R–lab

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1 Required packages and other preparations

```
library(TeachingDemos)
library(xlsx)
library(multtest)
library(Biobase)
library(plyr)
library(dplyr)
library(ggplot2)
```

2 Introduction and getting help

R is a software language for carrying out complicated (and simple) statistical analyses. It includes routines for data summary and exploration, graphical presentation and data modeling. The aim of this lab is to provide you with a basic fluency in the language. When you work in *R* you create objects that are stored in the current workspace (sometimes called image). Each object created remains in the image unless you explicitly delete it. At the end of the session the workspace will be lost unless you save it.

You can get your current working directory via `getwd()` and set it with `setwd()`. By default, it is usually your home directory.

Commands written in *R* are saved in memory throughout the session. You can scroll back to previous commands typed by using the "up" arrow key (and "down" to scroll back again). You finish an *R* session by typing `q()` at which point you will also be prompted as to whether or not you want to save the current workspace into your working directory. If you do not want to, it will be lost. Remember the ways to get help:

- Just ask!
- `help.start()` and the HTML help button in the Windows GUI.
- `help` and `?`: `help("data.frame")` or `?help`.
- `help.search()`, `apropos()`
- `browseVignettes("package")`
- rseek.org
- use tab–completion in RStudio, this will also display help–snippets

3 Basics – objects and arithmetic

R stores information in objects and operates on objects. The simplest objects are scalars, vectors and matrices. But there are many others: lists and data frames for example. In advanced use of *R* it can also be useful to define new types of objects, specific for particular application. We will stick with just the most commonly used objects here. An important feature of *R* is that it will do different things on different types of objects. For example, type:

```
4 + 6

#> [1] 10
```

So, *R* does scalar arithmetic returning the scalar value 10. In fact, *R* returns a vector of length 1 - hence the [1] denoting first element of the vector. We can assign objects values for subsequent use. For example:

```
x <- 6
y <- 4
z <- x+y
z

#> [1] 10
```

would do the same calculation as above, storing the result in an object called z. We can look at the contents of the object by simply typing its name. At any time we can list the objects which we have created:

```
ls()

#> [1] "x" "y" "z"
```

Notice that `ls` is actually an object itself. Typing `ls` would result in a display of the contents of this object, in this case, the commands of the function. The use of parentheses, `ls()`, ensures that the function is executed and its result — in this case, a list of the objects in the current environment — displayed. More commonly, a function will operate on an object, for example

```
sqrt(16)

#> [1] 4
```

calculates the square root of 16. Objects can be removed from the current workspace with the function `rm()`. There are many standard functions available in *R*, and it is also possible to create new ones. Vectors can be created in *R* in a number of ways. We can describe all of the elements:

```
z <- c(5,9,1,0)
```

Note the use of the function `c` to concatenate or "glue together" individual elements. This function can be used much more widely, for example

```
x <- c(5,9)
y <- c(1,0)
z <- c(x,y)
```

would lead to the same result by gluing together two vectors to create a single vector. Sequences can be generated as follows:

```
seq(1,9,by=2)

#> [1] 1 3 5 7 9

seq(8,20,length=6)

#> [1]  8.0 10.4 12.8 15.2 17.6 20.0
```

These examples illustrate that many functions in *R* have optional arguments, in this case, either the step length or the total length of the sequence (it doesn't make sense to use both). If you leave out both of these options, *R* will make its own default choice, in this case assuming a step length of 1. So, for example,

```
x <- seq(1,10)
```

also generates a vector of integers from 1 to 10. At this point it's worth mentioning the help facility again. If you don't know how to use a function, or don't know what the options or default values are, type `help(functionname)` or simply `?functionname` where `functionname` is the name of the function you are interested in. This will usually help and will often include examples to make things even clearer. Another useful function for building vectors is the `rep` command for repeating things. Examples:

```
rep(1:3,6)

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

## repeat each element six times
rep(1:3,c(6,6,6))

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

## simplified
rep(1:3,rep(6,3))

#>  [1] 1 1 1 1 1 1 2 2 2 2 2 2 3 3 3 3 3 3
```

As explained above, *R* will often adapt to the objects it is asked to work on. An example is the vectorized arithmetic used in *R*:

```
x <- 1:5; y <- 5:1
x

#> [1] 1 2 3 4 5

y
```

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

x + y

#> [1] 6 6 6 6 6

x^2

#> [1]  1  4  9 16 25

# another example
x <- c(6,8,9)
y <- c(1,2,4)
x + y

#> [1]  7 10 13

x * y

#> [1]  6 16 36
```

showing that *R* uses component-wise arithmetic on vectors. *R* will also try to make sense if objects are mixed. For example,

```
x <- c(6,8,9)
x + 2

#> [1]  8 10 11
```

Two particularly useful functions worth remembering are `length` which returns the length of a vector (i.e. the number of elements it contains) and `sum` which calculates the sum of the elements of a vector. *R* also has basic calculator capabilities:

- `a+b, a-b, a*b, a^b (or a**b), a %% b (a MOD b)`
- additionally: `sqrt(a), sin(a)` ...
- and some simple statistics:
  - `mean(a)`
  - `summary(a)`
  - `var(a)`
  - `min(a,b), max(a,b)`

Exercise: Simple R operations

(*a*) Define `x <- c(4,2,6)` and `y <- c(1,0,-1)` Decide what the result will be of the following:
  (*a*) `length(x)`
  (*b*) `sum(x)`
  (*c*) `sum(x^2)`
  (*d*) `x+y`
  (*e*) `x*y`
  (*f*) `x-2`
  (*g*) `x^2`
  Use *R* to check your answers.

(*b*) Decide what the following sequences are and use *R* to check your answers:
  (*a*) `7:11`
  (*b*) `seq(2,9)`
  (*c*) `seq(4,10,by=2)`
  (*d*) `seq(3,30,length=10)`
  (*e*) `seq(6,-4,by=-2)`

(*c*) Determine what the result will be of the following *R* expressions, and then use *R* to check you are right:
  (*a*) `rep(2,4)`

  (*b*) `rep(c(1,2),4)`
  (*c*) `rep(c(1,2),c(4,4))`
  (*d*) `rep(1:4,4)`
  (*e*) `rep(1:4,rep(3,4))`

(*d*) Use the rep function to define simply the following vectors in *R*.

  (*a*) `6,6,6,6,6,6`
  (*b*) `5,8,5,8,5,8,5,8`
  (*c*) `5,5,5,5,8,8,8,8`

Exercise: R as a calculator

Calculate the following expression, where `x` and `y` have values `-0.25` and `2` respectively. Then store the result in a new variable and print its content.

```
x + cos(pi/y)
```

4 Summaries, subscripting and useful vector functions

Let's suppose we've collected some data from an experiment and stored them in an object `x`. Some simple summary statistics of these data can be produced:

```
x <- c(7.5,8.2,3.1,5.6,8.2,9.3,6.5,7.0,9.3,1.2,14.5,6.2)
mean(x)

#> [1] 7.22

var(x)

#> [1] 11

summary(x)

#>    Min. 1st Qu.  Median    Mean 3rd Qu.    Max.
#>    1.20    6.05    7.25    7.22    8.48   14.50
```

It may be, however, that we subsequently learn that the first 6 data points correspond to measurements made in one experiment, and the second six on another experiment. This might suggest summarizing the two sets of data separately, so we would need to extract from `x` the two relevant subvectors. This is achieved by subscripting:

```
x[1:6]

#> [1] 7.5 8.2 3.1 5.6 8.2 9.3

x[7:12]

#> [1]  6.5  7.0  9.3  1.2 14.5  6.2

summary(x[1:6])

#>    Min. 1st Qu.  Median    Mean 3rd Qu.    Max.
#>    3.10    6.07    7.85    6.98    8.20    9.30

summary(x[7:12])

#>    Min. 1st Qu.  Median    Mean 3rd Qu.    Max.
#>    1.20    6.28    6.75    7.45    8.73   14.50
```

Other subsets can be created in the obvious way. For example:

```
x[c(2,4,9)]

#> [1] 8.2 5.6 9.3

x[-(1:6)]

#> [1]  6.5  7.0  9.3  1.2 14.5  6.2

# compare to
x[7:12]

#> [1]  6.5  7.0  9.3  1.2 14.5  6.2
```

Additionally, there are some useful commands to order and sort vectors

- `sort`: sort in increasing order
- `order`: orders the indexes is such a way that the elements of the vector are sorted, i.e `sort(v) = v[order(v)]`
- `rank`: gives the ranks of the elements of a vector, different options for handling *ties* are available.

```
x <- c(1.3,3.5,2.7,6.3,6.3)
sort(x)

#> [1] 1.3 2.7 3.5 6.3 6.3

order(x)

#> [1] 1 3 2 4 5

x[order(x)]

#> [1] 1.3 2.7 3.5 6.3 6.3

rank(x)

#> [1] 1.0 3.0 2.0 4.5 4.5
```

Exercise

(*a*) Define `x <- c(5,9,2,3,4,6,7,0,8,12,2,9)`
Decide what the result will be of the following:
  (*a*) `x[2]`
  (*b*) `x[2:4]`
  (*c*) `x[c(2,3,6)]`
  (*d*) `x[c(1:5,10:12)]`
  (*e*) `x[-(10:12)]`
Use *R* to check your answers.

(*b*) The `y <- c(33,44,29,16,25,45,33,19,54,22,21,49,11,24,56)` contain sales of milk in liters for 5 days in three different shops (the first 3 values are for shops 1,2 and 3 on Monday, etc.). Produce a statistical summary of the sales for each day of the week and also for each shop.

5 Classes, modes and types of objects

R is an object-oriented language, so every data item is an object in *R*. As in other programming languages, objects are instances of "blue-prints" called classes. There are the following elementary types or ("modes"):

(*a*) numeric: real number
(*b*) character: chain of characters, text
(*c*) factor: String or numbers, describing certain categories

(*d*) logical: TRUE, FALSE
(*e*) special values: NA (missing value), NULL (“empty object”), Inf, -Inf (infinity), NaN (not a number)

Data storage types includes matrices, lists and data frames, which will be introduced in the next section. Certain types can have different subtypes, e.g. numeric can be further subdivided into the integer, single and double types. Types can be checked by the `is.*` and changed (“casted”) by the `as.*` functions. Furthermore, the function `str` is very useful in order to obtain an overview of an (possibly complex) object at hand. The following examples will make this clear:

```
#assign value "9" to an object
a <- 9
# is a a string?
is.character(a)

#> [1] FALSE

# is a a number?
is.numeric(a)

#> [1] TRUE

# What's its type?
typeof(a)

#> [1] "double"

# now turn it into a factor
a <- as.factor(a)
# Is it a factor?
is.factor(a)

#> [1] TRUE

# assign an string to a:
a <- "NAME"
# what's a?
class(a)

#> [1] "character"

str(a)

#>  chr "NAME"
```

6 Matrices, lists, data frames and basic data handling

6.1 Matrices

Matrices can be created in *R* in a variety of ways. Perhaps the simplest is to create the columns and then glue them together with the command `cbind`. For example,

```
x <- c(5,7,9)
y <- c(6,3,4)
z <- cbind(x,y)
z

#>      x y
#> [1,] 5 6
#> [2,] 7 3
#> [3,] 9 4
```

```
## dimensions: 3 rows and 2 columns
dim(z)
```

```
#> [1] 3 2
```

```
### matrix constructor
z <- matrix(c(5,7,9,6,3,4),nrow=3)
```

There is a similar command, `rbind`, for building matrices by gluing rows together. The functions `cbind` and `rbind` can also be applied to matrices themselves (provided the dimensions match) to form larger matrices. Matrices can also be built by explicit construction via the function matrix. Notice that the dimension of the matrix is determined by the size of the vector and the requirement that the number of rows is 3 in the example above, as specified by the argument `nrow=3`. As an alternative we could have specified the number of columns with the argument `ncol=2` (obviously, it is unnecessary to give both). Notice that the matrix is "filled up" column-wise. If instead you wish to fill up row-wise, add the option `byrow=T`. For example:

```
z <- matrix(c(5,7,9,6,3,4),nr=3,byrow=T)
z
```

```
#>      [,1] [,2]
#> [1,]    5    7
#> [2,]    9    6
#> [3,]    3    4
```

Notice that the argument `nrow` has been abbreviated to `nr`. Such abbreviations are always possible for function arguments provided it induces no ambiguity – if in doubt always use the full argument name. As usual, *R* will try to interpret operations on matrices in a natural way. For example, with `z` as above, and

```
y <- matrix(c(1,3,0,9,5,-1),nrow=3,byrow=T)
y
```

```
#>      [,1] [,2]
#> [1,]    1    3
#> [2,]    0    9
#> [3,]    5   -1
```

```
y + z
```

```
#>      [,1] [,2]
#> [1,]    6   10
#> [2,]    9   15
#> [3,]    8    3
```

```
y * z
```

```
#>      [,1] [,2]
#> [1,]    5   21
#> [2,]    0   54
#> [3,]   15   -4
```

Notice that multiplication here is component–wise rather than conventional matrix multiplication. Indeed, conventional matrix multiplication is undefined for `y` and `z` as the dimensions fail to match. Actual matrix multiplication works like this:

```
x <- matrix(c(3,4,-2,6),nrow=2,byrow=T)
x
```

```
#>      [,1] [,2]
#> [1,]    3    4
#> [2,]   -2    6
```

```
y %*% x
```

```
#>      [,1] [,2]
#> [1,]   -3   22
#> [2,]  -18   54
#> [3,]   17   14
```

Other useful functions on matrices are `t` to calculate a matrix transpose and `solve` to calculate inverses:

```
t(z)
```

```
#>      [,1] [,2] [,3]
#> [1,]    5    9    3
#> [2,]    7    6    4
```

```
solve(x)
```

```
#>        [,1]   [,2]
#> [1,] 0.2308 -0.154
#> [2,] 0.0769  0.115
```

As with vectors it is useful to be able to extract sub-components of matrices. In this case, we may wish to pick out individual elements, rows or columns. As before, the `[ ]` notation is used to subscript. The following examples should make things clear:

```
z[1,1]
```

```
#> [1] 5
```

```
z[,2]
```

```
#> [1] 7 6 4
```

```
z[1:2,]
```

```
#>      [,1] [,2]
#> [1,]    5    7
#> [2,]    9    6
```

```
z[-1,]
```

```
#>      [,1] [,2]
#> [1,]    9    6
#> [2,]    3    4
```

```
z[-c(1,2),]
```

```
#> [1] 3 4
```

So, in particular, it is necessary to specify which rows and columns are required, whilst omitting the integer for either dimension implies that every element in that dimension is selected.

Exercise: Matrix operations

(*a*) Call `?matrix` to consult the *R* help on matrices.
(*b*) Create the variables $a = 3$ and $b = 4.5$.
(*c*) Test whether a and b are numeric or strings.
(*d*) Create the following matrices

$$A = \begin{pmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \\ 7 & 8 & 10 \end{pmatrix} \quad B = \begin{pmatrix} 1 & 4 & 7 \\ 2 & 5 & 8 \\ 3 & 6 & 9 \end{pmatrix} \quad y = \begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix}$$

(e) Calculate
  - $a^2 + 1/b$
  - $a * A$ Multiplication with a scalar
  - $A * B$ Matrix multiplication (R–command %*%)
  - Invert and transpose A. (R–commands `solve` and `t()`)
  - Fill the first row of B with ones

(f) Access the second element of the third column of A and the third element of the second column of B.

(g) Multiply the first row of A with the second column of B.

6.2 Data frames and lists

Data frames – "excel tables"

A data frame is essentially a matrix where the columns can have different data types. As such, it is usually used to represent a whole data set, where the rows represent the samples and columns the variables. Essentially, you can think of a data frame as an excel table.

This way columns are named and can be accessed by their name. If the rows have names, they can be be accessed by their names as well. Internally, a data frame is represented by a list.

Let's illustrate this by the small data set saved in comma–separated-format (csv) — `patients`. We load it in from a website using the function `read.csv`, which is used to read a data file in *comma separated format* — *csv* into *R*. In a .csv–file the data are stored row–wise, and the entries in each row are separated by commas.

```
pat <- read.csv("http://www-huber.embl.de/users/klaus/BasicR/Patients.csv")
pat

#>    Height Weight Gender
#> P1   1.65     80      f
#> P2   1.30     NA      m
#> P3   1.20     50      f

str(pat)

#> 'data.frame': 3 obs. of  3 variables:
#>  $ Height: num  1.65 1.3 1.2
#>  $ Weight: num  80 NA 50
#>  $ Gender: Factor w/ 2 levels " f"," m": 1 2 1

colnames(pat)

#> [1] "Height" "Weight" "Gender"

### equivalent
names(pat)

#> [1] "Height" "Weight" "Gender"

rownames(pat)

#> [1] "P1" "P2" "P3"

### a factor
pat$Gender

#> [1]  f  m  f
#> Levels:  f  m
```

It has weight, height and gender of three people. Notice that Gender is coded as a `factor`, which is the standard data type for categorical data.

warning: be careful about the StringsAsFactors option

When creating a `data.frame` strings are automatically coded as factors. This behavior is often not desirable and very often this setting causes problems. In order to turn it off, it is best to set `options(stringsAsFactors = FALSE)` globally or to specify this explicitly in the creation of the data frame as in:

```
pat <- read.csv("http://www-huber.embl.de/users/klaus/BasicR/Patients.csv",
              stringsAsFactors = FALSE)
### not a factor
pat$Gender

#> [1] " f" " m" " f"
```

However, when fitting regression models it is in general necessary to have the covariates as factors to obtain correct design matrices and model fits.

We can also use the function `read.xlsx` from the *xlsx* package to read in the data from an excel sheet. The `sheetIndex` specifies which subsheet of the file we want to read in. *comment: The packages requires a java installation. If it does not work, check this first.*

```
pat.xls<-read.xlsx("Patients.xls", sheetIndex=1)
pat.xls

#>   Patient Height Weight Gender
#> 1      P1   1.65     80      f
#> 2      P2   1.30             m
#> 3      P3   1.20     50      f

str(pat.xls)

#> 'data.frame': 3 obs. of  4 variables:
#>  $ Patient: Factor w/ 3 levels "P1","P2","P3": 1 2 3
#>  $ Height : num  1.65 1.3 1.2
#>  $ Weight : Factor w/ 3 levels "  ","50","80": 3 1 2
#>  $ Gender : Factor w/ 2 levels "f","m": 1 2 1
```

If you want to get the (row–) indexes of table entries with a certain property, you can use the function `which()` via `which(<condition>)`, where `<condition>` is a logical condition composed using logical operators:

- `Variable == value`: equal
- `Variable != value`: un–equal
- `Variable < value`: less
- `Variable > value`: greater
- &: *and*
- |: *or*
- !: negation
- %*in*%: is element?

We can illustrate the usage with the patient data. There are multiple ways to achieve the same output, of which using the `subset` function is the most general one and works also with other objects.

```
## which patients are  less than 1.5 tall?
which(pat$Height<1.5)

#> [1] 2 3

## How tall are they?
pat[which(pat$Height<1.5),]

#>    Height Weight Gender
#> P2    1.3     NA      m
#> P3    1.2     50      f
```

```
### recommended alternative that is less error prone
pat[pat$Height<1.5,]
```

```
#>    Height Weight Gender
#> P2    1.3     NA      m
#> P3    1.2     50      f
```

```
### access by rownames
low.height.rows <- subset(rownames(pat), pat$Height<1.5)
low.height.rows
```

```
#> [1] "P2" "P3"
```

```
pat[low.height.rows,]
```

```
#>    Height Weight Gender
#> P2    1.3     NA      m
#> P3    1.2     50      f
```

```
### access via subset
subset(pat, Height<1.5)
```

```
#>    Height Weight Gender
#> P2    1.3     NA      m
#> P3    1.2     50      f
```

Lists

Lists can be viewed as data frames with "columns" of possibly unequal length. although the elements of a list are not really ordered in columns anymore, but are rather a collection of vectors that don't have to be of the same length. List elements can either be accessed by their name or their position via a double bracket operator `[[]]`

```
L = list(one=1, two=c(1,2), five=seq(1, 4, length=5))
L
```

```
#> $one
#> [1] 1
#>
#> $two
#> [1] 1 2
#>
#> $five
#> [1] 1.00 1.75 2.50 3.25 4.00
```

```
names(L)
```

```
#> [1] "one"  "two"  "five"
```

```
 L$five + 10
```

```
#> [1] 11.0 11.8 12.5 13.2 14.0
```

```
## equivalent
L[[3]] + 10
```

```
#> [1] 11.0 11.8 12.5 13.2 14.0
```

Since data frames are just special lists, they can be accessed in the same way

```
pat$Height
```

```
#> [1] 1.65 1.30 1.20
```

```
#equivalent
pat[[1]]

#> [1] 1.65 1.30 1.20
```

6.3 Apply functions

A very useful class of functions in *R* are `apply` commands, which allows to apply a function to every row or column of a data matrix, data frame or list:

`apply(X, MARGIN, FUN, ...)`

- `MARGIN`: 1 (row-wise) or 2 (column-wise)
- `FUN`: The function to apply

The dots argument allows you to specify additional arguments that will be passed to `FUN`.

Special apply are functions include: `lapply` (lists), `sapply` (lapply wrapper trying to convert the result into a vector or matrix), `tapply` and aggregate (apply according to factor groups).

We can illustrate this again using the patients data set:

```
# Calculate mean for each of the first two columns
sapply(X = pat[,1:2], FUN = mean, na.rm = TRUE)

#> Height Weight
#>   1.38  65.00

# Mean height separately for each gender
tapply(X = pat$Height, FUN = mean, INDEX = pat$Ge)

#>    f    m
#> 1.42 1.30
```

Data handling can be much more elegantly performed by the *plyr* and *dplyr* packages, which will be introduced in another lab.

Exercise: Handling a small data set

(*a*) Read in the data set 'Patients.csv' from the website

`http://www-huber.embl.de/users/klaus/BasicR/Patients.csv`

(*b*) Check whether the read in data is actually a `data.frame`.
(*c*) Which variables are stored in the data frame and what are their values?
(*d*) Is there a missing weight value? If yes, replace it by the mean of the other weight values.
(*e*) Calculate the mean weight and height of all the patients.
(*f*) Calculate the BMI $=$ Weight/Height^2 of all the patients. Attach the BMI vector to the data frame using the function `cbind`.

7 Plotting in R

7.1 Plotting in base R

The default command for plotting is `plot()`, there are other specialized commands like `hist()` or `pie()`. A collection of such specialized commands (e.g. heatmaps and CI plots) can be found in the package *gplots*. Another useful visualization package is *LSD*, which includes a heat–scatterplot. The general `plot` command looks like this:

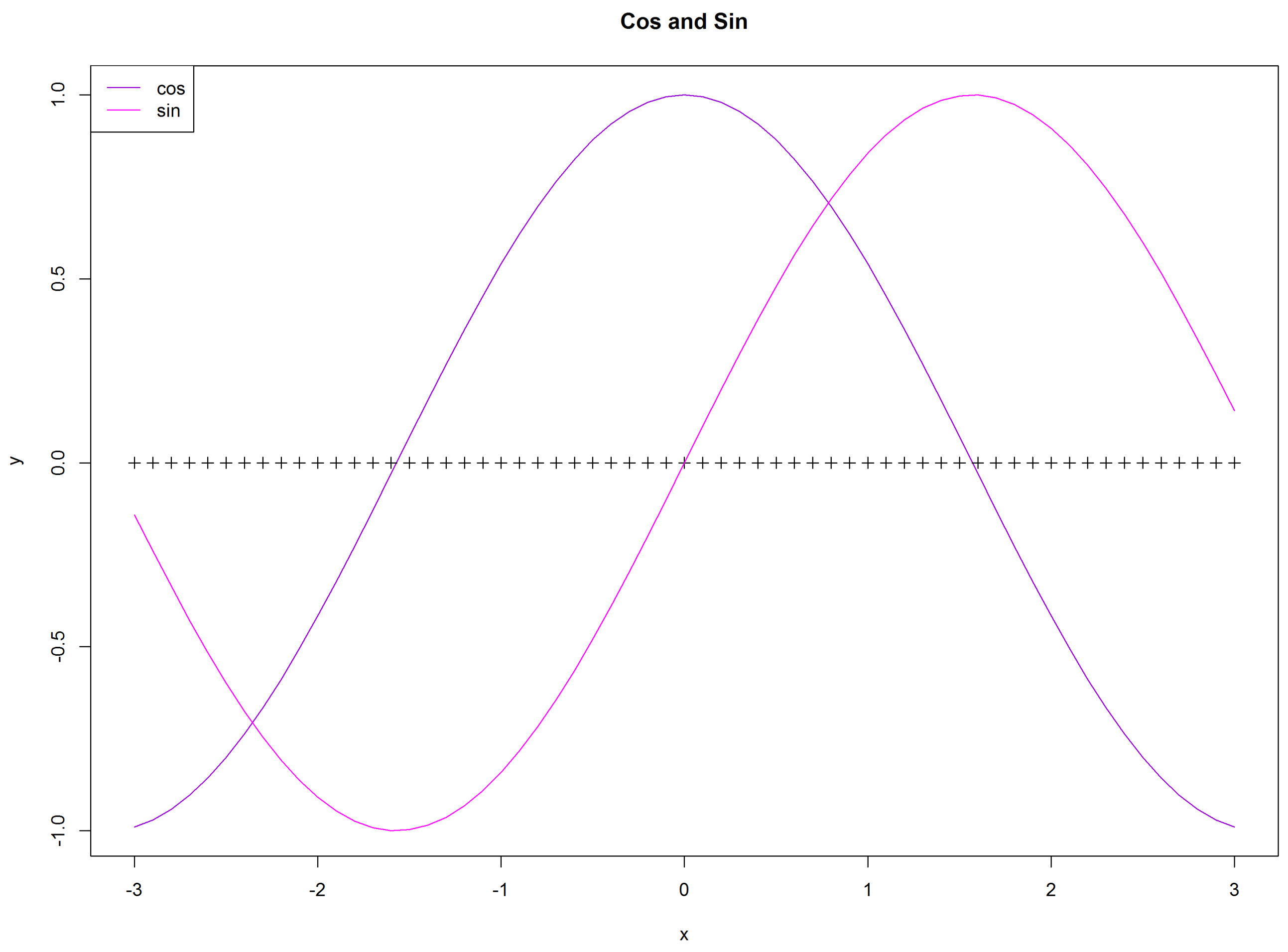
```
plot(x, y, type, main, par (...)  )
```

- `x:` x–axis data
- `y:` y–axis data (may be missing)
- `type=l,p,h,b` display lines / points / horizontal lines ...
- `main:` plot heading
- `par (...)` additional graphical parameters, see ?par for more info ...

The function `plot()` creates the plot. Additional lines, points and so on can be added by *R* commands of the same name: `lines()` and `points()`. The command `pdf` will open a pdf document as a "graphical device", subsequently everything will be plotted to the pdf. With `dev.off()` the device will be closed and the pdf will be viewable. A new graphical device can be opened by `dev.new()`. This allows you to create a new plot without overwriting the current active one. With the graphical option `par ( mfrow=c(<no.rows>, <no.columns>) )` you can produce an array of plots.

As a comprehensive example, the following code produces a sine / cosine plot and colors it:

```
#pdf(file="plot-example.pdf", width=12, height=6)
x <- seq(-3,3, by = 0.1); y <- cos(x); z <- sin(x)
plot(x,y, type="l", col="darkviolet", main="Cos and Sin")
points(x, rep(0, length(x)), pch=3)
lines(x,z, type="l", col="magenta")
legend("topleft", c("cos","sin"), col=c("darkviolet",
"magenta"), lty=1)
```



```
#dev.off()
```

7.2 ggplot2 and qplot

There's a quick plotting function in *ggplot2* called `qplot()` which is meant to be similar to the `plot()` function from base graphics. You can do a lot with `qplot()`, including splitting plots by factors, but in order to understand how *ggplot2* works, it is better to approach it from from the layering syntax.

All *ggplot2* plots begin with the function `ggplot()`. `ggplot()` takes two primary arguments, `data` is the data frame containing the data to be plotted and `aes( )` are the aesthetic mappings to pass on to the plot elements.

As you can see, the second argument, `aes()`, isn't a normal argument, but another function. Since we'll never use `aes()` as a separate function, it might be best to think of it as a special way to pass a list of arguments to the plot.

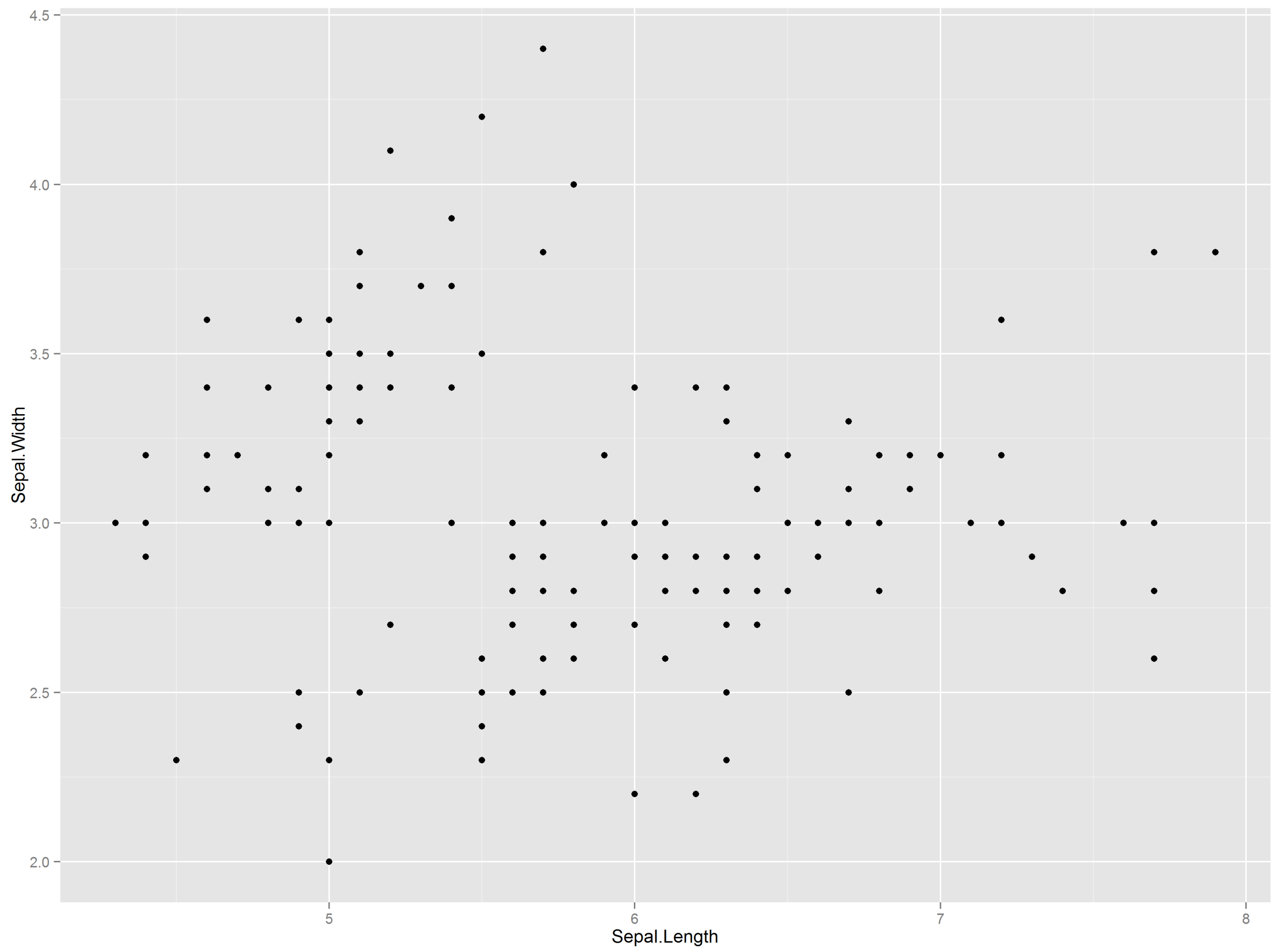
The first step in creating a plot is to add one or more layers. Let's start with the iris data set as an example. Note that *ggplot2* always requires the specification of the data frame from which the variables used in the plot are drawn.

```
    summary(iris)
#>   Sepal.Length    Sepal.Width     Petal.Length    Petal.Width          Species  
#>  Min.   :4.30   Min.   :2.00   Min.   :1.00   Min.   :0.1   setosa    :50  
#>  1st Qu.:5.10   1st Qu.:2.80   1st Qu.:1.60   1st Qu.:0.3   versicolor:50  
#>  Median :5.80   Median :3.00   Median :4.35   Median :1.3   virginica :50  
#>  Mean   :5.84   Mean   :3.06   Mean   :3.76   Mean   :1.2
#>  3rd Qu.:6.40   3rd Qu.:3.30   3rd Qu.:5.10   3rd Qu.:1.8
#>  Max.   :7.90   Max.   :4.40   Max.   :6.90   Max.   :2.5

    p <- ggplot(iris, aes(Sepal.Length, Sepal.Width) )
```

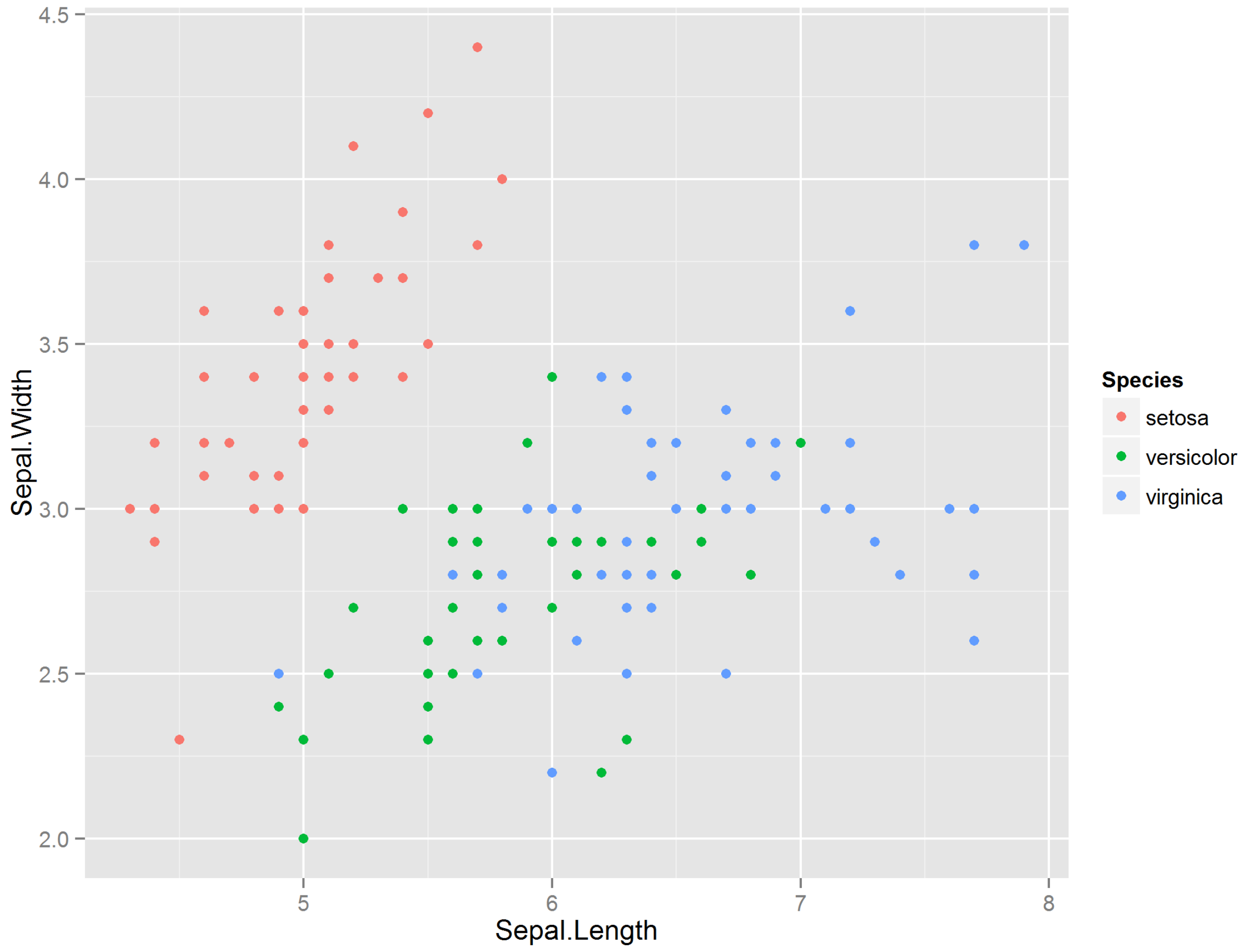
If you just type `p` or `print(p)`, you'll get back a warning saying that the plot lacks any layers. With the `ggplot()` function, we've set up a plot which is going to draw from the iris data, the Sepal.length variable will be mapped to the x–axis, and the Sepal.width variable is going to be mapped to the y–axis. However, we have not determined which kind of geometric object will represent the data. Let's add points, for a scatterplot.

```
p + geom_point()
```



Alternatively, this plot could have been produced with `qplot`. Additionally, you can map color to the species.

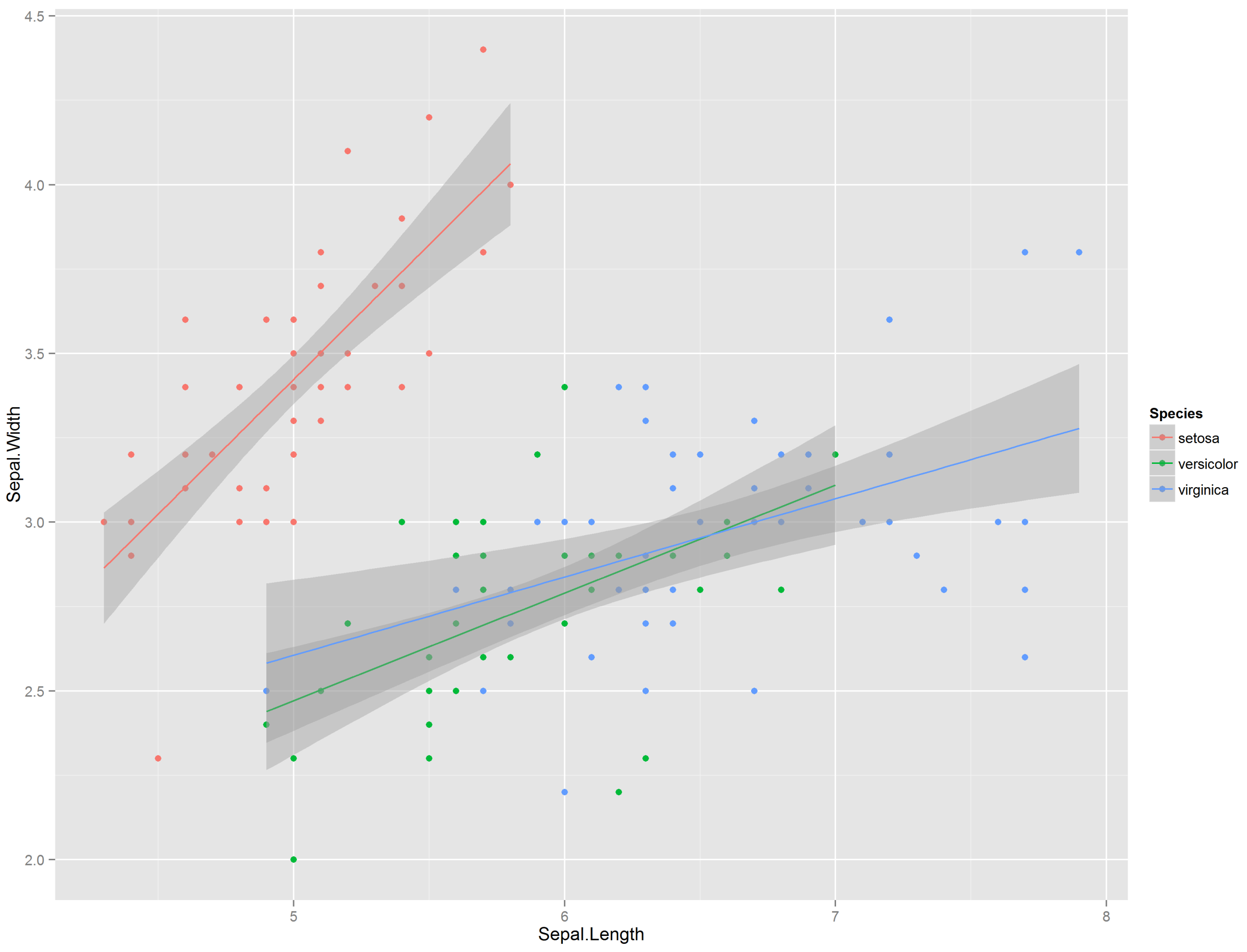
```
qplot(Sepal.Length, Sepal.Width, data = iris, color = Species)
```



We clearly see that the setosa plants have different Sepal.Length/Sepal.Width relationship compared to the other two species. The full documentation for *ggplot2* can be found at `http://docs.ggplot2.org/current/`. Apart from mapping data to aesthetics, *ggplot2* can handle statistical transformations of the data, i.e. easily create all the nice exploratory graphics we will look at below.

We will explore one of these transformations by adding a regression line to the data of each of the three plant species as a third layer.

```
ggsmooth <- (qplot(Sepal.Length, Sepal.Width, data = iris, color = Species)
+ stat_smooth(method = "lm"))
ggsmooth
```



The command `stat_smooth` first adds a statistical transformation to the existing data and then plots it using a certain geometry, in this case a special "smooth" geometry that is tailored to the plotting of regression fits. You can obtained the statistical transformations by looking at the saved plot and extracting the appropriate sublist.

```
transformed.data <- as.list(print(ggsmooth))$data[[2]]
```

Thus, you could also map the transformed data differently than the default geometry does it. This however does not make much sense in this case.

`qplot` and its most important options

`qplot` can be used much like plot, but has some additional features that are very useful, like facetting or coloring by condition. It represents an easy way to get started with *ggplot2*.

```
qplot(x, y = NULL, ..., data, facets = NULL, NA), ylim = c(NA, NA), log = "", main = NULL,
              xlab = deparse(substitute(x)), ylab = deparse(substitute(y)))
```

- `x:` x–axis data
- `y:` y–axis data (may be missing)
- `data:` `data.frame` containing the variables used in the plot
- `facets=` split the plot into facets, use a formula like . ~split to do wrapped splitting and row ~columns to split by rows and columns
- `main:` plot heading

- `color, fill` set to factor/string in the data set in order to color the plot depending on that factor. Use `I("colorname")` to use a specific color.
- `geom` specify a "geometry" to be used in the plots, examples include point, line, boxplot, histogram etc.
- `xlab, ylab, xlim, ylim` set the x–/y–axis parameters

Exercise: Plotting the normal density

The density of the normal distribution with expected value μ and variance σ^2 is given by:

$$f(x) = \frac{1}{\sigma^2\sqrt{\pi}} \exp\left(-\frac{1}{2}(\frac{x-\mu}{\sigma})^2\right)$$

In *R* it is implemented in the function `dnorm`.

(*a*) Call the *R* help to find out how to calculate density values.
(*b*) Determine the values of the standard normal distribution density ($\mu = 0$ and $\sigma^2 = 1$) at $-2, -1.8, -1.6, \ldots, +2$ and save it in a vector `stand.normal`.
(*c*) Plot the results obtained in the last exercise, play a bit with the plotting options!
(*d*) use `qplot` to produce the same plot and change the color of the density line using `color=I("darkgreen")`.

8 Calling functions and programming

8.1 Calling functions

Every *R*–function is following the pattern below:

```
function.name(arguments, optional arguments)
```

- `arguments`: Some function arguments are necessary to run the function
- `optional arguments`: Some function arguments can be changed, otherwise the default values are used. They are indicated by an equals sign.
- `?function.name`: Getting help
- `function.name`: Source code

As an example, look at the mean command:

```
mean(x, trim = 0, na.rm = FALSE)
```

- `x`: Data
- `trim = 0`: Trimmed mean (mean of the data without x% of extreme values)
- `na.rm = FALSE`: Remove missing values?

Here, `x` (usually a vector) has to be given in order to run the function, while the other arguments such as `trim` are optional, i.e. if you do not change them, their default values are used.

8.2 Creating your own functions

You can create your own functions very easily by adhering to the following template

```
function.name<-function(arguments, options) {
...
...
return(...)  }
```

- `{ }` : The source code of the function has to be in curly brackets
- By default *R* returns the result of the last line of the function, you can specify the return value directly with `return( )`. If you want to return multiple values, you can return a list.

As example, we look at the following currency converter function

```
euro.calc<-function(x, currency="US") {
  ## currency has a default argrument "US"
  if(currency=="US") return(x*1.33)
  if(currency=="Pounds") return(x*0.85)
}
euro.calc(100) ## how many dollars are 100 Euros?

#> [1] 133
```

Here `x` is a formal argument, necessary to execute the function. `currency:` is an optional argument, set to "US" by default.

8.3 Flow control

R offers the typical options for flow–control known from many other languages.

The most important one, the **if–statement** is used when certain computations should only be performed if a certain condition is met (and maybe something else should be performed when the condition is not met):

```
w= 3
        if( w < 5 ){
        d=2
        }else{
        d=10
        }
d

#> [1] 2
```

If you want do a computation for every entry of a list, you usually do the computations for one time step and then for the next and the next, etc. Because nobody wants to type the same commands over and over again, these computations are automated in **for–loops**. An example:

```
h <- seq(from = 1, to = 8)
s <- integer() # create empty integer vector
        for(i in 2:10)
        {
        s[i] <- h[i] * 10
        }
s

#>  [1] NA 20 30 40 50 60 70 80 NA NA
```

Another useful command is the **ifelse–command**, it replaces elements of a vector based on the evaluation of another logical vector of the same size. This is useful to replace missing values, or to binarize a vector.

```
s <- seq(from = 1, to = 10)
binary.s <- ifelse(s > 5, "high", "low")
binary.s

#>  [1] "low"  "low"  "low"  "low"  "low"  "high" "high" "high" "high" "high"
```

Exercise: Base calling errors

The function `readError(noBases)` simulates the base calling errors of a sequencing machine. The parameter `noBases` represents the number of positions in the genome sequenced and the function will return a vector, which has the entry "error" if a base calling error occurs at a certain position and "correct" if the base is read correctly. It can be obtained with the command

```
source("http://www-huber.embl.de/users/klaus/BasicR/readError.R")
```

(*a*) Let the sequencer read a thousand positions and try to infer a base calling error rate from this simulation HINT: The functions `table` and `prop.table` could be handy for this!
(*b*) Let us assume the technology improves and the machine is less prone to errors. Change the function accordingly!

9 Answers to exercises

Exercise: Simple R operations

Use the rep function to define simply the following vectors in *R*.

(*a*) `6,6,6,6,6,6`
(*b*) `5,8,5,8,5,8,5,8`
(*c*) `5,5,5,5,8,8,8,8`

Solution: Simple R operations

```
rep(6,6)
rep(c(5,8),4)
c(rep(5,4), rep(8,4))
```

Exercise: R as a calculator

Calculate the following expression, where `x` and `y` have values `-0.25` and `2` respectively. Then store the result in a new variable and print its content.

```
x + cos(pi/y)
```

Solution: R as a calculator

```
x <-  -0.25
y <- 2
x + cos(pi/y)
```

Exercise: milk sales

The `y<-c(33,44,29,16,25,45,33,19,54,22,21,49,11,24,56)` contain sales of milk in liters for 5 days in three different shops (the first 3 values are for shops 1,2 and 3 on Monday, etc.). Produce a statistical summary of the sales for each day of the week and also for each shop.

Solution: milk sales

```
y <- c(33,44,29,16,25,45,33,19,54,22,21,49,11,24,56)
# day of the week summary, example: Tuesday
Tuesday <- y[ (1:3) + 3 ]
summary(Tuesday)
## Shop 2 summary
Shop2 <- y[ seq(2, length(y), by = 3 )  ]
summary(Shop2)
```

Exercise: matrix operations

(*a*) Call `?matrix` to consult the *R* help on matrices.
(*b*) Create the variables $a = 3$ and $b = 4.5$.
(*c*) Test whether a and b are numeric or strings.
(*d*) Create the following matrices

$$A = \begin{pmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \\ 7 & 8 & 10 \end{pmatrix} \quad B = \begin{pmatrix} 1 & 4 & 7 \\ 2 & 5 & 8 \\ 3 & 6 & 9 \end{pmatrix} \quad y = \begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix}$$

(*e*) Calculate
- $a^2 + 1/b$
- $a * A$ Multiplication with a scalar
- $A * B$ Matrix multiplication (*R*–command `%*%`)
- Invert and transpose A. (*R*–commands `solve` and `t()`)
- Fill the first row of B with ones

(*f*) Access the second element of the third column of A and the third element of the second column of B.
(*g*) Multiply the first row of A with the second column of B.

Solution: matrix operations

```
#b
##########################################################################
a <- 3
b <- 4.5

#c
##########################################################################

is.numeric(a)
is.character(b)

#d
##########################################################################
```

```
A <- matrix(seq(1,9), nrow = 3, byrow = TRUE )
A[3,3] <- 10
#A<-matrix(c(1,2,3,4,5,6,7,8,10),nrow=3)

B <- matrix(seq(1,9), nrow = 3, byrow = FALSE)
#B<-matrix(c(1,2,3,4,5,6,7,8,10),nrow=3, byrow=TRUE)


y<-matrix(c(1,2,3), nrow=3)

#e
##########################################################################
a^2 + 1 /b
a*A
A %*% B

det(A)
#if the determinant of a matrix is zero, it cannot be inverted
solve(A)
t(A)

#f
##########################################################################

A[2,3]
B[3,2]

#g
##########################################################################

# element-wise
#A[1,]*B[,2]

# a^T * b
A[1,]%*%B[,2]

# b^T*a
fr.A <- as.matrix(A[1,])
sc.B <- as.matrix(t(B[,2]))

fr.A %*% sc.B
```

Exercise: Handling a small data set

(*a*) Read in the data set 'Patients.csv' from the website

http://www-huber.embl.de/users/klaus/BasicR/Patients.csv

(*b*) Check whether the read in data is actually a `data.frame`.
(*c*) Which variables are stored in the data frame and what are their values?
(*d*) Is there a missing weight value? If yes, replace it by the mean of the other weight values.

(*e*) Calculate the mean weight and height of all the patients.
(*f*) Calculate the BMI = Weight/Height^2 of all the patients. Attach the BMI vector to the data frame using the function `cbind`.

Solution: Handling a small data set

```r
#a
########################################################################

pat <- read.csv("http://www-huber.embl.de/users/klaus/BasicR/Patients.csv")
pat

#b
########################################################################

is.data.frame(pat)
summary(pat)
str(pat)

#c
########################################################################

head(pat)
pat
str(pat)
#d
########################################################################

summary(pat$Weight)
#There is a NA value, which is easy to spot, since the data set
# is really small!
#Otherwise, just use the which()-Funktion ...
which(is.na(pat$Weight))

## other NA methods
#?na.omit

## remove  NAs from Weight
na.omit(pat$Weight)

#e
########################################################################

#Pay attention to access the data set directly ...
pat[2,2] <- mean(pat$Weight, na.rm=TRUE)
pat


#f
########################################################################

BMI <- pat[,2] / pat[,1]^2
```

```
### alternatively

BMI = pat$Weight / pat$Height^2

pat$Weight[2] = mean(pat$Weight, na.rm=TRUE)

print(BMI)

### attach BMI to the data frame
pat <- cbind(pat, BMI)
pat
```

Exercise: Plotting the normal density

The density of the normal distribution with expected value μ and variance σ^2 is given by:

$$f(x) = \frac{1}{\sigma^2\sqrt{\pi}} \exp\left(-\frac{1}{2}(\frac{x-\mu}{\sigma})^2\right)$$

In *R* it is implemented in the function `dnorm`.

(*a*) Call the *R* help to find out how to calculate density values.
(*b*) Determine the values of the standard normal distribution density ($\mu = 0$ and $\sigma^2 = 1$) at $-2, -1.8, -1.6, \dots, +2$ and save it in a vector `stand.normal`.
(*c*) Plot the results obtained in the last exercise, play a bit with the plotting options!
(*d*) use `qplot` to produce the same plot and change the color of the density line using `color=I("darkgreen")`.

Solution: Plotting the normal density

```
x <- seq(from=-2, to=2, by=0.2)
length(x)
x
stand.normal <- dnorm(x, mean=0, sd=1)
# or: stand.normal<-dnorm(x)
length(stand.normal)
stand.normal

#visualize it
#
plot(x,stand.normal, type="l")

plot(x,stand.normal, type="b")
plot(x,stand.normal, type="h", col = "darkgreen")
plot(x,stand.normal, type="h", col = "darkgreen", main = "Standard Normal Density")

# use qplot
qplot(x, stand.normal, color = I("darkgreen"))
```

Exercise: Base calling errors

The function `readError(noBases)` simulates the base calling errors of a sequencing machine. The parameter `noBases` represents the number of positions in the genome sequenced and the function will return a vector, which has the entry "error" if a base calling error occurs at a certain position and "correct" if the base is read correctly. It can be obtained with the command

```
source("http://www-huber.embl.de/users/klaus/BasicR/readError.R")
```

(*a*) Let the sequencer read a thousand positions and try to infer a base calling error rate from this simulation HINT: The functions `table` and `prop.table` could be handy for this!

(*b*) Let us assume the technology improves and the machine is less prone to errors. Change the function accordingly!

Solution: Read errors

```
#a
########################################################################

source("http://www-huber.embl.de/users/klaus/BasicR/readError.R")

test <- readError(1000)
## number of errors
sum(test == "error")
##  error probability
sum(test == "error") / 1000

prop.table(table(test))


#b
########################################################################
readError2 <- function(noBases){

  positions <- integer(noBases) ## initialize vector
                for(i in 1:noBases){
                positions[i] <- rbinom(n=1, size = 1, prob = 0.05)
                }
  return(ifelse(positions, "correct", "error"))
        }



### equivalent function
rbinom(n=1000, size =1, prob = 0.05)
```

Session Info

```r
toLatex(sessionInfo())
```

- R version 3.2.0 (2015-04-16), `x86_64-w64-mingw32`
- Locale: `LC_COLLATE=English_United States.1252`, `LC_CTYPE=English_United States.1252`, `LC_MONETARY=English_United States.1252`, `LC_NUMERIC=C`, `LC_TIME=English_United States.1252`
- Base packages: base, datasets, graphics, grDevices, methods, parallel, stats, utils
- Other packages: Biobase 2.28.0, BiocGenerics 0.14.0, BiocInstaller 1.18.1, dplyr 0.4.1, ggplot2 1.0.1, knitr 1.10, magrittr 1.5, mgcv 1.8-6, multtest 2.24.0, nlme 3.1-120, plyr 1.8.2, reshape2 1.4.1, rJava 0.9-6, stringr 0.6.2, TeachingDemos 2.9, tidyr 0.2.0, xlsx 0.5.7, xlsxjars 0.6.1
- Loaded via a namespace (and not attached): assertthat 0.1, BiocStyle 1.6.0, codetools 0.2-11, colorspace 1.2-6, DBI 0.3.1, digest 0.6.8, evaluate 0.7, formatR 1.2, grid 3.2.0, gtable 0.1.2, highr 0.5, labeling 0.3, lattice 0.20-31, lazyeval 0.1.10, MASS 7.3-40, Matrix 1.2-0, munsell 0.4.2, proto 0.3-10, R6 2.0.1, Rcpp 0.11.5, scales 0.2.4, splines 3.2.0, stats4 3.2.0, survival 2.38-1, tools 3.2.0