Notes on using R

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Preface

This series of Notes cover different aspects of the use of R. They are meant to be use as a complement to a course, as explanations are short and terse.

1 R as a powerful calculator

1.1 Working at the R console

I assume that you are already familiar with RStudio. These examples use only the console window, and results are printed to the console. The values stored in the different variables are also visible in the Environment tab in RStudio.

In the console you can type commands at the > prompt. When you end a line by pressing the return key, if the line can be interpreted as an R command, the result will be printed in 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 + 4, if you enter in the console `1 + 2 +` 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.

When working at the command prompt, results are printed by default, but in other cases you may need to use the function `print` explicitly. The examples here rely on the automatic printing.

The idea with these examples is that you learn by working out how different commands work based on the results of the example calculations listed. The examples are designed so that they allow the rules, and also a few quirks, to be found by 'detective work'. This should hopefully lead to better understanding than just studying rules.

1.2 Examples with numbers

When working with arithmetic expression the normal precedence rules are followed and parentheses can be used to alter this order. In addition parentheses can be nested.

```
1 + 1

## [1] 2

2 * 2

## [1] 4

2 + 10 / 5

## [1] 4
```

```
(2 + 10) / 5

## [1] 2.4

10^2 + 1

## [1] 101

sqrt(9)

## [1] 3

pi # whole precision not shown when printing

## [1] 3.141593

print(pi, digits=22)

## [1] 3.1415926535897931

sin(pi) # oops! Read on for explanation.

## [1] 1.224606e-16

log(100)

## [1] 4.60517

log10(100)

## [1] 2

log2(8)

## [1] 3

exp(1)

## [1] 2.718282
```

One can use variables to store values. Variable names and all other names in R are case sensitive. Variables `a` and `A` are two different variables. Variable names can be quite long, but usually it is not a good idea to use very long names. Here I am using very short names, that is usually a very bad idea. However, in cases like these examples where the stored values have no real connection to the real world and are used just once or twice, these names emphasize the abstract nature.

```
a <- 1
a + 1

## [1] 2
```

```
a

## [1] 1

b <- 10
b <- a + b
b

## [1] 11

3e-2 * 2.0

## [1] 0.06
```

There are some syntactically legal 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 important thing is that you write commands consistently. `1 -> a` is valid but almost never used.

```
a <- b <- c <- 0.0
a

## [1] 0

b

## [1] 0

c

## [1] 0

1 -> a
a

## [1] 1

a = 3
a

## [1] 3
```

Numeric variables can contain more than one value. Even single numbers are vectors of length one. We will later see why this is important. 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 line.

One can use `c` 'concatenate' to create a vector of numbers from individual numbers.

```
a <- c(3,1,2)
a

## [1] 3 1 2
```

```r
b <- c(4,5,0)
b

## [1] 4 5 0

c <- c(a, b)
c

## [1] 3 1 2 4 5 0

d <- c(b, a)
d

## [1] 4 5 0 3 1 2
```

One can also create sequences, or repeat values:

```r
a <- -1:5
a

## [1] -1  0  1  2  3  4  5

b <- 5:-1
b

## [1]  5  4  3  2  1  0 -1

c <- seq(from = -1, to = 1, by = 0.1)
c

##  [1] -1.0 -0.9 -0.8 -0.7 -0.6 -0.5 -0.4 -0.3 -0.2
## [10] -0.1  0.0  0.1  0.2  0.3  0.4  0.5  0.6  0.7
## [19]  0.8  0.9  1.0

d <- rep(-5, 4)
d

## [1] -5 -5 -5 -5
```

Now something that makes R different from most other programming languages: vectorized arithmetic.

```r
a + 1 # we add one to vector a defined above

## [1] 0 1 2 3 4 5 6

(a + 1) * 2

## [1]  0  2  4  6  8 10 12

a + b

## [1] 4 4 4 4 4 4 4
```

```
a - a

## [1] 0 0 0 0 0 0 0
```

It can be seen in first line above, another peculiarity of R, that frequently called recycling: as vector `a` is of length 6, but the constant 1 is a vector of length 1, this 1 is extended by recycling into a vector of the same length as the longest vector in the statement.

Make sure you understand what calculations are taking place in the chunk above, and also the one below.

```
a <- rep(1, 6)
a

## [1] 1 1 1 1 1 1

a + 1:2

## [1] 2 3 2 3 2 3

a + 1:3

## [1] 2 3 4 2 3 4

a + 1:4

## Warning in a + 1:4:  longer object length is not a multiple of shorter
object length

## [1] 2 3 4 5 2 3
```

A couple on useful things to know: a vector can have length zero. One can remove variables from the workspace with `rm`. One can use `ls()` to list all objects in the environment, or by supplying a `pattern` argument, only the objects with names matching the `pattern`. The pattern is given as a regular expression, with `[ ]` enclosing alternative matching characters, `^` and `$` indicating the extremes of the name. For example `"^z$"` matches only the single character 'z' while `"^z"` matches any name starting with 'z'. In contrast `"^[zy]$"` matches both 'z' and 'y' but neither 'zy' nor 'yz', and `"^[a-z]"` matches any name starting with a lower case ASCII letter. If you are using RStudio, all objects are listed in the Environment pane, and the search box of the panel can be used to find a given object.

```
z <- numeric(0)
z

## numeric(0)

ls(pattern="^z$")

## [1] "z"
```

```
rm(z)
try(z)
ls(pattern="^z$")

## character(0)
```

There are some special values available for numbers. NA meaning 'not available' is used for missing values. Calculations can yield also the following values `NaN` 'not a number', `Inf` and `-Inf` for ∞ and $-\infty$. As you will see below, calculations yielding these values do **not** trigger errors or warnings, as they are arithmetically valid.

```
a <- NA
a

## [1] NA

-1 / 0

## [1] -Inf

1 / 0

## [1] Inf

Inf / Inf

## [1] NaN

Inf + 4

## [1] Inf
```

One thing to be aware of, and which we will discuss again later, is that numbers in computers are almost always stored with finite precision. This means that they not always behave as Real numbers as defined in mathematics. In R the usual numbers are stored as `double-precision floats`, which means that there are limits to the largest and smallest numbers that can be represented (approx. $-1 \cdot 10^{308}$ and $1 \cdot 10^{308}$), and the number of significant digits that can be stored (usually described as ϵ (epsilon, abbreviated `eps`, defined as the largest number for which $1 + \epsilon = 1$)). This can be sometimes important, and can generate unexpected results in some cases, especially when testing for equality. In the example below, the result of the subtraction is still exactly 1.

```
1 - 1e-20

## [1] 1
```

It is usually safer not to test for equality to zero when working with numeric values. One alternative is comparing against a suitably small number, which will depend on the situation, although `eps` is usualy a safe bet, unless the expected range of values is known to be small.

```
abs(x) < eps
abs(x) < 1e-100
```

The same applies to tests for equality, so whenever possible according to the logic of the calculations, it is best to test for inequalities, for example using `x <= 1.0` instead of `x == 1.0`. If this is not possible, then the tests should be treated as above, for example replacing `x == 1.0` with `abs(x - 1.0) < eps`.

When comparing integer values these problems do not exist, as integer arithmetic is not afected by loss of precision in calculations restricted to integers (the L comes from 'long' a name sometimes used for a machine represenation of intergers):

```
1L + 3L

## [1] 4

1L * 3L

## [1] 3

1L %/% 3L

## [1] 0

1L / 3L

## [1] 0.3333333
```

The last example above, using the 'usual' division operator yields a floating-point `numeric` result, while the integer division operator %/% yields an integer result.

1.3 Examples with logical values

What in maths are usually called Boolean values, are called `logical` values in R. They can have only two values TRUE and FALSE, in addition to NA. They are vectors. There are also logical operators that allow boolean algebra (and some support for set operations that we will not describe here).

```
a <- TRUE
b <- FALSE
a

## [1] TRUE

!a # negation

## [1] FALSE
```

```
a && b # logical AND

## [1] FALSE

a || b # logical OR

## [1] TRUE
```

Again vectorization is possible. I present this here, and will come back again to this, because this is one of the most troublesome aspects of the R language. The two types of 'equivalent' logical operators behave very differently, but use very similar syntax! The vectorized operators have single-character names & and |, while the non vectorized ones have two double-character names && and ||. There is only one version of the negation operator ! that is vectorized.

```
a <- c(TRUE,FALSE)
b <- c(TRUE,TRUE)
a

## [1]  TRUE FALSE

b

## [1] TRUE TRUE

a & b # vectorized AND

## [1]  TRUE FALSE

a | b # vectorized OR

## [1] TRUE TRUE

a && b # not vectorized

## [1] TRUE

a || b # not vectorized

## [1] TRUE
```

Functions `any` and `all` take a logical vector as argument, and return a single logical value 'summarizing' the logical values in the vector. `all` returns TRUE only if every value in the argument is TRUE, and `any` returns TRUE unless every value in the argument is FALSE.

```
any(a)

## [1] TRUE

all(a)
```

```
## [1] FALSE

any(a & b)

## [1] TRUE

all(a & b)

## [1] FALSE
```

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.

```
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
```

When using the vectorized operators on vectors of length greater than one, ‘short-cut’ evaluation still applies for the result obtained.

```
a & b & NA

## [1]    NA FALSE

a & b & c(NA, NA)

## [1]    NA FALSE

a | b | c(NA, NA)

## [1] TRUE TRUE
```

1.4 Comparison operators

Comparison operators yield as a result logical values.

```
1.2 > 1.0

## [1] TRUE

1.2 >= 1.0

## [1] TRUE

1.2 == 1.0 # be aware that here we use two = symbols

## [1] FALSE

1.2 != 1.0

## [1] TRUE

1.2 <= 1.0

## [1] FALSE

1.2 < 1.0

## [1] FALSE

a <- 20
a < 100 && a > 10

## [1] TRUE
```

Again these operators can be used on vectors of any length, the result is a logical vector.

```
a <- 1:10
a > 5

##  [1] FALSE FALSE FALSE FALSE FALSE  TRUE  TRUE
##  [8]  TRUE  TRUE  TRUE

a < 5

##  [1]  TRUE  TRUE  TRUE  TRUE FALSE FALSE FALSE
##  [8] FALSE FALSE FALSE

a == 5

##  [1] FALSE FALSE FALSE FALSE  TRUE FALSE FALSE
##  [8] FALSE FALSE FALSE

all(a > 5)
```

```
## [1] FALSE

any(a > 5)

## [1] TRUE

b <- a > 5
b

##  [1] FALSE FALSE FALSE FALSE FALSE  TRUE  TRUE
##  [8]  TRUE  TRUE  TRUE

any(b)

## [1] TRUE

all(b)

## [1] FALSE
```

Be once more aware of 'short-cut evaluation'. If the result would not be affected by the missing value then the result is returned. If the presence of the NA makes the end result unknown, then NA is returned.

```
c <- c(a, NA)
c > 5

##  [1] FALSE FALSE FALSE FALSE FALSE  TRUE  TRUE
##  [8]  TRUE  TRUE  TRUE    NA

all(c > 5)

## [1] FALSE

any(c > 5)

## [1] TRUE

all(c < 20)

## [1] NA

any(c > 20)

## [1] NA

is.na(a)

##  [1] FALSE FALSE FALSE FALSE FALSE FALSE FALSE
##  [8] FALSE FALSE FALSE

is.na(c)
```

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

any(is.na(c))

## [1] TRUE

all(is.na(c))

## [1] FALSE
```

This behaviour can be changed by using the optional argument `na.rm` which removes NA values **before** the function is applied. (Many functions in R have this optional parameter.)

```
all(c < 20)

## [1] NA

any(c > 20)

## [1] NA

all(c < 20, na.rm=TRUE)

## [1] TRUE

any(c > 20, na.rm=TRUE)

## [1] FALSE
```

You may skip this on first read, see page 10.

```
1e20 == 1 + 1e20

## [1] TRUE

1 == 1 + 1e-20

## [1] TRUE

0 == 1e-20

## [1] FALSE
```

In many situations, when writing programs one should avoid testing for equality of floating point numbers (‘floats’). Here we show how to handle gracefully rounding errors.

```
a == 0.0 # may not always work
```

```
##  [1] FALSE FALSE FALSE FALSE FALSE FALSE FALSE
##  [8] FALSE FALSE FALSE

abs(a) < 1e-15 # is safer

##  [1] FALSE FALSE FALSE FALSE FALSE FALSE FALSE
##  [8] FALSE FALSE FALSE

sin(pi) == 0.0 # angle in radians, not degrees!

## [1] FALSE

sin(2 * pi) == 0.0

## [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

.Machine$double.eps # see help for .Machine for explanation

## [1] 2.220446e-16

.Machine$double.neg.eps

## [1] 1.110223e-16
```

1.5 Character values

Character variables can be used to store any character. Character constants are written by enclosing characters in quotes. There are three types of quotes in the ASCII character set, double quotes `"`, single quotes `'`, and back ticks `` ` ``. The first two types of quotes can be used for delimiting characters.

```
a <- "A"
b <- letters[2]
```

```
c <- letters[1]
a

## [1] "A"

b

## [1] "b"

c

## [1] "a"

d <- c(a, b, c)
d

## [1] "A" "b" "a"

e <- c(a, b, "c")
e

## [1] "A" "b" "c"

h <- "1"
try(h + 2)
```

Vectors of characters are not the same as character strings.

```
f <- c("1", "2", "3")
g <- "123"
f == g

## [1] FALSE FALSE FALSE

f

## [1] "1" "2" "3"

g

## [1] "123"
```

One can use the ‘other’ type of quotes as delimiter when one want to include quotes in a string. Pretty-printing is changing what I typed into how the string is stored in R: I typed `b <- 'He said "hello" when he came in'`, try it.

```
a <- "He said 'hello' when he came in"
a

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

b <- 'He said "hello" when he came in'
b
```

```
## [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 sequences’. There are several of them, and here we will show just a few.

```
c <- "abc\ndef\txyz"
print(c)

## [1] "abc\ndef\txyz"

cat(c)

## abc
## def xyz
```

Above, you will not see any effect of these escapes when using `print`: `\n` represents ‘new line’ and `\t` means ‘tab’ (tabulator). The *scape codes* work only in some contexts, as when using `cat` to generate the output. They also are very useful when one wants to split an axis-label, title or label in a plot into two or more lines.

1.6 Finding the ‘mode’ of objects

Variables have *mode* that determines what can be stored in them. But differently to other languages, assignment of a variable of a different mode is allowed. However, there is a restriction that all elements in a vector, array or matrix, must be of the same mode, while this is not required for lists. Functions with names starting with `is.` are tests returning TRUE, FALSE or NA.

```
my_var <- 1:5
mode(my_var)

## [1] "numeric"

is.numeric(my_var)

## [1] TRUE

is.logical(my_var)

## [1] FALSE

is.character(my_var)

## [1] FALSE

my_var <- "abc"
mode(my_var)

## [1] "character"
```

1.7 Type conversions

The least intuitive ones are those related to logical values. All others are as one would expect. By convention, functions used to convert objects from one mode to a different one have names starting with `as.`.

```
as.character(1)

## [1] "1"

as.character(3.0e10)

## [1] "3e+10"

as.numeric("1")

## [1] 1

as.numeric("5E+5")

## [1] 5e+05

as.numeric("A")

## Warning:  NAs introduced by coercion

## [1] NA

as.numeric(TRUE)

## [1] 1

as.numeric(FALSE)

## [1] 0

TRUE + TRUE

## [1] 2

TRUE + FALSE

## [1] 1

TRUE * 2

## [1] 2

FALSE * 2

## [1] 0

as.logical("T")

## [1] TRUE
```

```
as.logical("t")

## [1] NA

as.logical("TRUE")

## [1] TRUE

as.logical("true")

## [1] TRUE

as.logical(100)

## [1] TRUE

as.logical(0)

## [1] FALSE

as.logical(-1)

## [1] TRUE
```

```
f <- c("1", "2", "3")
g <- "123"
as.numeric(f)

## [1] 1 2 3

as.numeric(g)

## [1] 123
```

Some tricks useful when dealing with results. Be aware that the printing is being done by default, these functions return numerical values.

```
round(0.0124567, 3)

## [1] 0.012

round(0.0124567, 1)

## [1] 0

round(0.0124567, 5)

## [1] 0.01246

signif(0.0124567, 3)

## [1] 0.0125
```

```
round(1789.1234, 3)

## [1] 1789.123

signif(1789.1234, 3)

## [1] 1790

a <- 0.12345
b <- round(a, 2)
a == b

## [1] FALSE

a - b

## [1] 0.00345

b

## [1] 0.12
```

1.8 Vectors

You already know how to create a vector. Now we are going to see how to get individual numbers out of a vector. They are accessed using an index. The index indicates the position in the vector, starting from one, following the usual mathematical tradition. What in maths would be x_i for a vector x, in R is represented as `x[i]`. (In R indexes (or subscripts) always start from one, while in some other programming languages indexes start from zero.)

```
a <- letters[1:10]
a

##  [1] "a" "b" "c" "d" "e" "f" "g" "h" "i" "j"

a[2]

## [1] "b"

a[c(3,2)]

## [1] "c" "b"

a[10:1]

##  [1] "j" "i" "h" "g" "f" "e" "d" "c" "b" "a"
```

The examples below demonstrate what is the result of using a longer vector of indexes than the indexed vector. The length of the indexing vector has no restriction, but the acceptable range of values for the indexes is given by the length of the indexed vector.

```
a[c(3,3,3,3)]

## [1] "c" "c" "c" "c"

a[c(10:1, 1:10)]

##  [1] "j" "i" "h" "g" "f" "e" "d" "c" "b" "a" "a"
## [12] "b" "c" "d" "e" "f" "g" "h" "i" "j"
```

Negative indexes have a special meaning, they indicate the positions at which values should be excluded.

```
a[-2]

## [1] "a" "c" "d" "e" "f" "g" "h" "i" "j"

a[-c(3,2)]

## [1] "a" "d" "e" "f" "g" "h" "i" "j"
```

Results from indexing with out-of-range values may be surprising.

```
a[11]

## [1] NA

a[1:11]

##  [1] "a" "b" "c" "d" "e" "f" "g" "h" "i" "j" NA
```

Results from indexing with special values may be surprising.

```
a[ ]

##  [1] "a" "b" "c" "d" "e" "f" "g" "h" "i" "j"

a[numeric(0)]

## character(0)

a[NA]

##  [1] NA NA NA NA NA NA NA NA NA NA

a[c(1, NA)]

## [1] "a" NA
```

```
a[NULL]

## character(0)

a[c(1, NULL)]

## [1] "a"
```

Another way of indexing, which is very handy, but not available in most other programming languages, is indexing with a vector of logical values. In practice, the vector of logical values used for ‘indexing’ is in most cases of the same length as the vector from which elements are going to be selected. However, this is not a requirement, and if the logical vector is shorter it is ‘recycled’ as discussed above in relation to operators.

```
a[TRUE]

##  [1] "a" "b" "c" "d" "e" "f" "g" "h" "i" "j"

a[FALSE]

## character(0)

a[c(TRUE, FALSE)]

## [1] "a" "c" "e" "g" "i"

a[c(FALSE, TRUE)]

## [1] "b" "d" "f" "h" "j"

a > "c"

##  [1] FALSE FALSE FALSE  TRUE  TRUE  TRUE  TRUE
##  [8]  TRUE  TRUE  TRUE

a[a > "c"]

## [1] "d" "e" "f" "g" "h" "i" "j"

selector <- a > "c"
a[selector]

## [1] "d" "e" "f" "g" "h" "i" "j"

which(a > "c")

## [1]  4  5  6  7  8  9 10

indexes <- which(a > "c")
a[indexes]

## [1] "d" "e" "f" "g" "h" "i" "j"

b <- 1:10
b[selector]

## [1]  4  5  6  7  8  9 10

b[indexes]

## [1]  4  5  6  7  8  9 10
```

1.9 Factors

Factors are used for indicating categories, most frequently the factors describing the treatments in an experiment, or categories in a survey. They can be created either from numerical or character vectors. The different possible values are called *levels*. Normal factors created with `factor` are unordered or categorical. R has ordered factors, that can be created with function `ordered`.

```
my.vector <- c("treated", "treated", "control", "control", "control", "treated")
my.factor <- factor(my.vector)
my.factor <- factor(my.vector, levels=c("treatment", "control"))
```

It is always preferable to use meaningful names for levels, although it is possible to use numbers. The order of levels becomes important when plotting data, as it affects the order of the levels along the axes, or in legends. Converting factors to numbers, even if the levels look like numbers when displayed, they are just character strings.

```
my.vector2 <- rep(3:5, 4)
my.factor2 <- factor(my.vector2)
as.numeric(my.factor2)

##  [1] 1 2 3 1 2 3 1 2 3 1 2 3

as.numeric(as.character(my.factor2))

##  [1] 3 4 5 3 4 5 3 4 5 3 4 5
```

Internally factor levels are stored as running numbers starting from zero, and those are the numbers returned by `as.numeric` applied to a factor.

Factors are very important in R. In contrast to other statistical software in which the role of a variable is set when defining a model to be fitted or setting up a test, in R models are specified exactly in the same way for ANOVA and regression analysis, as linear models. What 'decides' what type of model is fitted is whether the explanatory variable is a factor (giving ANOVA) or a numerical variable (giving regression). This makes a lot of sense, as in most cases, considering an explanatory variable as categorical or not, depends on the design of the experiment or survey, in other words, is a property of the data rather than of the analysis.

1.10 Lists

Elements of a `list` are not ordered, and can be of different type. Lists can be also nested. Elements in list are named, and normally are accessed by name. List are defined using function `list`.

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

## $x
## [1] 1 2 3 4 5 6
##
## $y
## [1] "a"
##
## $z
## [1]  TRUE FALSE

str(a.list)

## List of 3
##  $ x: int [1:6] 1 2 3 4 5 6
##  $ y: chr "a"
##  $ z: logi [1:2] TRUE FALSE

a.list$x

## [1] 1 2 3 4 5 6

a.list[["x"]]

## [1] 1 2 3 4 5 6

a.list[[1]]

## [1] 1 2 3 4 5 6

a.list[1]

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

a.list[c(1,3)]

## $x
## [1] 1 2 3 4 5 6
##
## $z
## [1]  TRUE FALSE

try(a.list[[c(1,3)]])

## [1] 3
```

Using double square brackets for indexing gives the element stored in the list, in its original mode, in the example above, `a.list[["x"]]` returns a numeric vector, while `a.list[1]` returns a list containing the numeric vector `x`. `a.list$x` returns the same value as `a.list[["x"]]`, a numeric vector. While `a.list[c(1,3)]` returns a list of length two, `a.list[[c(1,3)]]`.

1.11 Data frames

Data frames are a special type of list, in which each element is a vector or a factor of the same length. The are crested with function `data.frame` with a syntax similar to that used for lists. When a shorter vector is supplied as argument, it is recycled, until the full length of the variable is filled. This is very different to what we obtained in the previous section when we created a list.

```
a.df <- data.frame(x = 1:6, y = "a", z = c(TRUE, FALSE))
a.df

##   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

str(a.df)

## 'data.frame': 6 obs. of  3 variables:
##  $ x: int  1 2 3 4 5 6
##  $ y: Factor w/ 1 level "a": 1 1 1 1 1 1
##  $ z: logi  TRUE FALSE TRUE FALSE TRUE FALSE

a.df$x

## [1] 1 2 3 4 5 6

a.df[["x"]]

## [1] 1 2 3 4 5 6

a.df[[1]]

## [1] 1 2 3 4 5 6

class(a.df)

## [1] "data.frame"
```

R is an object oriented language, and objects belong to classes. With function `class` we can query the class of an object. As we saw in the two previous chunks lists and data frames objects belong to two different classes.

We can add also to lists and data frames.

```
a.df$x2 <- 6:1
a.df$x3 <- "b"
a.df

##   x y     z x2 x3
## 1 1 a  TRUE  6  b
## 2 2 a FALSE  5  b
## 3 3 a  TRUE  4  b
## 4 4 a FALSE  3  b
## 5 5 a  TRUE  2  b
## 6 6 a FALSE  1  b
```

We have added two columns to the data frame, and in the case of column `x3` recycling took place. Data frames are extremely important to anyone analysing or plotting data in R. One can think of data frames as tightly structured work-sheets, or as lists. As you may have guessed from the examples earlier in this section, there several different ways of accessing columns, rows, and individual observations stored in a data frame. The columns can to some extent be treated as elements in a list, and can be accessed both by name or index (position). When accessed by name, using `$` or double square brackets a single column is returned as a vector or factor. In contrast to lists, data frames are 'rectangular' and for this reason the values stored can be also accessed in a way similar to how elements in a matrix are accessed, using two indexes. As we saw for vectors indexes can be vectors of integer numbers or vectors of logical values. For columns they can be vectors of character strings matching the names of the columns. When using indexes it is extremely important to remember that the indexes are always given **row first**.

```
a.df[ , 1]   # first column

## [1] 1 2 3 4 5 6

a.df[ , "x"] # first column

## [1] 1 2 3 4 5 6

a.df[1, ]    # first row

##   x y    z x2 x3
## 1 1 a TRUE  6  b

a.df[1:2, c(FALSE, FALSE, TRUE, FALSE, FALSE)]

## [1]  TRUE FALSE

             # first two rows of the third column
a.df[a.df$z , ] # the rows for which z is true

##   x y    z x2 x3
## 1 1 a TRUE  6  b
## 3 3 a TRUE  4  b
## 5 5 a TRUE  2  b
```

```
a.df[a.df$x > 3, -3] # the rows for which x > 3 for

##   x y x2 x3
## 4 4 a  3  b
## 5 5 a  2  b
## 6 6 a  1  b

                  # all columns except the third one
```

When the names of data frames are long, complex conditions become awkward to write. 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.

```
subset(a.df, x > 3)

##   x y     z x2 x3
## 4 4 a FALSE  3  b
## 5 5 a  TRUE  2  b
## 6 6 a FALSE  1  b
```

When calling functions that return a vector, data farme, or other structure, the square brackets 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.

```
subset(a.df, x > 3)[ , -3]

##   x y x2 x3
## 4 4 a  3  b
## 5 5 a  2  b
## 6 6 a  1  b

subset(a.df, x > 3)$x

## [1] 4 5 6
```

None of the examples in the last three code chunks alter the original data frame `a.df`. We can store the returned value using a new name, if we want to preserve `a.df` unchanged, or we can assign the result to `a.df` deleting in the process the original `a.df`. The next to examples do assignment to `a.df`, but either to only one columns, or by indexing the individual values in both the 'right side' and 'left side' of the assignment. Another way to delete a column from a data frame is to assign NULL to it.

```
a.df[["x2"]] <- NULL
a.df$x3 <- NULL
a.df

##   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
```

In the previous code chuck we deleted the last two columns of the data frame `a.df`. Finally an esoteric trick for you think about.

```
a.df[1:6, c(1,3)] <- a.df[6:1, c(3,1)]
a.df

##   x y z
## 1 0 a 6
## 2 1 a 5
## 3 0 a 4
## 4 1 a 3
## 5 0 a 2
## 6 1 a 1
```

1.12 Simple built-in statistical functions

Being R's main focus in statistics, it provides functions for both simple and complex calculations, going from means and variances to fitting very complex models. we will start with the simple ones.

```
x <- 1:20
mean(x)

## [1] 10.5

var(x)

## [1] 35

median(x)

## [1] 10.5

mad(x)

## [1] 7.413

sd(x)

## [1] 5.91608

range(x)

## [1]  1 20
```

```
max(x)

## [1] 20

min(x)

## [1] 1

length(x)

## [1] 20
```

1.13 Functions and execution flow control

Although functions can be defined and used at the command prompt, we will discuss them when looking at scripts. We will do the same in the case of flow-control statements (e.g. repetition and conditional execution).

2 R Scripts and Programming

2.1 What is a script?

We call *script* to a text file that contains the same commands that you would type at the console prompt. A true script is not for example an MS-Word file where you have pasted or typed some R commands. A script file has the following characteristics.

- The script is a text file (ASCII or some other encoding e.g. UTF-8 that R uses in your set-up).
- The file contains valid R statements (including comments) and nothing else.
- Comments start at a # and end at the end of the line. (True end-of line as coded in file, the editor may wrap it or not at the edge of the screen).
- The R statements are in the file in the order that they must be executed.
- R scripts have file names ending in `.r`

It is good practice to write scripts so that they will run in a new R session, which means that the script should include library commands to load all the required packages.

2.2 How do we use a scrip?

A script can be sourced.

If we have a text file called `my.first.script.r`

```
# this is my first R script
print(3+4)
```

And then source this file:

```r
source("my.first.script.r")

## [1] 7
```

The results of executing the statements contained in the file will appear in the console. The commands themselves are not shown (the sourced file is not echoed) and the results will not be printed unless you include an explicit `print` command.

This also applies in many cases also to plots. A fig created with `ggplot` needs to be printed if we want to see it when the script is run.

From within RStudio, if you have an R script open in the editor, there will a "source" drop box (≠ DropBox) visible from where you can choose "source" as described above, or "source with echo" for the currently open file.

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 script file as argument directly at the command prompt of the operating system.

```
RScript my.first.script.r
```

You can open a '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 redirection.

```
RScript my.first.script.r > my.output.txt
```

Sourcing is very useful when the script is ready, however, while developing a script, or sometimes when testing things, one usually wants to run (= execute) one or a few statements at a time. This can be done using the "run" button after either locating the cursor in the line to be executed, or selecting the text that one would like to 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).

2.3 How to write a script?

The approach used, or mix of approaches will depend on your preferences, and on how confident you are that the statements will work as expected.

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 if moderately familiar with the problem One would write the script as above, but testing it, part by part as one is writing it. This is usually what I do.

If ones mostly playing around Then if one is using RStudio, one 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 and by pressing a single having copy and pasted to either the console prompt, or the cursor position in the file visible in the editor. In this way one can build a script by copying and pasting from the history to your script file the bits that have worked as you wanted.

2.4 The need to be understandable to people

When you write a script, it is either because you want to document what you have done or you want re-use it at a later time. In either case, the script itself although still meaningful for the computer could become very obscure to you, and even more to someone seeing it for the first time.

How does one achieve an understandable script or program?

- Avoid the unusual. People using a certain programming language tend to use some implicit or explicit rules of style. 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 explaining names are 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 just increase the length of the lines in the script, and one would spend more time typing without getting much in return.
- 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 in some contexts is "safer" as in special situations a dot may have a special meaning. What we call "camel case" is very rarely used in R programming but is common in other languages like Pascal. An example of camel case is `NumCols`. In some cases it can become a bit confusing as in `UVMean` or `UvMean`.

2.5 Exercises

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 'File' menu, "+" button, or by typing "Ctrl + Shift + N").
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.

2.6 Functions

When writing scripts, or any program, one should avoid repeating code (groups of statements). The reasons for this are: 1) if the code needs to be changed, you have to make changes in more than one place in the file, or in more than one file. Sooner or later, some copies will remain unchanged by mistake. 2) it makes the script file longer, and this makes debugging, commenting, etc. more tedious, and error prone.

How do we avoid repeating bits of code? We write a function containing the statements that we would need to repeat, and then `call` the function in their place.

Functions are defined by means of **function**, and saved like any other object in R by assignment a variable. `x` is a parameter, the name used within the function for an object that will be supplied as “argument” when the function is called. One can think of parameter names as place-holders.

```
my.prod <- function(x, y){x * y}
my.prod(4, 3)

## [1] 12
```

First some basic knowledge. In R, arguments are passed by copy. This is something very important to remember. Whatever you do within a function to the passed argument, its value outside the function will remain unchanged.

```
my.change <- function(x){x <- NA}
a <- 1
my.change(a)
a

## [1] 1
```

Any result that needs to be made available outside the function must be returned by the function. If the function `return` is not explicitly used, the value returned by the last statement within the body of the function will be returned.

```
print.x.1 <- function(x){print(x)}
print.x.1("test")

## [1] "test"

print.x.2 <- function(x){print(x); return(x)}
print.x.2("test")

## [1] "test"
## [1] "test"

print.x.3 <- function(x){return(x); print(x)}
print.x.3("test")

## [1] "test"
```

```
print.x.4 <- function(x){return(); print(x)}
print.x.4("test")

## NULL
```

We can assign to a variable defined outside a function with operator `<<-` but the usual recommendation is to avoid its use. This type of effects of calling a function are frequently called 'side-effects'.

Now we will define a useful function: a function for calculating the standard error of the mean from a numeric vector.

```
SEM <- function(x){sqrt(var(x)/length(x))}
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
```

For example in `SEM(a)` we are calling function SEM with `a` as argument.

The function we defined above may sometimes give a wrong answer because NAs will be counted by `length`, so we need to remove NAs before calling `length`.

```
SEM <- function(x) sqrt(var(x, na.rm=TRUE)/length(na.omit(x)))
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] 1.796988
```

R does not have a function for standard error, so the function above would be generally useful. If we would like to make this function both safe, and consistent with other R functions, one could define it as follows, allowing the user to provide a second argument which is passed as an argument to `var`:

```
SEM <- function(x, na.rm=FALSE){sqrt(var(x, na.rm=na.rm)/length(na.omit(x)))}
SEM(a)

## [1] 1.796988

SEM(a.na)

## [1] NA

SEM(a.na, TRUE)

## [1] 1.796988

SEM(x=a.na, na.rm=TRUE)

## [1] 1.796988

SEM(TRUE, a.na)

## Warning in if (na.rm) "na.or.complete" else "everything":  the condition
has length > 1 and only the first element will be used

## [1] NA

SEM(na.rm=TRUE, x=a.na)

## [1] 1.796988
```

In this example you can see that functions can have more than one parameter, and that parameters can have default values to be used if no argument is supplied. In addition if the name of the parameter is indicated, then arguments can be supplied in any order, but if parameter names are not supplied, then arguments are assigned to parameters based on their position. Once one parameter name is given, all later arguments need also to be explicitly matched to parameters. Obviously if given by position, then arguments should be supplied explicitly for all parameters at 'intermediate' positions.

2.7 R built-in functions

2.7.1 Plotting

The built-in generic function `plot` can be used to plot data. It is a generic function, that has suitable methods for different kinds of objects.

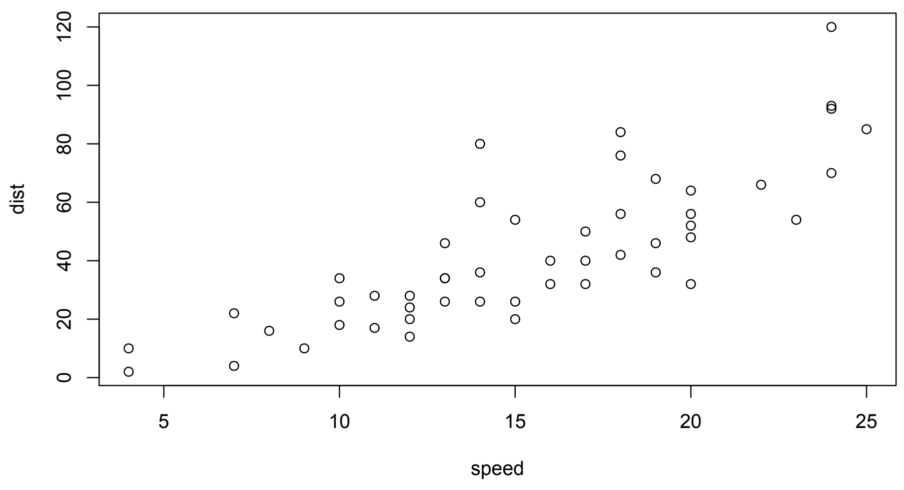
Before we can plot anything, we need some data.

```
data(cars)
names(cars)

## [1] "speed" "dist"
```

```
head(cars)

##   speed dist
## 1     4    2
## 2     4   10
## 3     7    4
## 4     7   22
## 5     8   16
## 6     9   10

tail(cars)

##    speed dist
## 45    23   54
## 46    24   70
## 47    24   92
## 48    24   93
## 49    24  120
## 50    25   85
```

`cars` is an example data set that is included in R. It is stored as a dataframe. Data frames are used for storing data, they consist in columns of equal length. The different columns can be different types (e.g. numeric and character). With `data` we load it; with `names` we obtain the names of the variables or columns. With head with can see the top several lines, and with tail the lines at the end.

```
plot(dist ~ speed, data=cars)
```

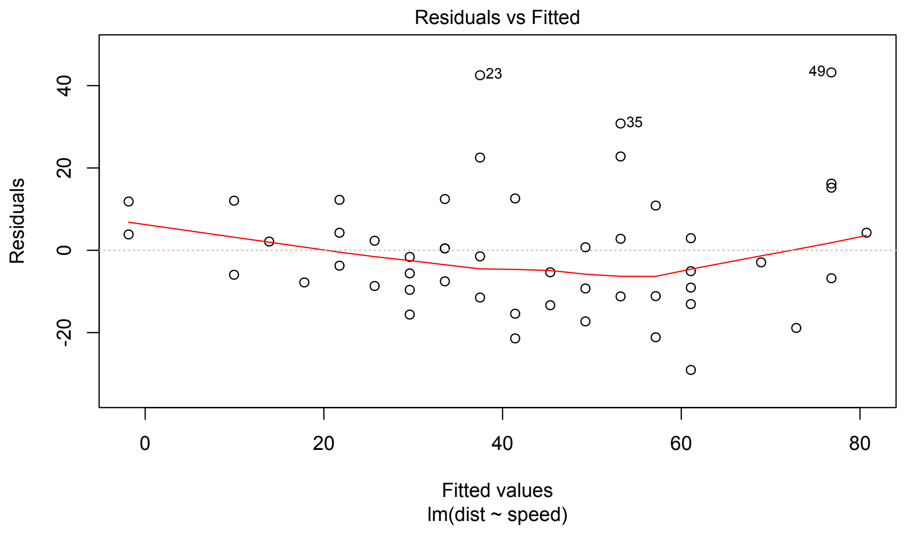


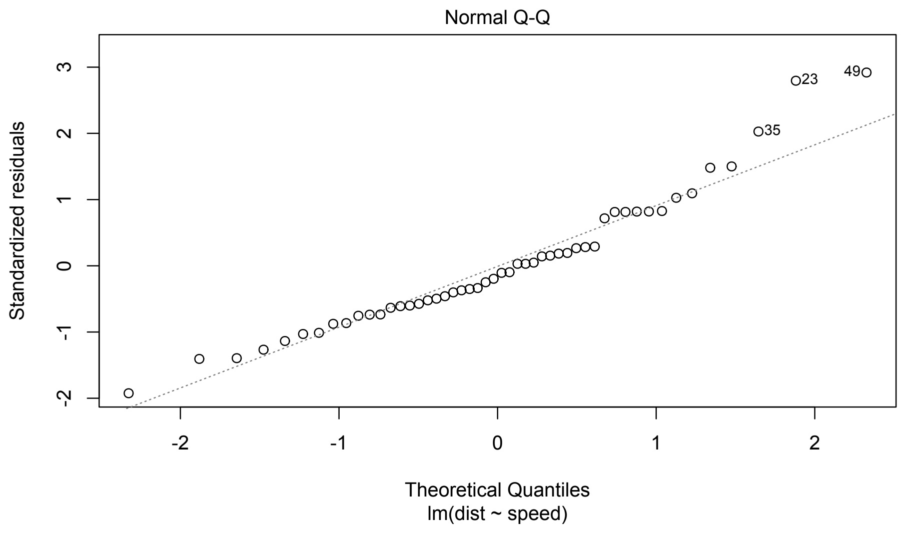
2.7.2 Fitting linear models

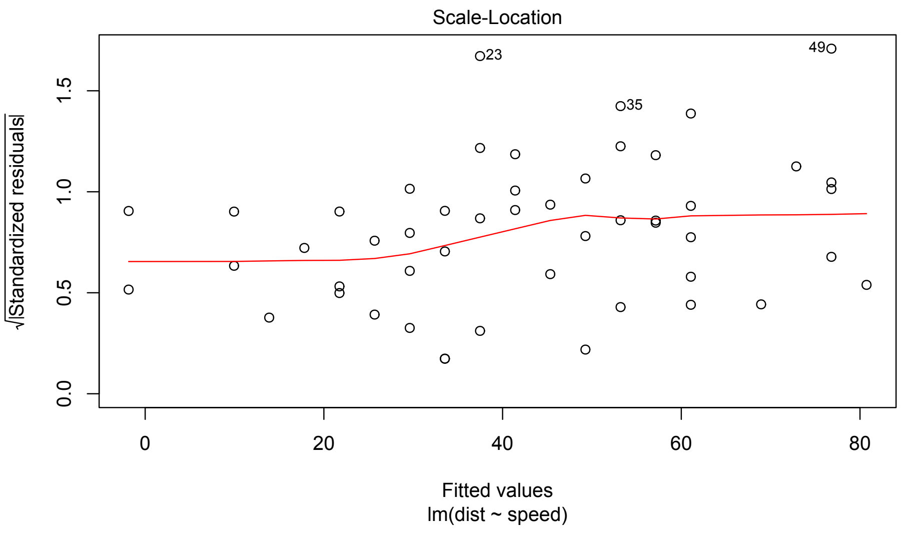
Regression

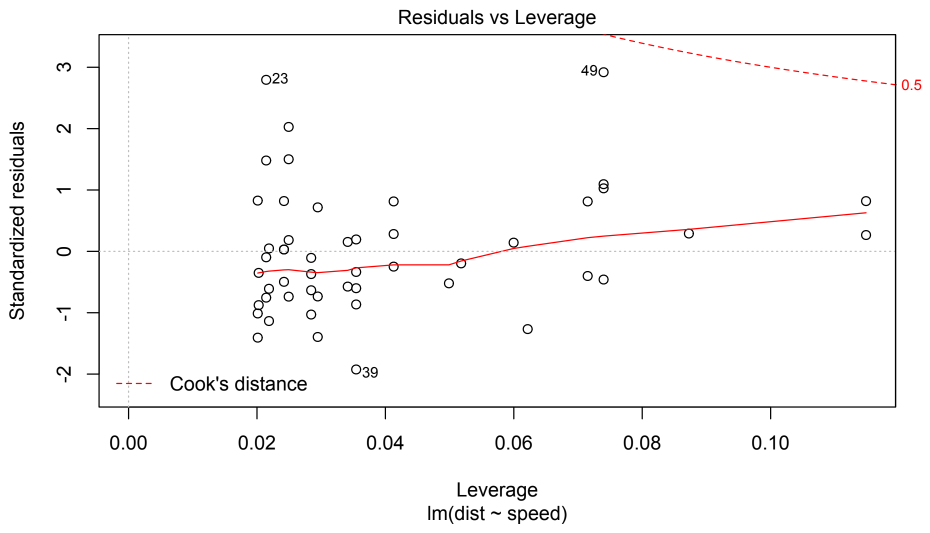
The R function `lm` is used next to fit a linear regression.

```
fm1 <- lm(dist ~ speed, data=cars) # we fit a model, and then save the result
plot(fm1) # we produce diagnosis plots
summary(fm1) # we inspect the results from the fit

##
## Call:
## lm(formula = dist ~ speed, data = cars)
##
## Residuals:
##     Min      1Q  Median      3Q     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   0.0123
## speed         3.9324     0.4155   9.464 1.49e-12
##
## (Intercept) *
## speed       ***
## ---
## 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

anova(fm1) # we calculate an ANOVA

## Analysis of Variance Table
##
## Response: dist
##           Df Sum Sq Mean Sq F value   Pr(>F)
## 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
```


Residuals vs Fitted
Residuals
Fitted values
lm(dist ~ speed)
23
49
35
40
20
0
-20
0
20
40
60
80


Normal Q-Q
Standardized residuals
Theoretical Quantiles
lm(dist ~ speed)
23
49
35
3
2
1
0
-1
-2
-2
-1
0
1
2

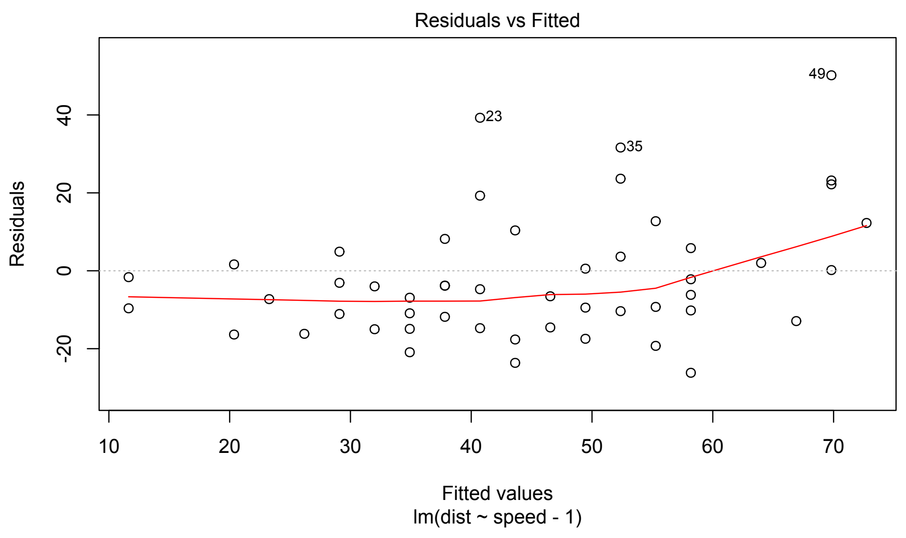


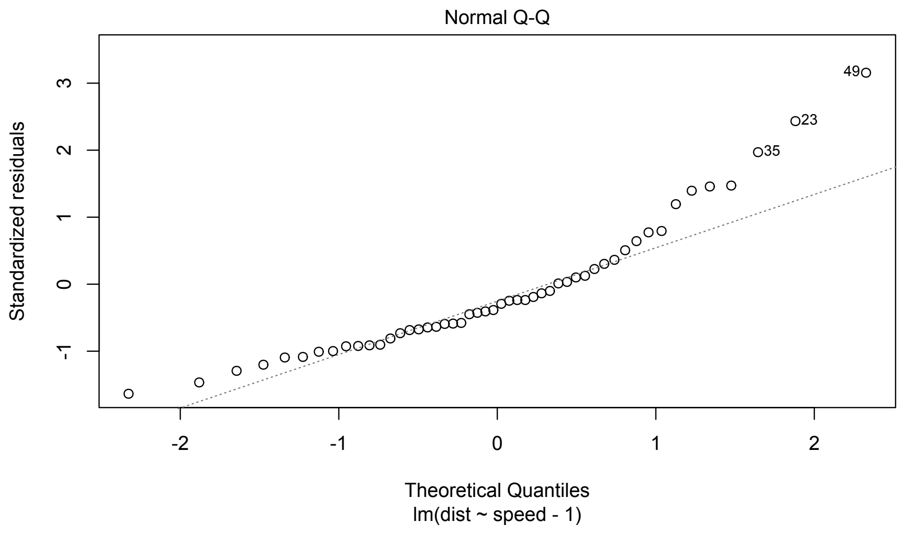


Let's look at each step separately: `dist` `speed` is the specification of the model to be fitted. The intercept is always implicitly included. To 'remove' this implicit intercept from the earlier model we can use `dist` `speed - 1`.

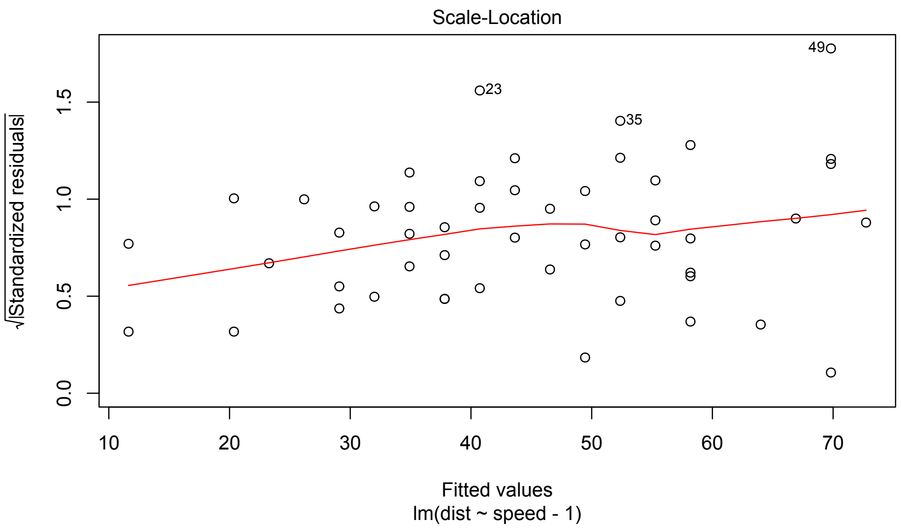
```
fm2 <- lm(dist ~ speed - 1, data=cars) # we fit a model, and then save the result
plot(fm2) # we produce diagnosis plots
summary(fm2) # we inspect the results from the fit

##
```

```
## 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

anova(fm2) # we calculate an ANOVA

## Analysis of Variance Table
##
## Response: dist
##           Df Sum Sq Mean Sq F value    Pr(>F)
## speed      1 111949  111949  423.47 < 2.2e-16 ***
## Residuals 49  12954     264
## ---
## Signif. codes:
## 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

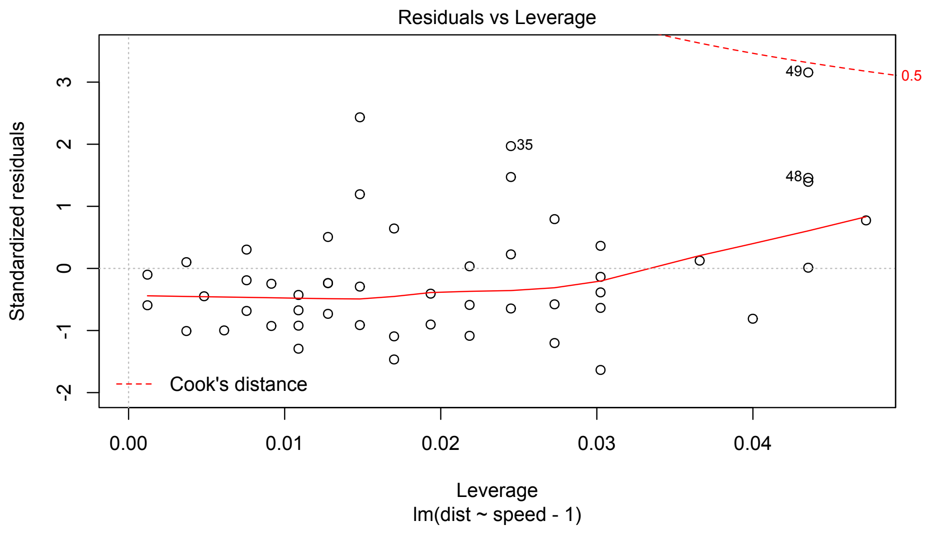




Normal Q-Q
Standardized residuals
Theoretical Quantiles
lm(dist ~ speed - 1)
49
23
35

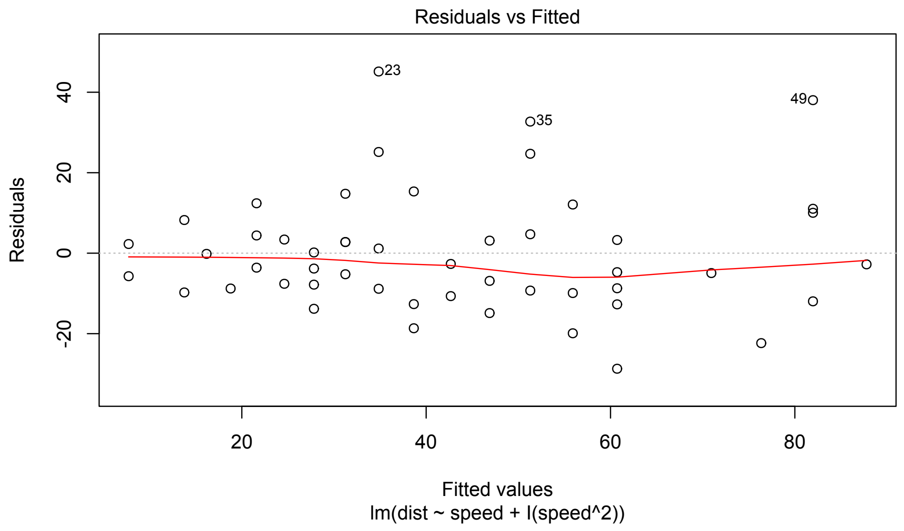


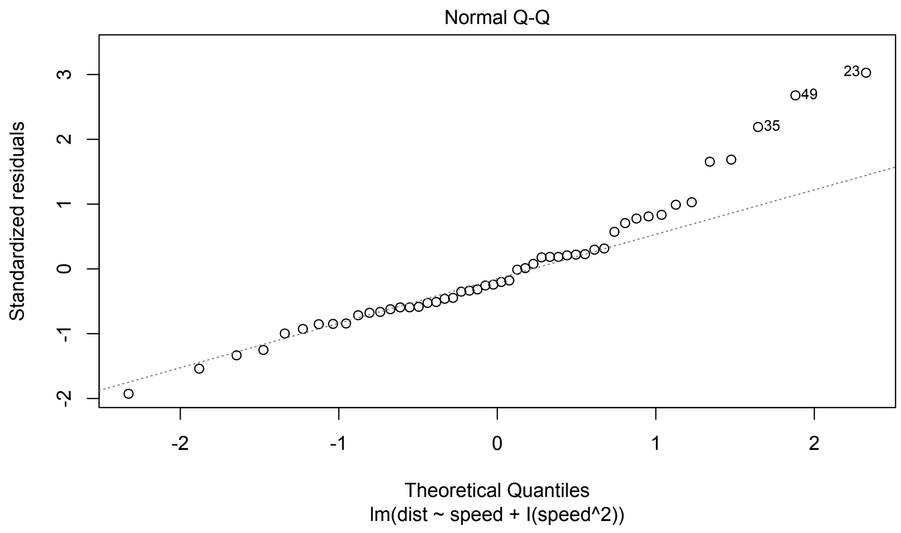
Scale-Location
√|Standardized residuals|
Fitted values
lm(dist ~ speed - 1)
49
23
35

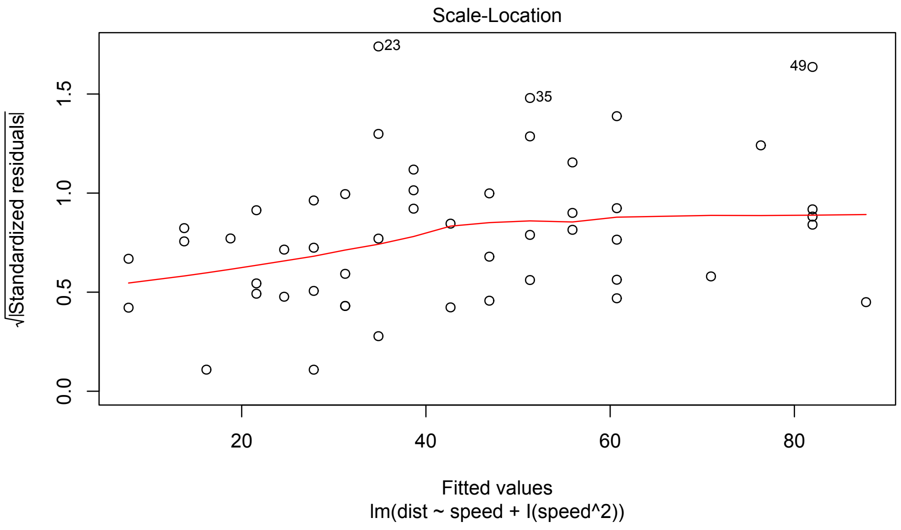


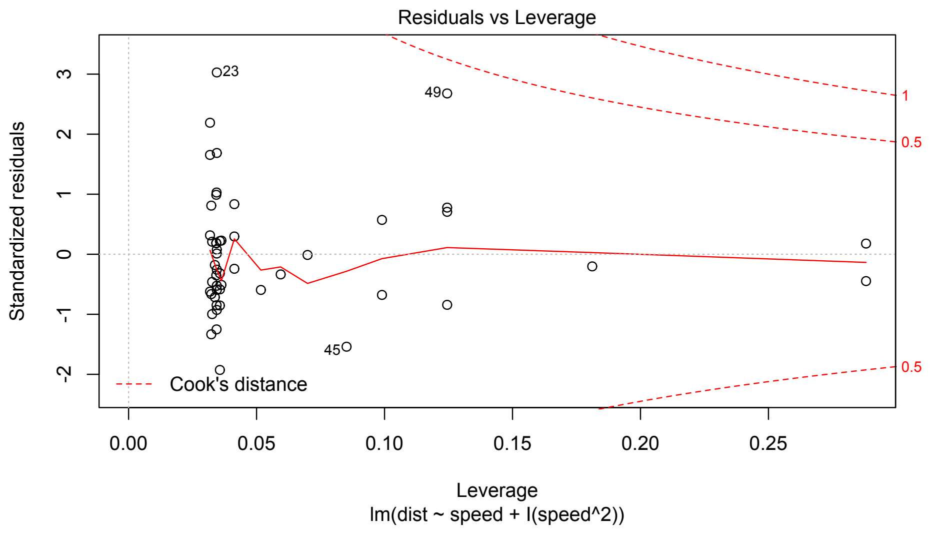
We now we fit a second degree polynomial.

```
fm3 <- lm(dist ~ speed + I(speed^2), data=cars) # we fit a model, and then save the result
plot(fm3) # we produce diagnosis plots
summary(fm3) # we inspect the results from the fit

##
## 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

anova(fm3) # we calculate an ANOVA

## Analysis of Variance Table
##
## Response: dist
##            Df  Sum Sq Mean Sq F value    Pr(>F)
## speed       1 21185.5 21185.5  91.986 1.211e-12
## I(speed^2)  1   528.8   528.8   2.296    0.1364
## Residuals  47 10824.7   230.3
##
## speed       ***
## I(speed^2)
## Residuals
## ---
## Signif. codes:
## 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```




Normal Q-Q
Standardized residuals
Theoretical Quantiles
lm(dist ~ speed + I(speed^2))
23
49
35
-2
-1
0
1
2
3


Scale-Location
√|Standardized residuals|
Fitted values
lm(dist ~ speed + I(speed^2))
23
49
35
0.0
0.5
1.0
1.5
20
40
60
80



We can also compare the two models.

```
anova(fm2, fm1)

## Analysis of Variance Table
##
## Model 1: dist ~ speed - 1
## Model 2: dist ~ speed
##   Res.Df   RSS Df Sum of Sq      F  Pr(>F)
## 1     49 12954
## 2     48 11354  1    1600.3 6.7655 0.01232 *
## ---
## Signif. codes:
## 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

Or three or more models. But be careful, as the order of the arguments matters.

```
anova(fm2, fm1, fm3)

## Analysis of Variance Table
##
## Model 1: dist ~ speed - 1
## Model 2: dist ~ speed
## Model 3: dist ~ speed + I(speed^2)
##   Res.Df   RSS Df Sum of Sq      F  Pr(>F)
## 1     49 12954
## 2     48 11354  1   1600.26 6.9482 0.01133 *
## 3     47 10825  1    528.81 2.2960 0.13640
## ---
## Signif. codes:
## 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

We can use different criteria to choose the best model: significance based on *P*-values or information criteria (AIC, BIC) that penalize the result 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.

2.8 Control of execution flow

2.8.1 Conditional execution

Non-vectorized

R has two types of "if" statements, non-vectorized and vectorized. We will start with the non-vectorized one, which is similar to what is available in most other computer programming languages.

Before this we need to explain compound statements. Individual statements can be grouped into compound statements by enclosed them in curly braces.

```
print("A")

## [1] "A"

{
  print("B")
  print("C")
}

## [1] "B"
## [1] "C"
```

The example above is pretty useless, but becomes useful when used together with 'control' constructs. The `if` construct controls the execution of one statement, however, this statement can be a compound statement of almost any length or complexity. Play with the code below by changing the value assigned to `printing`, including NA, and logical(0).

```
printing <- TRUE
if (printing) {
  print("A")
  print("B")
}

## [1] "A"
## [1] "B"
```

The condition '( )' can be anything yielding a logical vector, however, as this is not vectorized, only the first element will be used. Play with this example by changing the value assigned to `a`.

```
a <- 10.0
if (a < 0.0) 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"
```

As you can see above the statement immediately following `else` is executed if the condition is false. Later statements are executed independently of the condition.

Do you still remember the rules about continuation lines?

```
# 1
if (a < 0.0)
  print("'a' is negative") else
    print("'a' is not negative")
# 2 (not evaluated here)
if (a < 0.0) print("'a' is negative")
else print("'a' is not negative")
```

Why does only the second example above trigger an error?

Play with the use conditional execution, with both simple and compound statements, and also think how to combine `if` and `else` to select among more than two options.

There is in R a `switch` statement, that we will not describe here, that can be used to select among "cases", or several alternative statements, based on an expression evaluating to a number or a character string.

Vectorized

The vectorized conditional execution is coded by means of a **function** called `ifelse` (one word). This function takes three arguments: a logical vector, a result vector for TRUE, a result vector for FALSE. All three can be any construct giving the necessary argument as their result. In the case of result vectors, recycling will apply if they are not of the correct length. The length of the result is determined by the length of the logical vector in the first argument!.

```
a <- 1:10
ifelse(a > 5, 1, -1)

##  [1] -1 -1 -1 -1 -1  1  1  1  1  1

ifelse(a > 5, a + 1, a - 1)

##  [1]  0  1  2  3  4  7  8  9 10 11

ifelse(any(a>5), a + 1, a - 1) # tricky

## [1] 2
```

```
ifelse(logical(0), a + 1, a - 1) # even more tricky

## logical(0)

ifelse(NA, a + 1, a - 1) # as expected

## [1] NA
```

Try to understand what is going on in the previous example. Create your own examples to test how `ifelse` works.

Exercise: write using `ifelse` a single statement to combine numbers from a and b into a result vector d, based on whether the corresponding value in c is the character "a" or "b".

```
a <- rep(-1, 10)
b <- rep(+1, 10)
c <- c(rep("a", 5), rep("b", 5))
# your code
```

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 have clear what each parameter does.

2.8.2 Why using vectorized functions and operators is important

If you have written programs in other languages, it would feel to you natural to use loops (for, repeat while, repeat until) for many of the things for which we have been using vectorization. When using the R language it is best to use vectorization whenever possible, because it keeps the listing of scripts and programs shorter and easier to understand (at least for those with experience in R). However, there is another very important reason: execution speed. The reason behind this is that R is an interpreted language. In current versions of R it is possible to byte-compile functions, but this is rarely used for scripts, and even byte-compiled loops are much slower and vectorized functions.

However, there are cases were we need to repeatedly execute statements in a way that cannot be vectorized, or when we do not need to maximize execution speed. The R language does have loop constructs, and we will describe them next.

2.8.3 Repetition

The most frequently used type of loop is a `for` loop. These loops work in R are based on lists or vectors of values to act upon.

```
b <- 0
for (a in 1:5) b <- b + a
b
```

```
## [1] 15

b <- sum(1:5) # built-in function
b

## [1] 15
```

Here the statement `b <- b + a` is executed five times, with a sequentially taking each of the values in `1:5`. Instead of a simple statement used here, also a compound statement could have been used.

Here are a few examples that show some of the properties of `for` loops and functions, combined with the use of a function.

```
test.for <- function(x) {
  for (i in x) {print(i)}
}
test.for(numeric(0))
test.for(1:3)

## [1] 1
## [1] 2
## [1] 3

test.for(NA)

## [1] NA

test.for(c("A", "B"))

## [1] "A"
## [1] "B"

test.for(c("A", NA))

## [1] "A"
## [1] NA

test.for(list("A", 1))

## [1] "A"
## [1] 1

test.for(c("z", letters[1:4]))

## [1] "z"
## [1] "a"
## [1] "b"
## [1] "c"
## [1] "d"
```

In contrast to other languages, in R function arguments are not checked for ‘type’ when the function is called. The only requirement is that the function code can handle the argument provided. In this example you can see that the same function works with numeric and character vectors, and with lists. We haven't seen lists before. As earlier discussed all elements in a vector should have the same type. This is not the case for lists. It is also interesting to note that a list or vector of length zero is a valid argument, that triggers no error, but that as one would expect, causes the statements in the loop body to be skipped.

Some examples of use of `for` loops — and of how to avoid there use.

```
a <- c(1, 4, 3, 6, 8)
for(x in a) x*2 # result is lost
for(x in a) print(x*2) # print is needed!

## [1] 2
## [1] 8
## [1] 6
## [1] 12
## [1] 16

b <- for(x in a) x*2 # doesn't work as expected, but triggers no error
b

## NULL

for(x in a) b <- x*2 # a bit of a surprise, as b is not a vector!
b

## [1] 16

for(i in seq(along=a)) {
  b[i] <- a[i]^2
  print(b)
}

## [1] 1
## [1]  1 16
## [1]  1 16  9
## [1]  1 16  9 36
## [1]  1 16  9 36 64

b # is a vector!

## [1]  1 16  9 36 64

# a bit faster if we first allocate a vector of the required length
b <- numeric(length(a))
for(i in seq(along=a)) {
  b[i] <- a[i]^2
  print(b)
}

## [1] 1 0 0 0 0
## [1]  1 16  0  0  0
## [1]  1 16  9  0  0
## [1]  1 16  9 36  0
## [1]  1 16  9 36 64
```

```
b # is a vector!

## [1]  1 16  9 36 64

# vectorization is simplest and fastest
b <- a^2
b

## [1]  1 16  9 36 64
```

Look at the results from the above examples, and try to understand where does the returned value come from in each case.

We sometimes may not be able to use vectorization, or may be easiest to not use it. However, whenever working with large data sets, or many similar datasets, we will need to take performance into account. As vectorization usually also makes code simpler, it is good style to use it whenever possible.

```
b <- numeric(length(a)-1)
for(i in seq(along=b)) {
  b[i] <- a[i+1] - a[i]
  print(b)
}

## [1] 3 0 0 0
## [1]  3 -1  0  0
## [1]  3 -1  3  0
## [1]  3 -1  3  2

# although in this case there were alternatives, there
# are other cases when we need to use indexes explicitly
b <- a[2:length(a)] - a[1:length(a)-1]
b

## [1]  3 -1  3  2

# or even better
b <- diff(a)
b

## [1]  3 -1  3  2
```

`seq(along=b)` builds a new numeric vector with a sequence of the same length as the length as the vector given as argument for parameter 'along'.

`while` loops are quite frequently also useful. Instead of a list or vector, they take a logical argument, which is usually an expression, but which can also be a variable. For example the previous calculation could be also done as follows.

```
a <- c(1, 4, 3, 6, 8)
i <- 1
while (i < length(a)) {
  b[i] <- a[i]^2
  print(b)
  i <- i + 1
}

## [1]  1 -1  3  2
## [1]  1 16  3  2
## [1]  1 16  9  2
## [1]  1 16  9 36

b

## [1]  1 16  9 36
```

Here is another example. In this case we use the result of the previous iteration in the current one. In this example you can also see, that it is allowed to put more than one statement in a single line, in which case the statements should be separated by a semicolon (;).

```
a <- 2
while (a < 50) {print(a); a <- a^2}

## [1] 2
## [1] 4
## [1] 16

print(a)

## [1] 256
```

Make sure that you understand why the final value of `a` is larger than 50.

`repeat` is seldom used, but adds flexibility as `break` can be in the middle of the compound statement.

```
a <- 2
repeat{
  print(a)
  a <- a^2
  if (a > 50) {print(a); break()}
}

## [1] 2
## [1] 4
## [1] 16
## [1] 256

# or more elegantly
a <- 2
repeat{
  print(a)
  if (a > 50) break()
  a <- a^2
}
```

```
## [1] 2
## [1] 4
## [1] 16
## [1] 256
```

Please, make sure you understand what is happening in the previous examples.

2.8.4 Nesting

All the execution-flow control statements seen above can be nested. We will show an example with two `for` loops. We first need a matrix of data to work with:

```
A <- matrix(1:50, 10)
A

##       [,1] [,2] [,3] [,4] [,5]
##  [1,]    1   11   21   31   41
##  [2,]    2   12   22   32   42
##  [3,]    3   13   23   33   43
##  [4,]    4   14   24   34   44
##  [5,]    5   15   25   35   45
##  [6,]    6   16   26   36   46
##  [7,]    7   17   27   37   47
##  [8,]    8   18   28   38   48
##  [9,]    9   19   29   39   49
## [10,]   10   20   30   40   50

A <- matrix(1:50, 10, 5)
A

##       [,1] [,2] [,3] [,4] [,5]
##  [1,]    1   11   21   31   41
##  [2,]    2   12   22   32   42
##  [3,]    3   13   23   33   43
##  [4,]    4   14   24   34   44
##  [5,]    5   15   25   35   45
##  [6,]    6   16   26   36   46
##  [7,]    7   17   27   37   47
##  [8,]    8   18   28   38   48
##  [9,]    9   19   29   39   49
## [10,]   10   20   30   40   50

# argument names used for clarity
A <- matrix(1:50, nrow = 10)
A

##       [,1] [,2] [,3] [,4] [,5]
##  [1,]    1   11   21   31   41
##  [2,]    2   12   22   32   42
##  [3,]    3   13   23   33   43
##  [4,]    4   14   24   34   44
##  [5,]    5   15   25   35   45
##  [6,]    6   16   26   36   46
##  [7,]    7   17   27   37   47
##  [8,]    8   18   28   38   48
##  [9,]    9   19   29   39   49
## [10,]   10   20   30   40   50

A <- matrix(1:50, ncol = 5)
A

##       [,1] [,2] [,3] [,4] [,5]
##  [1,]    1   11   21   31   41
##  [2,]    2   12   22   32   42
##  [3,]    3   13   23   33   43
##  [4,]    4   14   24   34   44
##  [5,]    5   15   25   35   45
##  [6,]    6   16   26   36   46
##  [7,]    7   17   27   37   47
##  [8,]    8   18   28   38   48
##  [9,]    9   19   29   39   49
## [10,]   10   20   30   40   50

A <- matrix(1:50, nrow = 10, ncol = 5)
A

##       [,1] [,2] [,3] [,4] [,5]
##  [1,]    1   11   21   31   41
##  [2,]    2   12   22   32   42
##  [3,]    3   13   23   33   43
##  [4,]    4   14   24   34   44
##  [5,]    5   15   25   35   45
##  [6,]    6   16   26   36   46
##  [7,]    7   17   27   37   47
##  [8,]    8   18   28   38   48
##  [9,]    9   19   29   39   49
## [10,]   10   20   30   40   50
```

All the statements above are equivalent, but some are easier to read than others.

```
row.sum <- numeric() # slower as size needs to be expanded
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
```

```
row.sum <- numeric(nrow(A)) # faster
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
```

Look at the output of these two examples to understand what is happening differently with `row.sum`.

The code above is very general, it will work with any size of two dimensional matrix, which is good programming practice. However, sometimes we need more specific calculations. `A[1, 2]` selects one cell in the matrix, the one on the first row of the second column. `A[1, ]` selects row one, and `A[ , 2]` selects column two. In the example above 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.

Exercises: 1) modify the example above to add up only the first three columns of A, 2) modify the example above to add the last three columns of A.

Will the code you wrote continue working as expected if the number of rows in A changed? and what if the number of columns in A changed, and the required results still needed to be calculated for relative positions? 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 think how to improve the code, at least so that wrong results are not produced.

Vectorization can be achieved in this case easily for the inner loop.

```
row.sum <- numeric(nrow(A)) # faster
for (i in 1:nrow(A)) {
  row.sum[i] <- sum(A[i, ])
}
print(row.sum)

##  [1] 105 110 115 120 125 130 135 140 145 150
```

`A[i, ]` selects row `i` and all columns. In R, the row index always comes first, which is not the case in all programming languages.

Full vectorization can be achieved with `apply` functions.

```
row.sum <- apply(A, MARGIN = 1, sum) # MARGIN=1 inidcates rows
print(row.sum)

##  [1] 105 110 115 120 125 130 135 140 145 150
```

How would you change this last example, so that only the last three columns are added up? (Think about use of subscripts to select a part of the matrix.)

There are many variants of `apply` functions, both in base R and in contributed packages.

2.9 Packages

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. The function `library` is used to load packages, already installed in the local R library, into the current session, while the function `install.packages` is used to install packages, either from a file, or directly from the internet into the library. When using RStudio it is easiest to use RStudio commands (which call `install.packages` and `update.packages`) to install and update packages.

```
library(graphics)
```

Currently there are thousands of packages available. The most reliable source of packages is CRAN, as only packages that pass strict tests and are actively maintained are included. In some cases you may need or want to install less stable code, and this is also possible.

R packages can be installed either from source, or from already built 'binaries'. Installing from sources, depending on the package, may require quite a lot of additional software to be available. Under MS-Windows, very rarely the needed shell, commands and compilers are already available. Installing then is not too difficult (you will need RTools, and MiKTeX). For this reason it is the norm to install packages from binary .zip files. Under Linux most tools will be available, or very easy to install, so it is not unusual to install from sources. For OS X (Mac) the situation is somewhere in-between. If the tools are available, packages can be very easily installed from source from within RStudio.

The development of packages is beyond the scope of the current course, but it is still interesting to know a few things about packages. Using RStudio it is relatively easy to develop your own packages. Packages can be of very different sizes. Packages use a relatively rigid structure of folder for storing the different types of files, and there is a built-in help system, that one needs to use, so that the package documentation gets linked to the R help system when the package is loaded. In addition to R code, packages can call C, C++, FORTRAN, Java, etc. functions and routines, but some kind of 'glue' is needed, as data is stored differently. At least for C++, the recently developed Rcpp R package makes the gluing extremely easy.

In addition to some packages from CRAN, later in the course we will use a suite of packages for photobiology that I have developed during the last couple of years. Some of the functions in these packages are very simple, and others more complex. In one of the packages, I included some C++ functions to improve performance. Replacing some R for loops with C++ for loops and iterators, resulted in a huge speed increase. The reason for this is that R is an interpreted language and C++ is compiled into machine code. Recent versions of R allow byte-compilation which can give some speed improvement, without need to switch to another language.

The source code for the photobiology and many other packages is freely available, so if you are interested you can study it. For any function defined in R, typing at the command prompt the name of the function without the parentheses lists the code.

```
length  # a function defined in C within R itself

## function (x)  .Primitive("length")

SEM # the function we defined earlier

## function(x, na.rm=FALSE){sqrt(var(x, na.rm=na.rm)/length(na.omit(x)))}
```

One good way of learning how R works, is by experimenting with it, and whenever using a certain function looking at the help, to check what are all the available options.

3 Storing and manipulating data with R

3.1 Packages used in this chapter

For executing the examples listed in this chapter you need first to load the following packages from the library:

```r
library(data.table)
```

3.2 Introduction

Data frames have been discussed in 1 and data tables are also data frames. In other words they are 'derived' from data frames, so they can be used whenever data frames are expected as input. Package `data.frame` is under active development but it is already a better option than data frames in many contexts, specially when working with large data sets. The reason for this is that because of the way the R language is defined, data frames are are very frequently copied in whole even when a small part of the data is altered, or when passed as arguments to many functions. This has a very large impact on performance. The `data.table` avoids or delays copying as much as possible, and also implements fast search, sort, etc. operations. This makes a huge difference for large data sets. For smaller data set the main advantage is the new (additional) syntax that is more concise, though not in all cases easier to understand.

3.3 Differences between `data.tables` and `data.frames`

Data tables are also data frames, and if one operates on them with the usual data-frame syntax, in most cases they behave identically to data frames. To achieve the full advantage in performance one should be careful of one codes scripts and functions. Data tables can created in a similar way as data frames.

```r
my.dt <- data.table(x = 1:10, y = rnorm(10))
class(my.dt)

## [1] "data.table" "data.frame"
```

We can 'convert' in place, without any copying, a data frame into a data table using `setDT`, and with `setDF` 'convert' a data table into a data frame.

```
my.df <- data.frame(x = 1:10, y = rnorm(10))
class(my.df)

## [1] "data.frame"

setDT(my.df)
class(my.df)

## [1] "data.table" "data.frame"

setDF(my.df)
class(my.df)

## [1] "data.frame"
```

An assignment of a data frame is equivalent to a copy, and in most cases results in the whole data frame being copyed from one location in memory to a different one.

```
my.cp.df <- my.df
identical(my.cp.df, my.df)

## [1] TRUE

my.cp.df$y <- 1
identical(my.cp.df, my.df)

## [1] FALSE
```

With data tables, assignment with `<-` just creates a new name for the same object. However, if we use 'data.frame' syntax to alter the new name, a copy is done at that moment, and yields the same result as a true data frame.

```
my.cp.dt <- my.dt
identical(my.cp.dt, my.dt)

## [1] TRUE

my.cp.dt$y <- my.cp.dt$y + 1
identical(my.cp.dt, my.dt)

## [1] FALSE
```

However, if we use the special syntax introduced by the `data.frame` package, no copy is done, and both names continue pointing to the same, now modified data table.

```
my.cp.dt <- my.dt
identical(my.cp.dt, my.dt)

## [1] TRUE
```

```
my.cp.dt[ , y := y + 1]

##      x         y
##  1:  1 0.9041652
##  2:  2 1.2999309
##  3:  3 2.0708793
##  4:  4 0.8692864
##  5:  5 2.4332193
##  6:  6 1.2191764
##  7:  7 0.6761261
##  8:  8 0.1673908
##  9:  9 1.2405094
## 10: 10 1.0210096

identical(my.cp.dt, my.dt)

## [1] TRUE

my.cp.dt

##      x         y
##  1:  1 0.9041652
##  2:  2 1.2999309
##  3:  3 2.0708793
##  4:  4 0.8692864
##  5:  5 2.4332193
##  6:  6 1.2191764
##  7:  7 0.6761261
##  8:  8 0.1673908
##  9:  9 1.2405094
## 10: 10 1.0210096

my.dt

##      x         y
##  1:  1 0.9041652
##  2:  2 1.2999309
##  3:  3 2.0708793
##  4:  4 0.8692864
##  5:  5 2.4332193
##  6:  6 1.2191764
##  7:  7 0.6761261
##  8:  8 0.1673908
##  9:  9 1.2405094
## 10: 10 1.0210096
```

The assignemnt of the value ‘1’ using the new syntax, changed the only object, pointed at by both names. When using data table syntax, if we really want a copy, then we should use the function `copy`.

```
my.cp.dt <- copy(my.dt)
identical(my.cp.dt, my.dt)
```

```
## [1] TRUE

my.cp.dt[ , y := y - 1]

##      x           y
##  1:  1 -0.09583481
##  2:  2  0.29993089
##  3:  3  1.07087932
##  4:  4 -0.13071359
##  5:  5  1.43321926
##  6:  6  0.21917637
##  7:  7 -0.32387388
##  8:  8 -0.83260916
##  9:  9  0.24050940
## 10: 10  0.02100964

identical(my.cp.dt, my.dt)

## [1] FALSE

my.cp.dt

##      x           y
##  1:  1 -0.09583481
##  2:  2  0.29993089
##  3:  3  1.07087932
##  4:  4 -0.13071359
##  5:  5  1.43321926
##  6:  6  0.21917637
##  7:  7 -0.32387388
##  8:  8 -0.83260916
##  9:  9  0.24050940
## 10: 10  0.02100964

my.dt

##      x         y
##  1:  1 0.9041652
##  2:  2 1.2999309
##  3:  3 2.0708793
##  4:  4 0.8692864
##  5:  5 2.4332193
##  6:  6 1.2191764
##  7:  7 0.6761261
##  8:  8 0.1673908
##  9:  9 1.2405094
## 10: 10 1.0210096
```

For fast access of large data sets one can set a 'key' based on one or more columns, using function `setkey`.

```
setkey(my.dt, y)
my.dt
```

```
##       x         y
##   1:  8 0.1673908
##   2:  7 0.6761261
##   3:  4 0.8692864
##   4:  1 0.9041652
##   5: 10 1.0210096
##   6:  6 1.2191764
##   7:  9 1.2405094
##   8:  2 1.2999309
##   9:  3 2.0708793
##  10:  5 2.4332193

setkey(my.dt, x)
my.dt

##       x         y
##   1:  1 0.9041652
##   2:  2 1.2999309
##   3:  3 2.0708793
##   4:  4 0.8692864
##   5:  5 2.4332193
##   6:  6 1.2191764
##   7:  7 0.6761261
##   8:  8 0.1673908
##   9:  9 1.2405094
##  10: 10 1.0210096
```

There is also an special `print` method for datables, that is used automatically by default, that instead of printing the whole data.table, only prints the 'head' and the 'tail' of the tables, unless the table has few rows. In the examples above all rows were printed because, there were not many of them.

```
data.table(x = 1:1000, y = runif(1000))

##           x         y
##     1:    1 0.4034798
##     2:    2 0.1633459
##   ---
##   999:  999 0.7787175
##  1000: 1000 0.7784970
```

3.4 Using `data.frames` and `data.tables`

Adding new columns based on other columns, or other variables, uses the same syntax shown above for modifying column 'y'.

```
my.cp.dt[ , z := y + x * 2]

##       x           y          z
##  1:  1 -0.09583481  1.904165
##  2:  2  0.29993089  4.299931
##  3:  3  1.07087932  7.070879
##  4:  4 -0.13071359  7.869286
##  5:  5  1.43321926 11.433219
##  6:  6  0.21917637 12.219176
##  7:  7 -0.32387388 13.676126
##  8:  8 -0.83260916 15.167391
##  9:  9  0.24050940 18.240509
## 10: 10  0.02100964 20.021010
```

```r
try(detach(package:data.table))
```