Package 'readxl' supports reading of MS-Excel workbooks, and selecting worksheets and regions within worksheets specified in ways similar to those used by MS-Excel itself. The interface is simple, and the package easy to install. We will import a file that in MS-Excel looks like the screen capture below.



We first list the sheets contained in the workbook file with excel\_sheets().

```
sheets <- excel_sheets("extdata/Book1.xlsx")
sheets
## [1] "my data"</pre>
```

In this case, the argument passed to sheet is redundant, as there is only a single worksheet in the file. It is possible to use either the name of the sheet or a positional index (in this case 1 would be equivalent to "my data"). We use function read\_excel() to import the worksheet. Being part of the 'tidyverse' the returned value is a tibble and character columns are returned as is.

```
Book1.df <- read_excel("extdata/Book1.xlsx",</pre>
                        sheet = "my data")
Book1.df
## # A tibble: 10 x 3
    sample group observation
##
      <db1> <chr>
                          <db1>
## 1
          1 a
                              1
          2 a
                              5
## 2
## 3
          3 a
                              7
## # i 7 more rows
```

We can also read a region instead of the whole worksheet.

Of the remaining arguments, the most useful ones have the same names and play similar roles as in 'readr' (see section 10.6.2 on page 378). For example, we can set new names to the columns instead of reading their names from the worksheet.

```
Book1_region.df <- read_excel("extdata/Book1.xlsx",</pre>
                                sheet = "my data",
                                range = "A2:B8",
                                col_names = c("A", "B"))
Book1_region.df
## # A tibble: 7 x 2
##
         A B
##
     <dbl> <chr>
## 1
         1 a
## 2
         2 a
## 3
         3 a
## # i 4 more rows
```

#### 10.9.3 'xlsx'

Package 'xlsx' can be more difficult to install as it uses Java functions to do the actual work. However, it is more comprehensive, with functions both for reading and writing MS-Excel worksheets and workbooks, in different formats including the older binary ones. Similar to 'readr' it allows selected regions of a worksheet to be imported.

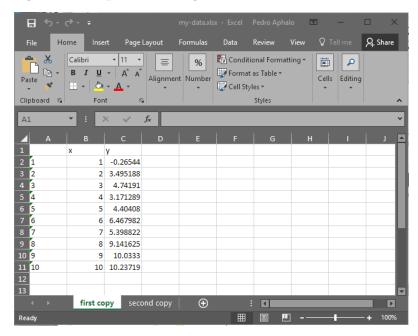
Here we use function read.xlsx(), indexing the worksheet by name. The returned value is a data frame, and following the expectations of R package 'utils', character columns are converted into factors by default.

```
Book1_xlsx.df <- read.xlsx("extdata/Book1.xlsx",</pre>
                              sheetName = "my data")
Book1_xlsx.df
##
      sample group observation
## 1
            1
                  a
                              1.0
## 2
            2
                              5.0
                  a
                              7.0
## 3
            3
                  a
## 4
            4
                              2.0
                  a
## 5
            5
                              5.0
                  а
## 6
            6
                  b
                              0.0
## 7
                  b
                              2.0
## 8
            8
                  b
                              3.0
## 9
            9
                              1.0
## 10
           10
                              1.5
```

With function write.xlsx() we can write data frames out to Excel worksheets and even append new worksheets to an existing workbook.

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When opened in Excel, we get a workbook containing two worksheets, named using the arguments we passed through sheetName in the code chunk above.



10.12 If you have some worksheet files available, import them into R to get a feel for how the way in which data is organized in the worksheets affects how easy or difficult it is to import them into R.

#### 10.9.4 'readODS'

Package 'readODS' provides functions for reading data saved in files that follow the *Open Documents Standard*. Function read\_ods() has a similar but simpler user interface to that of read\_excel() and reads one worksheet at a time, with support only for skipping top rows. The value returned is a data frame.

```
## 3 3 a 7
## # i 7 more rows
```

Function write\_ods() writes a data frame into an ODS file.

#### 10.10 Statistical software

There are two different comprehensive packages for importing data saved from other statistical programs such as SAS, Statistica, SPSS, etc. The longtime "standard" is package 'foreign' included in base R, and package 'haven' is a newer contributed extension. In the case of files saved with old versions of statistical programs, functions from 'foreign' tend to be more robust than those from 'haven'.

#### 10.10.1 'foreign'

Functions in package 'foreign' allow us to import data from files saved by several statistical analysis programs, including SAS, Stata, SPSS, Systat, Octave among others, and a function for writing data into files with formats native to SAS, Stata, and SPSS. R documents the use of these functions in detail in the *R Data Import/Export* manual. As a simple example, we use function read.spss() to read a .sav file, saved a few years ago with the then current version of SPSS. We display only the first six rows and seven columns of the data frame, including a column with dates, which appears as numeric.

```
my_spss.df <- read.spss(file = "extdata/my-data.sav", to.data.frame = TRUE)</pre>
my_spss.df[1:6, c(1:6, 17)]
##
     block
                 treat mycotreat water1 pot harvest harvest_date
## 1
         0 Watered, EM
                                1
                                       1 14
                                                    1 13653705600
         0 Watered, EM
## 2
                                       1 52
                                                      13653705600
                                1
                                                    1
## 3
         0 Watered, EM
                                1
                                       1 111
                                                      13653705600
                                                    1
## 4
         0 Watered, EM
                                1
                                       1 127
                                                       13653705600
                                                    1
         0 Watered, EM
                                1
                                       1 230
                                                    1
                                                       13653705600
         0 Watered, EM
                                       1 258
                                                    1 13653705600
```

A second example, this time with a simple .sav file saved 15 years ago.

```
thiamin.df <- read.spss(file = "extdata/thiamin.sav", to.data.frame = TRUE)
head(thiamin.df)
     THIAMIN CEREAL
##
## 1
         5.2
             wheat
  2
##
         4.5
             wheat
## 3
         6.0 wheat
## 4
         6.1 wheat
## 5
         6.7
             wheat
         5.8 wheat
## 6
```

Another example, for a Systat file saved on an PC more than 20 years ago, and read with read.systat().

```
my_systat.df <- read.systat(file = "extdata/BIRCH1.SYS")
head(my_systat.df)
## CONT DENS BLOCK SEEDL VITAL BASE ANGLE HEIGHT DIAM</pre>
```

```
## 1
         1
               1
                      1
                             2
                                                         1
                                                              53
## 2
                             2
                                   41
                                                              70
         1
               1
                      1
                                          2
                                                 1
                                                         2
## 3
                             2
                                   21
                                          2
                                                         1
         1
               1
                      1
                                                              65
## 4
         1
               1
                      1
                             2
                                   15
                                          3
                                                 0
                                                         1
                                                              79
## 5
         1
               1
                      1
                             2
                                   37
                                          3
                                                 0
                                                         1
                                                              71
                             2
## 6
               1
                      1
                                   29
                                          2
                                                 1
                                                         1
                                                              43
```

Not all functions in 'foreign' return data frames by default, but all of them can be coerced to do so.

#### 10.10.2 'haven'

Package 'haven' is less ambitious with respect to the number of formats supported, or their vintages, providing read and write functions for only three file formats: SAS, Stata and SPSS. On the other hand, 'haven' provides flexible ways to convert the different labeled values that cannot be directly mapped to R modes. They also decode dates and times according to the idiosyncrasies of each of these file formats. In cases when the imported file contains labeled values the returned tibble object needs some additional attention from the user. Labeled numeric columns in SPSS are not necessarily equivalent to factors, although they sometimes are. Consequently, conversion to factors cannot be automated and must be done manually in a separate step.

We can use function <code>read\_sav()</code> to import a <code>.sav</code> file saved by a recent version of SPSS. As in the previous section, we display only the first six rows and seven columns of the data frame, including a column <code>treat</code> containing a labeled numeric vector and <code>harvest\_date</code> with dates encoded as R date values.

```
my_spss.tb <- read_sav(file = "extdata/my-data.sav")</pre>
my_spss.tb[1:6, c(1:6, 17)]
## # A tibble: 6 x 7
     block treat
                           mycotreat water1
                                               pot harvest harvest_date
     <dbl> <dbl+1bl>
                                <fdb> <fdb> <fdb>
                                                      <dbl> <date>
## 1
         0 1 [Watered, EM]
                                   1
                                                14
                                                         1 2015-06-15
                                           1
## 2
         0 1 [Watered, EM]
                                    1
                                           1
                                                52
                                                         1 2015-06-15
## 3
         0 1 [Watered, EM]
                                    1
                                           1
                                               111
                                                         1 2015-06-15
## # i 3 more rows
```

In this case, the dates are correctly decoded.

Next, we import an SPSS's .sav file saved 15 years ago.

```
thiamin.tb <- read_sav(file = "extdata/thiamin.sav")</pre>
thiamin.tb
## # A tibble: 24 x 2
##
     THIAMIN CEREAL
##
       <dbl> <dbl+1bl>
## 1
         5.2 1 [wheat]
## 2
         4.5 1 [wheat]
## 3
         6
             1 [wheat]
## # i 21 more rows
thiamin.tb <- as_factor(thiamin.tb)</pre>
thiamin.tb
## # A tibble: 24 x 2
##
     THIAMIN CEREAL
##
       <dbl> <fct>
```

```
## 1 5.2 wheat
## 2 4.5 wheat
## 3 6 wheat
## # i 21 more rows
```

10.13 Compare the values returned by different read functions when applied to the same file on disk. Use names(), str() and class() as tools in your exploration. If you are brave, also use attributes(), mode(), dim(), dimnames(), nrow() and ncol().

10.14 If you use or have in the past used other statistical software or a general-purpose language like Python, look for some old files and import them into R.

#### 10.11 NetCDF files

In some fields, including geophysics and meteorology, NetCDF is a very common format for the exchange of data. It is also used in other contexts in which data is referenced to a grid of locations, like with data read from Affymetrix microarrays used to study gene expression. NetCDF files are binary but use a format that allows the storage of metadata describing each variable together with the data itself in a well-organized and standardized format, which is ideal for exchange of moderately large data sets measured on a spatial or spatio-temporal grid.

Officially described as follows:

NetCDF is a set of software libraries [from Unidata] and self-describing, machine-independent data formats that support the creation, access, and sharing of array-oriented scientific data.

As sometimes NetCDF files are large, it is good that it is possible to selectively read the data from individual variables with functions in packages 'ncdf4' or 'RNetCDF'. On the other hand, this implies that contrary to other data file reading operations, reading a NetCDF file is done in two or more steps—i.e., opening the file, reading metadata describing the variables and spatial grid, and finally reading the data of interest.

#### 10.11.1 'ncdf4'

Package 'ncdf4' supports reading of files using NetCDF version 4 or earlier formats. Functions in 'ncdf4' not only allow reading and writing of these files, but also their modification.

We first read metadata to obtain an index of the file contents, and in additional steps, read a subset of the data. With print() we can find out the names and characteristics of the variables and attributes. In this example, we read long-term averages for potential evapotranspiration (PET).

We first open a connection to the file with function nc\_open().

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```
meteo_data.nc <- nc_open("extdata/pevpr.sfc.mon.ltm.nc")</pre>
str(meteo_data.nc, max.level = 1)
## List of 15
  $ filename : chr "extdata/pevpr.sfc.mon.ltm.nc"
  $ writable : logi FALSE
## $ id
               : int 65536
## $ error
               : logi FALSE
## $ safemode : logi FALSE
               : chr "NC_FORMAT_NETCDF4_CLASSIC"
## $ format
## $ is_GMT
               : logi FALSE
## $ groups
                :List of 1
##
  $ fqqn2Rindex:List of 1
              : num 4
##
  $ ndims
   $ natts
                : num 8
   $ dim
                :List of 4
   $ unlimdimid : num −1
                : num 3
   $ nvars
   $ var
                :List of 3
   - attr(*, "class")= chr "ncdf4"
```

10.15 Increase max.level in the call to str() above and study the connection object stores information on the dimensions and for each data variable. You can also print(meteo\_data.nc) for a more complete printout once you have understood the structure of the object.

The dimensions of the array data are described with metadata, in our examples mapping indexes to a grid of latitudes and longitudes and into a time vector as a third dimension. The dates are returned as character strings. We get here the variables one at a time with function ncvar\_get().

```
time.vec <- ncvar_get(meteo_data.nc, "time")
head(time.vec)
## [1] -657073 -657042 -657014 -656983 -656953 -656922
longitude <- ncvar_get(meteo_data.nc, "lon")
head(longitude)
## [1] 0.000 1.875 3.750 5.625 7.500 9.375
latitude <- ncvar_get(meteo_data.nc, "lat")
head(latitude)
## [1] 88.5420 86.6531 84.7532 82.8508 80.9473 79.0435</pre>
```

The time vector is rather odd, as it contains only monthly data as these are long-term averages, but expressed as days from 1800-01-01 corresponding to the first day of each month of year 1. We use package 'lubridate' for the conversion.

We construct a tibble object with PET values for one grid point, taking advantage of the *recycling* of short vectors.

If we want to read in several grid points, we can use several different approaches. However, the order of nesting of dimensions can make adding the dimensions as columns error prone. It is much simpler to use package 'tidync' described next.

#### 10.11.2 'tidync'

Package 'tidync' provides functions that make it easier to extract subsets of the data from an NetCDF file. We start by doing the same operations as in the examples for 'ncdf4'.

We open the file creating an object and simultaneously activating the first grid.

```
meteo_data.tnc <- tidync("extdata/pevpr.sfc.mon.ltm.nc")</pre>
meteo_data.tnc
##
## Data Source (1): pevpr.sfc.mon.ltm.nc ...
## Grids (5) <dimension family> : <associated variables>
##
       D0,D1,D2: pevpr, valid_yr_count
## [1]
                                         **ACTIVE GRID** ( 216576 values per variable)
                 : climatology_bounds
## [2]
         D3,D2
## [3]
                  : 1on
         D0
## [4]
         D1
                  : lat
## [5]
         D2
                  : time
##
## Dimensions 4 (3 active):
##
##
    dim name length
                          min
                                 max start count
                                                   dmin
                                                           dmax unlim coord_dim
##
    <chr> <chr> <dbl>
                          <fdb>>
                                 <dbl> <int> <int> <dbl>
                                                             <dbl> <lgl> <lgl>
                                          1 192 0
## 1 D0
                    192 0
                                 3.58e2
                                                             3.58e2 FALSE TRUE
          lon
                                            1 94 -8.85e1 8.85e1 FALSE TRUE
## 2 D1
           lat
                     94 -8.85e1 8.85e1
                                                 12 -6.57e5 -6.57e5 FALSE TRUE
## 3 D2
          time
                     12 -6.57e5 -6.57e5
                                            1
##
## Inactive dimensions:
##
##
         name length
                          min
                                max unlim coord_dim
     <chr> <chr> <dbl> <dbl> <dbl> <lgl> <lgl><</pre>
           nbnds
                            1
                                  2 FALSE FALSE
hyper_dims(meteo_data.tnc)
## # A tibble: 3 x 7
    name length start count
                                 id unlim coord_dim
     <chr>
           <dbl> <int> <int> <lgl> <lgl>
## 1 lon
              192
                      1
                          192
                                  0 FALSE TRUE
## 2 lat
               94
                      1
                           94
                                  1 FALSE TRUE
## 3 time
               12
                           12
                                  2 FALSE TRUE
hyper_vars(meteo_data.tnc)
## # A tibble: 2 x 6
        id name
                          type
                                   ndims natts dim_coord
```

We extract a subset of the data into a tibble in long (or tidy) format, and add the months using a pipe operator from 'wrapr' and methods from 'dplyr'.

```
hyper_tibble(meteo_data.tnc,
             lon = signif(lon, 1) == 9,
             lat = signif(lat, 2) == 87) %.>%
  mutate(.data = ., month = month(ymd("1800-01-01") + days(time))) %.>%
  select(.data = ., -time)
## # A tibble: 12 x 5
##
     pevpr valid_yr_count
                            lon
                                  lat month
##
     <dbl>>
                    <dbl> <dbl> <dbl> <dbl> <
                 1.19e-39 9.38 86.7
## 1 4.28
## 2 5.72
                 1.19e-39 9.38
                                86.7
                                          1
## 3 4.38
                 1.29e-39 9.38
                                          2
                                 86.7
## # i 9 more rows
```

In this second example, we extract data for all grid points along latitudes. To achieve this we need only to omit the test for lat from the chunk above. The tibble is assembled automatically and columns for the active dimensions added. The decoding of the months remains unchanged.

```
hyper_tibble(meteo_data.tnc,
             lon = signif(lon, 1) == 9) %.>%
  mutate(.data = ., month = month(ymd("1800-01-01") + days(time))) %.>%
  select(.data = ., -time)
## # A tibble: 1,128 x 5
     pevpr valid_yr_count
                            lon
                                  lat month
##
     < Idb>
                    <dbl> <dbl> <dbl> <dbl> <
## 1
                 1.19e-39
     1.02
                          9.38
                                 88.5
##
      4.28
                 1.19e-39
                           9.38
                                 86.7
                                          12
## 3
     3.03
                 9.18e-40
                           9.38
                                 84.8
                                          12
## # i 1,125 more rows
```

10.16 Instead of extracting data for one longitude across latitudes, extract data across longitudes for one latitude near the Equator.

## 10.12 Remotely located data

Many of the functions described above accept an URL address in place of a file name. Consequently files can be read remotely without having to first download and save a copy in the local file system. This can be useful, especially when file names are generated within a script. However, one should avoid, especially in the case of servers open to public access, repeatedly downloading the same file as this unnecessarily increases network traffic and workload on the remote server. Because of this, our first example reads a small file from my own web site. See section 10.6 on page 372 for details on the use of these and other functions for reading text files.

```
logger.df <-
      read.csv2(file = "http://r4photobiology.info/learnr/logger_1.txt",
               header = FALSE,
               col.names = c("time", "temperature"))
sapply(logger.df, class)
         time temperature
## "character"
                "numeric"
sapply(logger.df, mode)
         time temperature
## "character"
                "numeric"
logger.tb <-</pre>
   read_csv2(file = "http://r4photobiology.info/learnr/logger_1.txt",
             col_names = c("time", "temperature"))
## i Using "','" as decimal and "'.'" as grouping mark. Use `read_delim()` for
more control.
## Rows: 723 Columns: 2
## -- Column specification -----
## Delimiter: ";"
## chr (1): time
## dbl (1): temperature
## i Use `spec()` to retrieve the full column specification for this data.
## i Specify the column types or set `show_col_types = FALSE` to quiet this
message.
sapply(logger.tb, class)
         time temperature
## "character"
                "numeric"
sapply(logger.tb, mode)
         time temperature
## "character"
                "numeric"
```

While functions in package 'readr' support the use of URLs, those in packages 'readxl' and 'xlsx' do not. Consequently, we need to first download the file and save a copy locally, that we can read as described in section 10.9.2 on page 389. Function download.file() in the R 'utils' package can be used to download files using URLs. It supports different modes such as binary or text, and write or append, and different methods such as "internal", "wget" and "libcurl".

For portability, MS-Excel files should be downloaded in binary mode, setting mode = "wb", which is required under MS-Windows.

Functions in package 'foreign', as well as those in package 'haven', support URLs. See section 10.10 on page 392 for more information about importing this kind of data into R.

```
##
     THIAMIN CEREAL
## 1
         5.2
              wheat
##
         4.5
              wheat
         6.0 wheat
## 3
## 4
              wheat
         6.1
## 5
         6.7
              wheat
## 6
         5.8 wheat
remote_my_spss.tb <-</pre>
    read_sav(file = "http://r4photobiology.info/learnr/thiamin.sav")
remote_my_spss.tb
## # A tibble: 24 x 2
##
     THIAMIN CEREAL
##
       <dbl> <dbl+1bl>
## 1
         5.2 1 [wheat]
## 2
         4.5 1 [wheat]
## 3
         6
            1 [wheat]
## # i 21 more rows
```

In this example we use a downloaded NetCDF file of long-term means for potential evapotranspiration from NOOA, the same used above in the 'ncdf4' example. This is a moderately large file at 444 KB. In this case, we cannot directly open the connection to the NetCDF file, and we first download it (commented out code, as we have a local copy), and then we open the local file.

For portability, NetCDF files should be downloaded in binary mode, setting mode = "wb", which is required under MS-Windows.

## 10.13 Data acquisition from physical devices

Numerous modern data acquisition devices based on microcontrollers, including internet-of-things (IoT) devices, have servers (or daemons) that can be queried over a network connection to retrieve either real-time or logged data. Formats based on XML schemas or in JSON format are commonly used.

### 10.13.1 'jsonlite'

We give here a simple example using a module from the *YoctoPuce* (http://www.yoctopuce.com/) family using a software hub running locally. We retrieve logged data from a YoctoMeteo module.

1 This example needs setting the configuration of the YoctoPuce module be-

forehand. Fully reproducible examples, including configuration instructions, will be provided online.

Here we use function from JSON() from package 'jsonlite' to retrieve logged data from one sensor.

The minimum, mean, and maximum values for each logging interval need to be split from a single vector. We do this by indexing with a logical vector (recycled). The data returned is in long form, with quantity names and units also returned by the module, as well as the time.

Most YoctoPuce input modules have a built-in datalogger, and the stored data can also be downloaded as a csv file through a physical or virtual hub. As shown above, it is possible to control them through the HTML server in the physical or virtual hubs. Alternatively the R package 'reticulate' can be used to control YoctoPuce modules by means of the Python library giving access to their API.

#### 10.14 Databases

One of the advantages of using databases is that subsets of cases and variables can be retrieved, even remotely, making it possible to work in R both locally and remotely with huge data sets. One should remember that R natively keeps whole objects in RAM, and consequently, available machine memory limits the size of data sets with which it is possible to work. Package 'dbplyr' provides the tools to work with data in databases using the same verbs as when using 'dplyr' with data stored in memory (RAM) (see chapter 8). This is an important subject, but extensive enough to be outside the scope of this book. We provide a few simple examples

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to show the very basics but interested readers should consult *R for Data Science* (Wickham and Grolemund 2017).

The additional steps compared to using 'dplyr' start with the need to establish a connection to a local or remote database. We will use R package 'RSQLite' to create a local temporary SQLite database. 'dbplyr' backends supporting other database systems are also available. We will use meteorological data from 'learnrbook' for this example.

```
library(dplyr)
con <- DBI::dbConnect(RSQLite::SQLite(), dbname = ":memory:")</pre>
copy_to(con, weather_wk_25_2019.tb, "weather",
        temporary = FALSE,
        indexes = list(
          c("month_name", "calendar_year", "solar_time"),
          "sun_elevation",
          "was_sunny",
          "day_of_year"
          "month_of_year"
weather.db <- tbl(con, "weather")</pre>
colnames(weather.db)
    [1] "time"
                          "PAR_umol"
                                            "PAR_diff_fr"
                                                              "global_watt"
        "day_of_year"
                          "month_of_year"
                                            "month_name"
                                                              "calendar_year"
##
    [5]
                          "sun_elevation" "sun_azimuth"
        "solar_time"
                                                              "was_sunny"
##
    [9]
                          "wind_direction" "air_temp_C"
        "wind_speed"
                                                              "air_RH"
## [13]
        "air_DP"
                          "air_pressure"
                                            "red_umol"
                                                              "far_red_umol"
## [17]
## [21] "red_far_red"
weather.db %.>%
  filter(., sun_elevation > 5) %.>%
  group_by(., day_of_year) %.>%
  summarise(., energy_wh = sum(global_watt, na.rm = TRUE) * 60 / 3600)
               SQL [?? x 2]
## # Database: sqlite 3.41.2 [:memory:]
##
     day_of_year energy_Wh
##
           <dbl>
                      <dbl>
## 1
             162
                      7500.
             163
## 2
                      6660.
             164
## 3
                      3958.
## # i more rows
```

- Package 'dbplyr' translates data pipes that use 'dplyr' syntax into SQL queries to databases, either local or remote. As long as there are no problems with the backend, the use of a database is almost transparent to the R user.
- It is always good to clean up, and in the case of the book, the best way to test that the examples can be run in a "clean" system.

```
unlink("./data", recursive = TRUE)
unlink("./extdata", recursive = TRUE)
```

# 10.15 Further reading

Since this is the end of the book, I recommend as further reading the writings of Burns as they are full of insight. Having arrived at the end of *Learn R: As a Language* you should read *S Poetry* (Burns 1998) and *Tao Te Programming* (Burns 2012). If you want to never get caught unaware by R's idiosyncrasies, read also *The R Inferno* (Burns 2011).

- Aho, A. V. and J. D. Ullman (1992). *Foundations of computer science*. Computer Science Press. ISBN: 0716782332.
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