Applied Methods in Statistics

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Chapter 1

Practical Information

Exercises in this site is relevant for Stat340 course which discusses some of the applied topics in statistics. For the exercises, we will use open source R statistical software along with RStudio, an integrated development environment for R. We advise student to install the latest version of R and RStudio on their laptop computer. In addition, we will use few packages in R which we will discuss during the exercise period. Students are highly encouraged to complete these exercises on their own and also participate in Group Exercises. Follow the link below to install R and RStudio.

Install R and Install RStudio

See: Lecture and Exercise Plan and Reference Books

Lecture and Exercise Plan

Week	Topics	Exercises
Week 6 (Feb. 05)	Overview, R and R Studio	Getting Started
Week 7 (Feb. 12)	Regression Analysis	Exercise 1
Week 8 (Feb. 19)	Analysis of Variance	Exercise 2
Week 9 (Feb. 26)	Principal Component Analysis	Exercise 3
Week 10 (Mar. 05)	Multivariate Statistics (PCR, PLS)	Exercise 4
Week 11 (Mar. 12)	Cluster Analysis	Exercise 5
Week 12 (Mar. 19)	Classification	Exercise 6
Week 14 - 15 (Apr. 2, Apr. 9)	Generalized Linear Models	Exercise 7-8
Week 16 (Apr. 16)	Random Effects Models	Exercise 9
Week 17 (Apr. 23)	Mixed Effects Models	Exercise 10

See: Practical Information | Reference Books

Reference Books

See: Practical Information | Lecture and Exercise Plan

Chapter 2

Getting Started

In this secion, we will dive into R and RStudio and get used to with it to some extent. We will continue learning about R and RStudio as we go on. R is an open source programming language basically used in data analysis. In R there are many packages that are created for specific purposes and they have made R rich and powerful. In this course, apart from default R package (that is installed and already loaded), we will use few other packages which we will install and load as we go through our exercises. We can use following command to install a package. Below, a `car` package is used as an example:

```
install.packages("car")
```

To load the package we use `library` function as,

```
library(car)
```

Following screenshot help you to install package using RStudio IDE,

Exercise 1: Create New Project

Creating a project allows us to organize the files and related materials during our study. File => New Project opens a window to create new project. It will be easier to access all the resources, if all the scripts and datasets are within a main folder, i.e. the project folder.

The examples in this exercise uses the project folder as the main folder. Although it is not necessary, but throughout the exercises we will use `_data` folder as a folder containing all

the data that we are using in the course.

Exercise 2: Importing data in R

The usual data sources can be a text file in `txt` or `csv` format or spreadsheet(excel) file in `xls` or `xlsx`. Data and R-objects can also be imported from `rds`, `rda` or `rdata`. Below, we will discuss these in detail. In addition you can also find some animated images showing how we can import data in RStudio for each of these file formats.

Import `txt` or `csv`

Base R-package has `read.table` and `read.csv` for importing a text or comma separated file (csv) files. Download `bodydata.txt` and to import it in R as,

```
bodydata <- read.table("_data/bodydata.txt", header = TRUE)
```

Here the argument `header` is `TRUE` if the data has header in its first row. The argument `sep` takes `\t`, `,` or `;` based on if the columns in the text data are tab-separated, comma-separated or separated by semi-colons. If the decimal values in the data are represented by `,`, the `dec` argument takes the value `,`. For further help see: `?read.table`

Import Microsoft Excel spreadsheet

An R-package `readxl` helps to import excel file. If it is not installed, you should install it as,

```
install.packages("readxl")
```

Download `bodydata.xlsx` from canvas and load it to R as,

```
library(readxl)
bodydata <- read_excel("_data/bodydata.xlsx", sheet = 1)
```

For further help and arguments on this function load the library as `library(readxl)` and see: `?read_excel` or `?read_xlsx`.

Load `rdata`, `rda` or `rds`

One can save data, models and other R-objects in `rdata` or `rds` format. In order to load `rdata`, we can use `load` function. Download `bodydata.rdata` from canvas and load it to R.

```
load("_data/bodydata.rdata")
```

Reading data from clipboard ("pasting" copied data into an R object)

You can import data in clipboard in R. For example the data you copied in Excel or Word files.

```
bodydata <- read.table(file = "clipboard", header = TRUE)
```

In Mac, you need to do,

```
bodydata <- read.table(file = pipe("pbpaste"), header = TRUE)
```

This allows us to get the data from anywhere just after they are copied.

After every import in above examples, we have saved our imported data in `bodydata` variable. This an R-object that holds any kind of data-structures such as `matrix`, `data.frame`, `list` or fitted models. We can find these R-objects in "Environment" tab in RStudio.

Exercise 3: Exporting data to a file

To export an r-object to a file, `write.table` function is used. For example, we can export the `bodydata` table we just imported as a text file named `bodydata-export.txt` as,

```
write.table(bodydata, file = "_data/bodydata-export.txt",
            row.names = FALSE, quote = FALSE)
```

We can also use `write.csv` function to export the data in `csv` format. The `txt` and `csv` file format only holds data in tabular structures. Sometimes we need to save other R-objects

such as fitted models or list for which we can use `Rdata` format. We can save our `bodydata` objects in `Rdata` format as,

```
save(bodydata, file = "_data/bodydata-export.rdata")
```

This will export bodydata object to a file named `bodydata-export.rdata` in `_data` folder in your project directory.

Exercise 4: Data Structure in R

The dataset we imported in Exercise 2: Importing data in R is a data frame. DataFrame is a structure that R uses to keep the data in that particular format. If you do `class(bodydata)` for the data we have imported before, we can see `data.frame` as its class. There are other data structures in R. Some basic structure that R uses are discussed below:

Vector

A vector is a one-dimensional object where you can store elements of different modes such as "logical" (TRUE or FALSE), "integer", "numeric", "character" etc. All elements of a vector must be of same mode. For example,

```
x <- c(TRUE, FALSE, FALSE, TRUE, TRUE)
y <- c("TRUE", "FALSE", "Not Sure")
z <- c(2, 3, 5, 6, 10)
```

Here, `x`, `y` and `z` are of class logical, character and numeric respectively. Although in vector `y` we have `TRUE` and `FALSE` they are in `character` format. The function `c` is used to define a vector. However functions that are used to create sequences also gives us a vector. For example,

```
(a_sequence <- seq(from = 0, to = 10, by = 2))
```

```
[1]  0  2  4  6  8 10
```

```
(b_sequence <- 1:10)
```

```
 [1]  1  2  3  4  5  6  7  8  9 10
```

Here both `a_sequence` and `b_sequence` are vector. Give special attention to the way we have created the sequence of numbers. It will be useful in many situations in future exercises.

Matrix

A matrix is a two dimensional structure with row and column. As this is an extension of vector structure, matrix must have elements of same mode as in a vector. For example:

```
(a_matrix <- matrix(1:25, nrow = 5, ncol = 5))
```

```
     [,1] [,2] [,3] [,4] [,5]
[1,]    1    6   11   16   21
[2,]    2    7   12   17   22
[3,]    3    8   13   18   23
[4,]    4    9   14   19   24
[5,]    5   10   15   20   25
```

```
(b_matrix <- diag(1:5))
```

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

Here, `a_matrix` is created from a vector of sequence of 1 to 25 in 5 rows and 5 columns. We can also define a diagonal matrix as `b_matrix` with numbers from 1 to 5 in its diagonal.

Array

An array is an extension of Matrix structure in three or more dimension. We can define an array as,

```
(an_array <- array(1:24, dim = c(2, 4, 3)))
```

```
, , 1
```

```
     [,1] [,2] [,3] [,4]
[1,]    1    3    5    7
[2,]    2    4    6    8

, , 2

     [,1] [,2] [,3] [,4]
[1,]    9   11   13   15
[2,]   10   12   14   16

, , 3

     [,1] [,2] [,3] [,4]
[1,]   17   19   21   23
[2,]   18   20   22   24
```

List

All the above structure we discussed require that the the elements in them to be of same mode such as `numeric`, `character` and `logical`. Sometimes it is necessary to keep objects of different modes in same place. List is a structure that helps in such situation. A list can contain `list`, `matrix`, `vector`, `numeric` or any other data structure as its elements. For example:

```
a_list <- list(
  a_matrix = matrix(1:6, nrow = 2, ncol = 3),
  a_vector = 2:7,
  a_list = list(a = 1, b = 3:6),
  a_logical = c(TRUE, FALSE, TRUE, NA)
)
a_list
```

```
$a_matrix
     [,1] [,2] [,3]
[1,]    1    3    5
```

```
[2,]    2    4    6

$a_vector
[1] 2 3 4 5 6 7

$a_list
$a_list$a
[1] 1

$a_list$b
[1] 3 4 5 6


$a_logical
[1]  TRUE FALSE  TRUE    NA
```

In above example, `a_list` contains a matrix, a numeric vector, a list and a logical vector.

Data Frame

Data Frame is a list kept in tabular structure. Every column of a data frame has a name assigned to it. The `bodydata` dataset we have imported is an example of data frame. Data frame is the most used data structure to keep data in tabular format. Lets create a data frame:

```
a_dataframe <- data.frame(
  character = c("a", "b", "c"),
  numeric = 1:3,
  logical = c(TRUE, FALSE, NA)
)
a_dataframe
```

```
  character numeric logical
1         a       1    TRUE
2         b       2   FALSE
3         c       3      NA
```

Every column of a data.frame is a vector. Different columns of a data frame can contain element of different modes. For example: the first column can be a character vector while the second column can be a numeric vector as in the example above.

Exercise 5: Exploring the data

Structure of an R-object

The first command you need to learn is `str` function in order to explore any object in R. Lets apply this to our `bodydata`,

```
str(bodydata)
```

```
'data.frame':   407 obs. of  4 variables:
 $ Weight       : num  65.6 80.7 72.6 78.8 74.8 86.4 78.4 62 81.6 76.6 ...
 $ Height       : num  174 194 186 187 182 ...
 $ Age          : num  21 28 23 22 21 26 27 23 21 23 ...
 $ Circumference: num  71.5 83.2 77.8 80 82.5 82 76.8 68.5 77.5 81.9 ...
```

This output shows us that `bodydata` is a `data.frame` with 407 rows and 4 numeric variables - Weight, Height, Age, Circumference.

Accessing elements from R-objects

Different data structure have different way of accessing elements from them.

Extracting elements from `vector`, `matrix` and `array`

For vector, matrix and arraywe can use `[` for accessing their elements. Lets create a vector, a matrix and an array as follows,

```
a_vector <- c("one", "two", "three", "four", "five")
a_matrix <- matrix(1:24, nrow = 3, ncol = 8)
an_array <- array(1:24, dim = c(2, 3, 4))
```

Extracting element at position 3 to 5 in `a_vector` `a_vector[3:5]` with give three, four, five, the elements at postion index 3, 4, and 5. In R, position index starts from 1.

Extracting element in rows 2, 3 and columns 2, 4, 6, 8 from `a_matrix` This is a two dimensional structure, we give row-index and column-index inside `[` operator separated by comma as,

```
a_matrix[c(2, 3), c(2, 4, 6, 8)]
```

```
     [,1] [,2] [,3] [,4]
[1,]    5   11   17   23
[2,]    6   12   18   24
```

We can also write this as,

```
a_matrix[2:3, seq(from = 2, to = 8, by = 2)]
```

```
     [,1] [,2] [,3] [,4]
[1,]    5   11   17   23
[2,]    6   12   18   24
```

Here `seq(from = 2, to = 8, by = 2)` create sequence even integer from 2 to 8 which is used as column index for extracting elements from `a_matrix`.

Extracting first element of `an_array`: Here `an_array` is an array structure of dimension three. So, we have to use three index vector inside `[` operator in order to extract element from it. For instance `an_array[1, 1, 1]` gives 1 as its first element of the array.

In all these structures we can only supply index of one or more dimension. For example, `a_matrix[1:2,]` where we have only mentioned the row index, will give elements in *first* and *second* row from all columns. i.e.

```
a_matrix[1:2, ]
```

```
     [,1] [,2] [,3] [,4] [,5] [,6] [,7] [,8]
[1,]    1    4    7   10   13   16   19   22
[2,]    2    5    8   11   14   17   20   23
```

Extracting elements from `data.frame` and `list`

Lets create a `data.frame` and a `list` as,

```
a_dataframe <- data.frame(
  fertilizer = c("Low", "Low", "High", "High"),
  yield = c(12.5, 13.1, 15.3, 16.2)
)
a_list <- list(
  facebook = data.frame(
    name = c("Gareth", "Raju", "Marek", "Franchisco"),
    has_profile = c(TRUE, TRUE, FALSE, TRUE)
  ),
  twitter = c("@gareth", "@raju", "@marek", "franchisco")
)
```

Extracting third and fourth row of `fertilizer` from `a_dataframe` Same as extracting elements as matrix as discussed above we can use row and column index as `a_dataframe[3:4, 1]`. We have used `1` in place of column index since `fertilizer` is in first column. We can also use name instead as `a_dataframe[3:4, "fertilizer"]`.

```
a_dataframe[3:4, "fertilizer"]
```

```
[1] High High
Levels: High Low
```

Extracting first element of `a_list` We can use `[[` for extracting elements from `a_list`. For example `a_list[[1]]` will give the first element of the list. Here in our list we have two elements with names `facebook` and `twitter`. So, we can also use their names as `a_list[["facebook"]]` which is not possible if they do not have any name.

```
a_list[["facebook"]]
```

```
        name has_profile
1     Gareth        TRUE
2       Raju        TRUE
3      Marek       FALSE
4 Franchisco        TRUE
```

We can also use `$` operator to extract elements from named list and a data frame. For example, `bodydata$Weight` extracts `Weight` variable from `bodydata` dataset.

View Data in RStudio

Newer version of RStudio support viewing data in different structures. To view `bodydata` we have imported in Exercise 2: Importing data in R, we can use `View(bodydata)`. If you have not imported the, you need to follow the exercise and import the data first. We can also click the data in "Environment" tab to view it.

Summary of data

We can compute basic descriptive summary statistics using `summary` function as,

```
summary(bodydata)
```

```
     Weight          Height          Age        Circumference
 Min.   : 42.0   Min.   :150   Min.   :18.0   Min.   : 57.9
 1st Qu.: 58.5   1st Qu.:164   1st Qu.:23.0   1st Qu.: 68.0
 Median : 68.6   Median :171   Median :27.0   Median : 75.6
 Mean   : 69.2   Mean   :171   Mean   :29.9   Mean   : 76.9
 3rd Qu.: 78.8   3rd Qu.:178   3rd Qu.:35.0   3rd Qu.: 84.3
 Max.   :108.6   Max.   :198   Max.   :67.0   Max.   :113.2
```

Dimension of data

The number of elements in a data structure like vector and list we can use `length` function. For example: if we extract `Weight` variable from `bodydata` we will get a numeric vector. The length of this vector is,

```
length(bodydata$Weight)
```

A multi-dimensional data structure like matrix, array and data frame has dimension. We can use `dim` function to find the dimension.

```
dim(bodydata)
```

```
[1] 407   4
```

Here, the first and second item refers to the number of rows and number of columns of bodydata. Similarly, we can use `nrow(bodydata)` and `ncol(bodydata)`to obtain these

number individually.

Lets Practice

1) Take a look at the top 5 rows of `bodydata`
2) Take a look at the top 5 rows of `Height` and `Circumference` variables of `bodydata`
3) Apply `summary` function on `Age` variable of `bodydata`

Exercise 6: Subsets of data and logical operators

Logical vector and index vector

A lot of times we want to get a subset of data filtering rows or columns of a dataframe. For which we can perform logical test and get `TRUE` or `FALSE` as result. This vector of logical can then be used to subset the observations from a dataframe.

For example, Lets extract observation from `bodydata` with Weight greater than 80. You might be wondering why following code does not work,

```
isHeavy <- Weight > 80
```

```
Error in eval(expr, envir, enclos): object 'Weight' not found
```

But remember that, the variable `Weight` is a part of `bodydata`. We have to extract `Weight` from the `bodydata` first. In R, `with` and `within` function helps you in this respect. In the following code, `with` function goes inside `bodydata` and execute the expression `Weight > 80`.

```
isHeavy <- with(bodydata, Weight > 80)
```

Here the logical vector `isHeavy` is computed by performing a logical operation on `Weight` variable within `bodydata`. The same operation can be done as,

```
isHeavy <- bodydata$Weight > 80
```

Take a look at this variable, what is it? :

```
head(isHeavy)
```

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

Yes, it is a vector of `TRUE` and `FALSE` with same length as `Weight`. Here the condition has compared each element of `Weight` results `TRUE` if it is greater than 80 and `FALSE` if it is less than 80.

Identify the elements We can identify which observations that are heavy by the `which()` function

```
HeavyId <- which(isHeavy)
```

This will return a vector of row index for the observations that are heavy, i.e. greater than 80. So how many are heavy? To find the size of a vector we can use `length` function.

```
length(HeavyId)
```

```
[1] 94
```

Here, 94 observations have Weight larger than 80.

Exercise

1) Identify who are taller than 180 and save this logical vector as an object called `isTall`.

```
isTall <- with(bodydata, Height > 180)
```

2) How many observations have height taller than 180?

```
TallId <- which(isTall)
length(TallId)
```

```
[1] 76
```

3) How many observations are both tall and heavy? Here, you can use `length` function as above to find how many person are taller than 180.

```
isBoth <- isHeavy * isTall
```

How is this computation done? Here `isHeavy` and `isTall` contains `TRUE` and `FALSE`. The multiplication of logical operator results a logical vector with `TRUE` only if both the vectors are `TRUE` else `FALSE`.

Alternatively :

```
isBoth <- which(isHeavy & isTall)
```

The `&` operator result `TRUE` if both `isHeavy` and `isTall` are `TRUE` else, `FALSE` which is same as previous.

Subsetting data frame

Example 1

Lets create a subset of the data called `bodydataTallAndHeavy` containing only the observations for tall and heavy persons as defined by isBoth.

```
bodydataTallAndHeavy <- bodydata[isBoth, ]
```

For other logical tests see help file `?Comparison`

Example 2

Lets create a random subset of 50 observations. For this we first sample 50 row index randomly from all rows in `bodydata`. The `sample` function is used for the purpose. In the following code, `nrow(bodydata)` return the number of rows in `bodydata`. The `sample` function takes two argument `x` which can be a vector or a integer and `size` which is the size of the sample to be drawn.

```
idx <- sample(x = nrow(bodydata), size = 50)
```

Here, 50 rows are sampled from the total number of rows and the index of the selected rows are saved on vector `idx`.

Using this vector we can select the observations in `bodydata` to create a new data set called `bodydataRandom` as,

```
bodydataRandom <- bodydata[idx, ]
```

Here is the first five rows of `bodydataRandom` dataset.

```
head(bodydataRandom, n = 5)
```

```
    Weight Height Age Circumference
215   77.7    176  27          85.8
280   83.0    176  22          85.0
315   75.7    174  47          83.0
325   45.9    155  48          63.0
189   73.6    175  60          90.5
```

Exercise

Create a subset of dataset `bodydata` including the observation with `Age` larger an 55 and `Circumference` larger than 80. Save this dataset named `subdata`.

```
idx <- with(bodydata, Age > 55 & Circumference > 80)
subdata <- bodydata[idx, ]
subdata
```

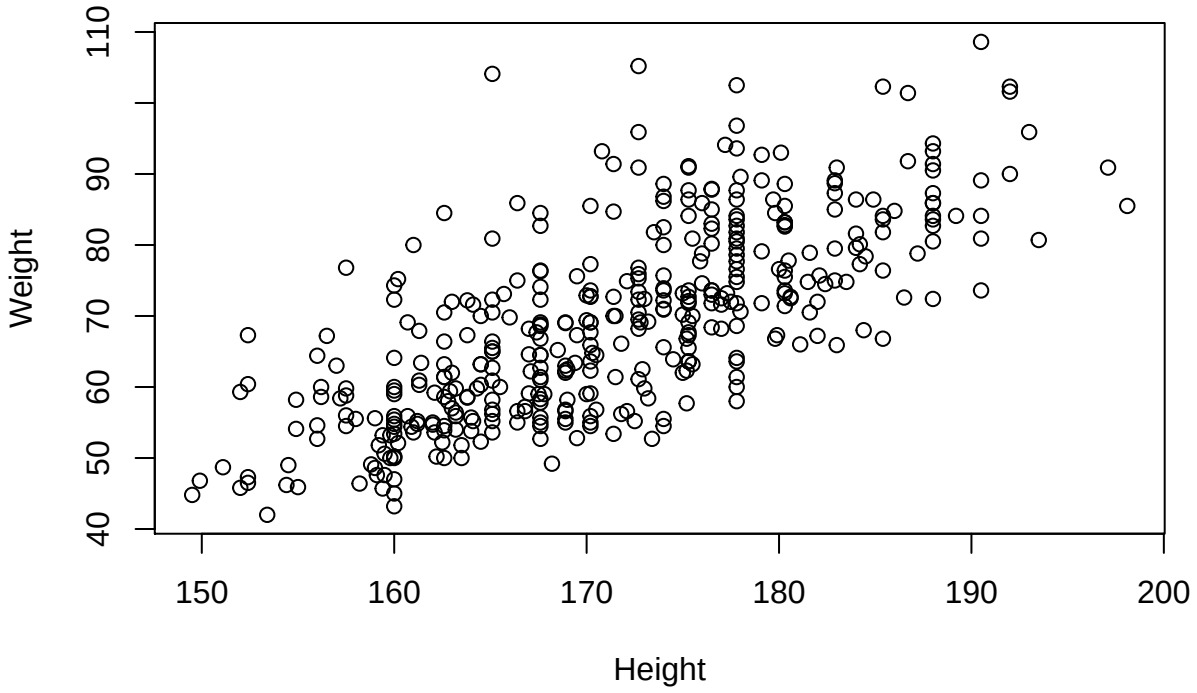
```
    Weight Height Age Circumference
136   76.4    185  62          94.8
189   73.6    175  60          90.5
207   66.8    168  62          81.5
231   80.0    174  65          98.6
```

For those who are interested in playing more with data, have a look at http://r4ds.had.co.nz/transform.html

Exercise 7: Graphics

Plot the heights versus the weights for all observations in bodydata.

```
with(bodydata, plot(x = Height, y = Weight))
```



Spice up the plot

Check out the presentation for lesson 1 to see how to spice up the plot

Explore the `?par` help file

Use the `isBoth` variable to create a color vector

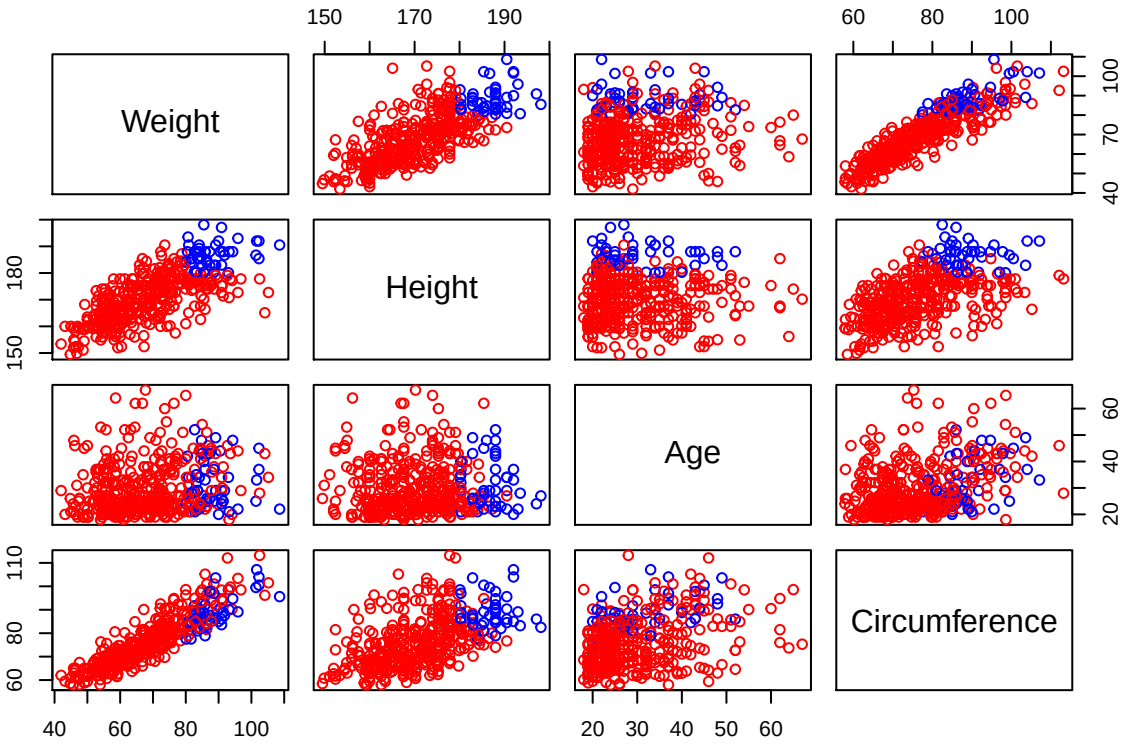
```
mycolors <- ifelse((isHeavy & isTall), "blue", "red")
```

Here, `isHeady & isTall` returns a logical vector. The `ifelse` function returns `blue` if `TRUE`and `red` if `FALSE` for each elements of the logical vector. The colors are then used in the plot so that all the Heavy and Tall person will be colored "blue" and rest as "red".

Use "`mycolors`" in the `col` argument of the plot function to mark the tall and heavy individuals

Plot all variables against each other

```
pairs(bodydata, col = mycolors)
```



Which variables seem to be most correlated to each other?

Here, `Weight` and `Circumference` seems to have highest correlation.

Which variables are least correlated to each other?

`Age` and `Height` variables seems to have least correlation.

Check by,

```
cor(bodydata)
```

```
              Weight Height    Age Circumference
Weight         1.000 0.7208 0.1870         0.899
Height         0.721 1.0000 0.0482         0.545
Age            0.187 0.0482 1.0000         0.355
Circumference  0.899 0.5448 0.3547         1.000
```

This returns the correlation matrix for the variables, and the guess made earlier true. Further, check out the help file for pairs, and the examples at the end. Try to make a pairs plot with scatter plots with smoothed lines in the lower left triangle, histograms on the diagonal, and correlation numbers in the upper right triangle.

Lets first create a function which create histogram. The function will later be used in the `pairs` function to create its diagonal plots.

```
panel.hist <- function(x, ...) {
    usr <- par("usr"); on.exit(par(usr))
    par(usr = c(usr[1:2], 0, 1.5) )
    h <- hist(x, plot = FALSE)
    breaks <- h$breaks; nB <- length(breaks)
    y <- h$counts; y <- y/max(y)
    rect(breaks[-nB], 0, breaks[-1], y, col = "cyan", ...)
}
```

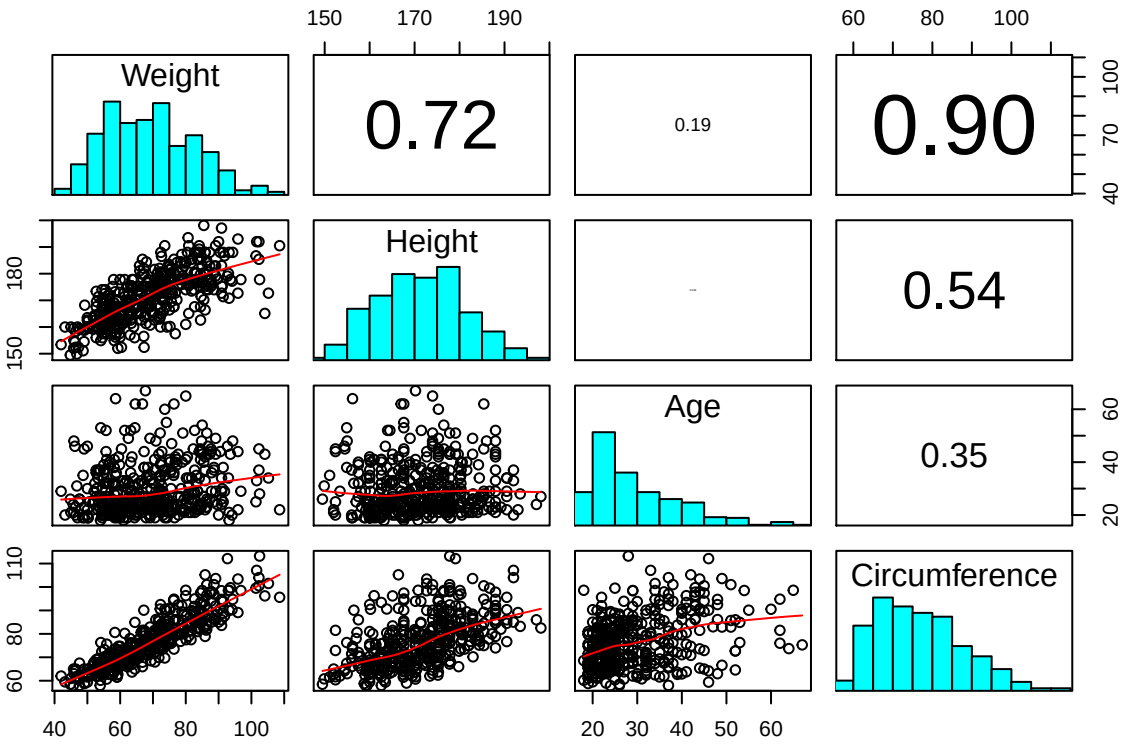
Now, create a function that will display correlation on `pairs` plot.

```
panel.cor <- function(x, y, digits = 2, prefix = "", cex.cor, ...) {
    usr <- par("usr"); on.exit(par(usr))
    par(usr = c(0, 1, 0, 1))
    r <- abs(cor(x, y))
    txt <- format(c(r, 0.123456789), digits = digits)[1]
    txt <- paste0(prefix, txt)
    if (missing(cex.cor)) cex.cor <- 0.8 / strwidth(txt)
    text(0.5, 0.5, txt, cex = cex.cor * r)
}
```

Now, the above functions are implemented on the `pairs` plot,

```
pairs(bodydata,
      lower.panel = panel.smooth,
```

```
      upper.panel = panel.cor,
      diag.panel = panel.hist)
```



Here the `panel.smooth` deals with the smooth line on the lower panel of `pairs` plot.

Note:: Chapter 5 of the R book contains numerous examples of graphics. **Note::** For those interested in playing around with plots in R checkout: http://r4ds.had.co.nz/data-visualisation.html

Chapter 3

Regression Analysis

In this exercise we will use `birth.rdata` and `bodydata.rdata` datasets. We can load those data as below:

```
load("_data/birth.rdata")
load("_data/bodydata.rdata")
load("_data/mtcars.rdata")
```

Least Sqaures App

Play around with the least squares app on Play around with the least squares app on http://solve.shinyapps.io/LeastSquaresApp

1. Use `N=10`
2. Try to adjust manually the intercept and the slope to minimize the sum of squared errors, `K`.
3. Display the least square estimate to see how close you were.
4. Display the true model. Were you close?

Once Again,

1. Increase to `N=100`
2. Repeat the procedure.
3. Are you closer to the true model now?

Dataset: birth

The dataset `birth` records 189 birth weights from Massachusetts, USA, and some additional variables. The variables are,

Var	Description
`LOW`	Equals `YES` if birth weight is below 2500g and `NO` otherwise.
`AGE`	Age of the mother in years.
`LWT`	Weight in pounds of mother.
`SMK`	`YES` if mother smokes and `NO` otherwise.
`BWT`	Birth weight in g (RESPONSE).

The data appears in fronter as `birth.rdata`. Download the data into your STAT340 course folder and load the data set in RStudio.

Overview of data

- Take a look at the top 10 rows of the data using the `head()` function

```
head(birth, n = 10)
```

```
   LOW AGE LWT SMK  BWT
1  YES  28 120 YES  709
2  YES  29 130  NO 1021
3  YES  34 187 YES 1135
4  YES  25 105  NO 1330
5  YES  25  85  NO 1474
6  YES  27 150  NO 1588
7  YES  23  97  NO 1588
8  YES  24 128  NO 1701
9  YES  24 132  NO 1729
10 YES  21 165 YES 1790
```

- Use the `summary()` function to get a short summary of the variables.

```
summary(birth)
```

```
 LOW          AGE             LWT        SMK          BWT
NO :130   Min.   :14.0   Min.   : 80   NO :115   Min.   : 709
YES: 59   1st Qu.:19.0   1st Qu.:110   YES: 74   1st Qu.:2414
          Median :23.0   Median :121             Median :2977
          Mean   :23.2   Mean   :130             Mean   :2945
          3rd Qu.:26.0   3rd Qu.:140             3rd Qu.:3475
          Max.   :45.0   Max.   :250             Max.   :4990
```

- What is the proportion of smoking mothers in the data set?

The proportion of smoking mother is 0.39

- What is the average age of a mother giving birth?

The average age of mother giving birth is 23.2 years.

- What is the average birth weight of children from non-smoking and smoking mothers?

```
tapply(birth$BWT, INDEX = birth$SMK, FUN = mean)
```

```
  NO  YES
3055 2773
```

The function returns the mean birth weight for children of non-smoking and smoking mothers.

- What is the standard deviation of birth weight of children from non-smoking and smoking mothers?

```
tapply(birth$BWT, INDEX = birth$SMK, FUN = sd)
```

```
 NO YES
752 660
```

The `sd()` function computes the sample standard deviation of a vector of observations.

Linear Regression

Run a simple linear regression model with BWT as response and LWT as predictor, like this,

```
birth1 <- lm(BWT ~ LWT, data = birth)
summary(birth1)
```

```
Call:
lm(formula = BWT ~ LWT, data = birth)

Residuals:
    Min      1Q  Median      3Q     Max
-2192.2  -503.6    -3.9   508.3  2075.5

Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept)  2369.67     228.43   10.37   <2e-16 ***
LWT             4.43       1.71    2.59     0.01 *
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

s: 718 on 187 degrees of freedom
Multiple R-squared: 0.0345,
Adjusted R-squared: 0.0294
F-statistic: 6.69 on 1 and 187 DF,  p-value: 0.0105
```

Here, the regression model is,

$$\text{BWT} = \beta_0 + \beta_1 \text{LWT} + \epsilon$$

where $\epsilon \sim N(0, \sigma^2)$

Test the significance of LWT on BWT with a 5% test level and at a 1% level

What is the hypothesis you are testing?

The hypothesis for testing the significance of LWT on BWT is,

$$H_0 : \beta_1 = 0 \text{ vs } H_1 : \beta_1 \neq 0$$

- What is the conclusion?

The p-value corresponding to β_1 is less than 0.05 but greater than 0.01. So, at 5% test level, LWT is significant while at 1% test level, it is not significant.

- Find the R-squared. Do you think the model fits the data well?

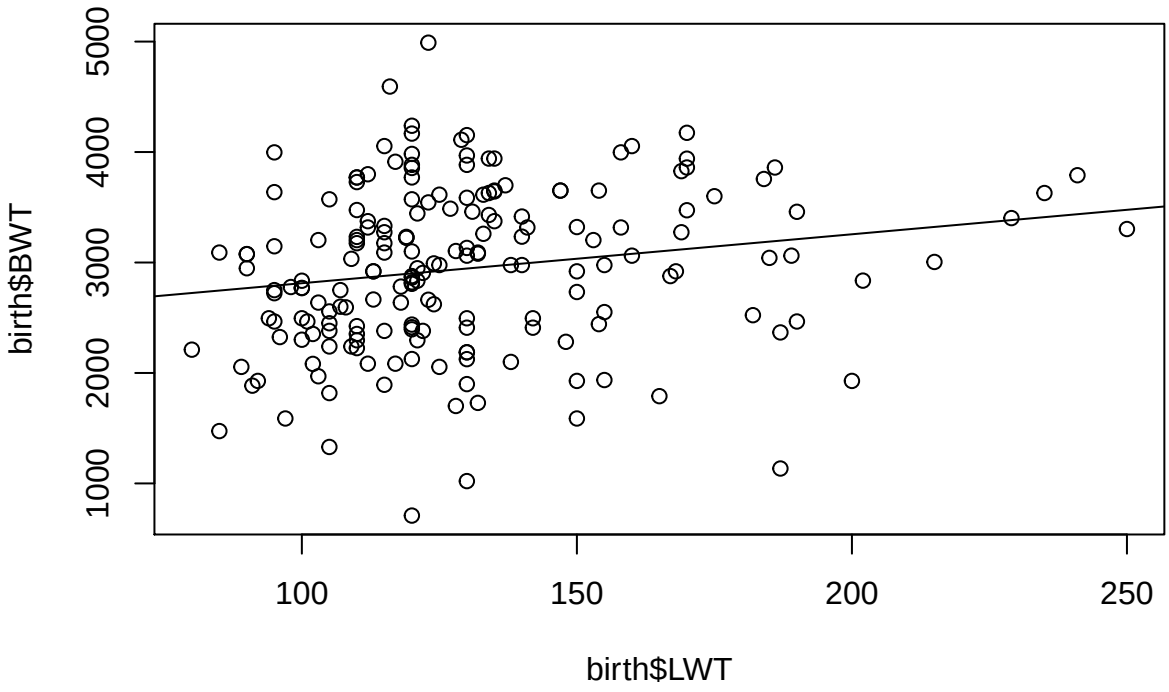
The r-squared (R^2) for the model is 0.03, this shows that only 3% of variation present in birth weight (BWT) is explained by weight of mother (LWD). Here, the model fits the data poorely.

Scatter Plot

- Make a scatter plot of LWT vs BWT

The scatter plot of LWT and BWT is,

```
plot(x = birth$LWT, y = birth$BWT)
abline(birth1)
```



- Make a comment to the plot in light of the output of your analyses.

1. The intercept for the regression line is 2369.67 and the slope is 4.43.
2. The data-points are scattered around the regression line where BWT vary most
3. Since the data-points are scattered much, the model could only explain small variation present in BWT with LWT.

Confidence Intervals

- Find 95% confidence intervals for the regression coefficients of the `birth1` model

```
confint(birth1)
```

```
                2.5 %  97.5 %
(Intercept) 1919.04 2820.30
LWT            1.05    7.81
```

- Also find 99% confidence intervals

```
confint(birth1, level = 0.99)
```

```
                 0.5 %  99.5 %
(Intercept) 1775.2097 2964.13
```

```
LWT           -0.0287    8.89
```

- Comment on the intervals

1. It is 95% certain that the interval (1.05, 7.809) covers the true β_1. Similary, it is 99% certain that the interval (-0.029, 8.887) covers the true β_1.
2. The 99% confidence is larger than 95% confidence. In other words, being more certain about the true value needs larger confidence interval.
3. Moreover, the 95% does not include zero while 99% interval includes zero. This is equivalent with the result that β_1 cofficient is significant at a 5% test level, but not significant at a 1% test level.

Regression with categories

Here we will fit a separate regression for smoking and non-smoking groups. You can identify the observation numbers of the smokers by:

```
smokeYes <- which(birth$SMK == "YES")
```

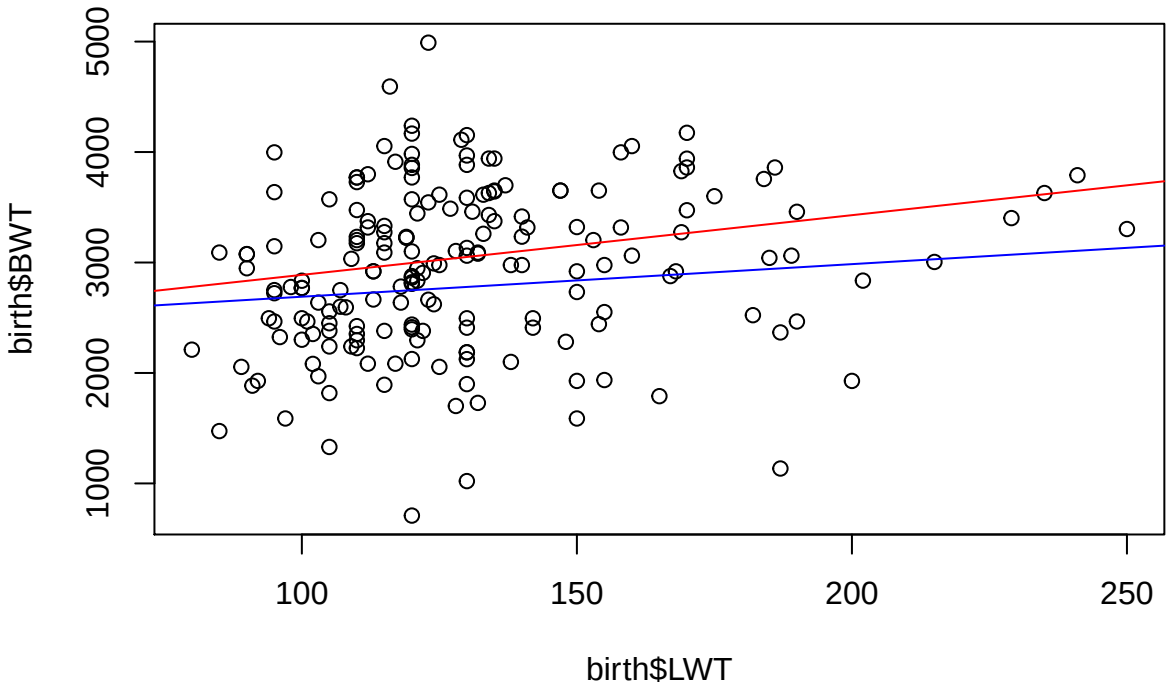
Fit the same model as `birth1`, but separate models for non-smokers and smokers, and call the models `birth2` and `birth3`. (Hint: select observations by the subset argument in the `lm`-function using the `smokeYes` variable.)

```
birth2 <- lm(BWT ~ LWT, data = birth, subset = -smokeYes)
birth3 <- lm(BWT ~ LWT, data = birth, subset = smokeYes)
```

Interpreate these models

- Make a scatter plot of LWT vs BWT and add two fitted lines form the model fitted above.

```
plot(x = birth$LWT, y = birth$BWT)
abline(birth2, col = "red")
abline(birth3, col = "blue")
```



- Comment on the plot

Fitted lines for both non-smokers and smokers seems very similar, but it is difficult to tell whether they are significantly different. We will later se how we can model both mother-groups simultaneously and be able to test this difference.

- Is LWT significant at a 5% level on BWT for the smokers?

```
summary(birth3)
```

```
Call:
lm(formula = BWT ~ LWT, data = birth, subset = smokeYes)

Residuals:
    Min      1Q  Median      3Q     Max
-2040.3  -416.3    33.9   472.2  1488.7

Coefficients:
            Estimate Std. Error t value       Pr(>|t|)
(Intercept)  2395.37     301.47    7.95 0.000000000019 ***
LWT             2.95       2.28    1.30            0.2
---
```

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

s: 657 on 72 degrees of freedom
Multiple R-squared: 0.0228,
Adjusted R-squared: 0.00921
F-statistic: 1.68 on 1 and 72 DF,  p-value: 0.199
```

The hypothesis for testing the significance of LWT is,

$$H_0 : \beta_1 = 0 \text{ vs } H_1 : \beta_1 \neq 0$$

From the summary of model `birth3` above, p-value corresponding to LWT is higher than 0.05 and we fail to reject H_0, which suggests that LWT is not significant for smokers group. In other words, LWT does not have any linear relationship with BWT at 95% confidence level for smokers group.

Assume a model with both LWT and AGE as predictors for BWT using all observations.

- Write up the model and the model assumptions.

$$\text{BWT} = \beta_0 + \beta_1 \text{LWT} + \beta_2 \text{AGE} + \epsilon$$

Assumptions:

The error term ϵ follows $N(0, \sigma^2)$ iid, i.e error terms are independently normally distributed with mean 0 and constant variance σ^2.

- What is the interpretation of the regression coefficients?

1. β_1 gives the expected amount of change in BWT for unit change in LWT when AGE is held constant, i.e. if LWT increases by 1 pound, BWT will increase by β_1 grams for people of the same AGE.
2. β_2 gives the expected amount of change in BWT (in grams) if AGE increase by 1 year and LWT is held constant.

Fit the model in RStudio, call it `birth4` and comment on the results.

```
birth4 <- lm(BWT ~ LWT + AGE, data = birth)
summary(birth4)
```

```
Call:
lm(formula = BWT ~ LWT + AGE, data = birth)

Residuals:
    Min      1Q  Median      3Q     Max
-2232.8  -500.5    32.1   520.3  1899.3

Coefficients:
            Estimate Std. Error t value        Pr(>|t|)
(Intercept)  2215.76     299.24     7.4 0.0000000000044 ***
LWT             4.18       1.74     2.4           0.018 *
AGE             8.02      10.06     0.8           0.426
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

s: 719 on 186 degrees of freedom
Multiple R-squared: 0.0378,
Adjusted R-squared: 0.0275
F-statistic: 3.65 on 2 and 186 DF,  p-value: 0.0278
```

The summary output shows that LWT is significant at 5% level of significance but not at 1%. AGE has very high p-value and thus is not significant, i.e. there is not any linear relationship of AGE with BWT. The explained variation is still very low with an $R^2 = 0.038$.

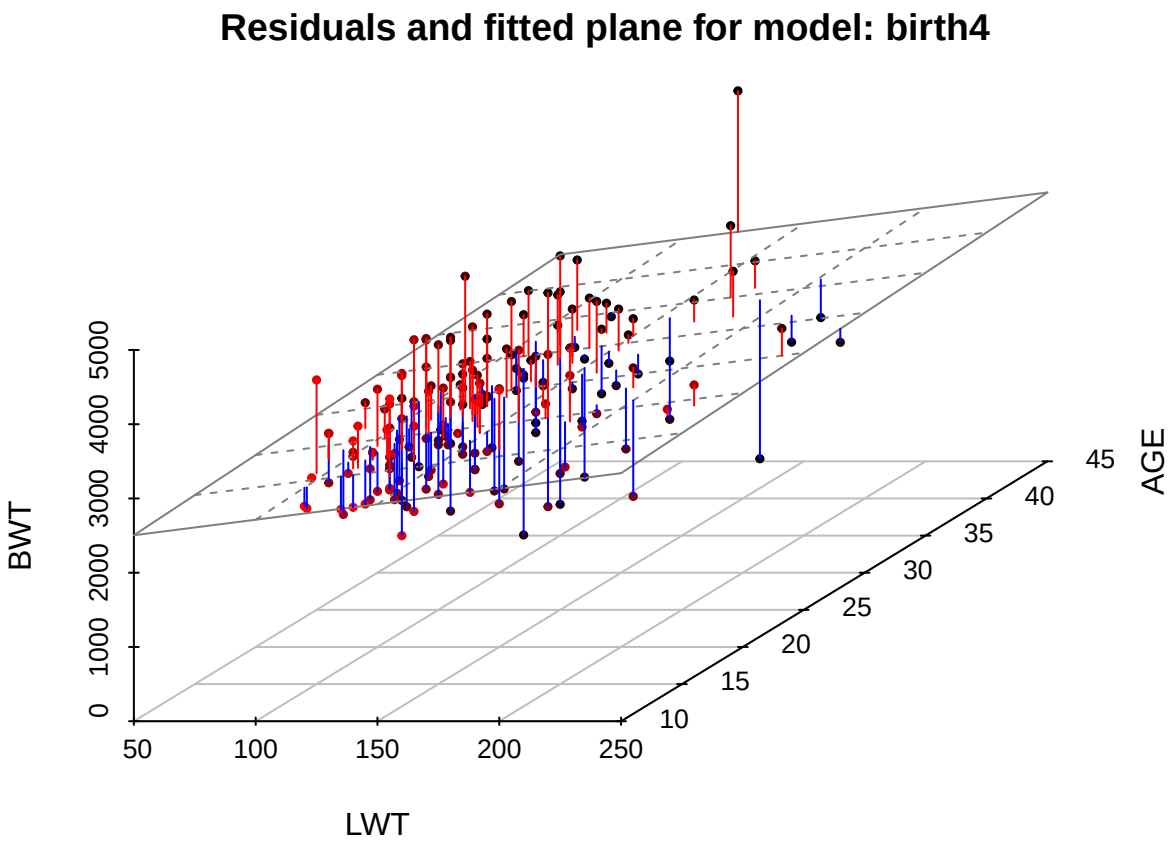
Optional:

Look at the presentation file Regression.Rmd from lecture 2 and produce for the `birth4-model` a similar 3D-plot as on page 15. You may need to install the R-packages: `rgl`, `nlme`, `mgcv` and `car` first. Use the figure to get an understanding of the effects of LWT and AGE on BWT.

A 3D plot

```
library(scatterplot3d)
with(birth, {
```

```
  # Start Plot
  plot3d <- scatterplot3d(LWT, AGE, BWT, type = "p", highlight.3d = TRUE,
                          mar = c(3, 3, 2, 3), pch = 19, cex.symbols = 0.5,
                          main = "Residuals and fitted plane for model: birth4",
                          angle = 45, box = FALSE)
  # Add fitted plane for model birth4
  plot3d$plane3d(birth4, col = "grey50", lty.box = "solid", polygon_args = list(bg = "li
  # True Values
  true <- plot3d$xyz.convert(LWT, AGE, BWT)
  # Predicted Values
  fitted <- plot3d$xyz.convert(LWT, AGE, fitted(birth4))
  # Is the residuals negative?
  neg_res <- 1 + (resid(birth4) > 0)
  # Add segment for the residuals
  segments(true$x, true$y, fitted$x, fitted$y, col = c("blue", "red")[neg_res])
})
```



An interactive 3D plot

```
library(car)
scatter3d(BWT ~ LWT + AGE, data = birth, axis.ticks = TRUE, revolutions = 1)
```

For grouped: Smoking vs Non-Smoking:

```
car::scatter3d(BWT ~ LWT + AGE, data = birth, axis.ticks = TRUE,
               revolutions = 1, groups = birth$SMK)
```

Interpretation

- What is the interpretation of the estimated regression coefficients for LWT and AGE in this model?

From the summary output of `birth4` model, the β coefficient for LWT is 4.179 and AGE is 8.021. This shows that, if weight of mother (LWT) increases by 1 pound, the birth weight (BWT) is estimated to increase by 4.179 grams if AGE is held constant. Similary, if the age of a mother (AGE) increases by 1 year, the birth weight (BWT) is estimated to increase by 8.021 grams, if LWT is held constant. The regression coefficients are therefore equal to the slopes of the gridlines of the surface in the figure.

Dataset: bodydata

Training Samples

Create a training data set called bodytrain containing the first 20 observations only, by:

```
bodytrain <- bodydata[1:20,]
```

Fitting Model

Fit one at a time three simple regression models with Weight as response and each of Height, Age and Circumference as predictors, name the models `Model1`, `Model2` and `Model3`, respectively. Use the `summary()` function on each model to print out a summary of the fitted models. Use the first 20 observations as your training data.

```
model1 <- lm(Weight ~ Height, data = bodytrain)
model2 <- lm(Weight ~ Age, data = bodytrain)
model3 <- lm(Weight ~ Circumference, data = bodytrain)
```

Understanding the fitted Model

- Test whether the three predictors are significant. Use a 5% test level.

The summary result for `model1` is,

```
summary(model1)
```

```
Call:
lm(formula = Weight ~ Height, data = bodytrain)

Residuals:
    Min      1Q  Median      3Q     Max
-11.516  -2.596   0.026   2.914  11.745

Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept)  -38.231     38.360   -1.00   0.3322
Height         0.639      0.212    3.01   0.0076 **
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

s: 5.84 on 18 degrees of freedom
Multiple R-squared: 0.334,
Adjusted R-squared: 0.297
F-statistic: 9.04 on 1 and 18 DF,  p-value: 0.00757
```

Here, at 5% test level, Height is significant (p-value for Height is less than 0.05). The summary result for `model2` is,

```
summary(model2)
```

```
Call:
lm(formula = Weight ~ Age, data = bodytrain)

Residuals:
    Min      1Q  Median      3Q     Max
-15.084  -3.918   0.898   4.251  12.439

Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept)   80.745     14.563    5.54 0.000029 ***
Age           -0.159      0.625   -0.25      0.8
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

s: 7.14 on 18 degrees of freedom
Multiple R-squared: 0.00359,
Adjusted R-squared: -0.0518
F-statistic: 0.0648 on 1 and 18 DF,  p-value: 0.802
```

Here, at 5% test level, Age is not significant (p-value for age is greater than 0.05). Finally, the summary result for `model3` is,

```
summary(model3)
```

```
Call:
lm(formula = Weight ~ Circumference, data = bodytrain)

Residuals:
   Min     1Q Median     3Q    Max
-8.937 -3.540  0.038  2.956  8.659

Coefficients:
              Estimate Std. Error t value Pr(>|t|)
(Intercept)      3.674     17.104    0.21  0.83234
Circumference    0.914      0.212    4.30  0.00043 ***
```

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

s: 5.03 on 18 degrees of freedom
Multiple R-squared: 0.507,
Adjusted R-squared: 0.479
F-statistic: 18.5 on 1 and 18 DF,  p-value: 0.000431
```

Here, at 5% test level, Circumference is significant (p-value for circumference is less than 0.05).

- Which model gives a better linear fit in terms of R-squared?

The model with `Circumference` as predictor has highest R^2 among the models. This model explains 50.67 percent of variation present in the response `Weight`.

Compute the correlation matrix of the bodydtrain data by:

```
cormat <- cor(bodytrain)
```

You can square the correlations by:

```
cormat ^ 2
```

```
                Weight  Height        Age Circumference
Weight        1.00000 0.33440 0.00358748    0.50671271
Height        0.33440 1.00000 0.00167276    0.06116116
Age           0.00359 0.00167 1.00000000    0.00000422
Circumference 0.50671 0.06116 0.00000422    1.00000000
```

- Compare the squared correlations under the `Weight` column with the R-squared values from the three models.

The square of correlation between each predictor variable with response is equals to the R^2 obtained in `model1`, `model2` and `model3`. However, this only applies to simple regression with one predictor.

If we "predict" the same observations as was used to fit the model, we get the so-called fitted values. These can be retrieved from the `model1` by `model1$fitted.values`

- Compute the squared correlations between the `weights` of `bodytrain` and the fitted values of `model1`.

```
cors <- cor(bodytrain[ , 1], model1$fitted.values)
cors ^ 2
```

```
[1] 0.334
```

- Compare with the R-squared of `model1`

The square of correlation between the fitted values from a model with the response is equal to the R^2 obtained from the model. This is a result which extends to multiple regression.

- For each model locate and compare the estimates for the error variance, σ^2.

By applying the anova() function to each model object we obtain the analysis of variance tables containing the MSE, i.e. the Mean Sum of Squares of the Error (Residuals), which is the estimator for the error variance.

```
anova(model1)
```

```
Analysis of Variance Table

Response: Weight
          Df Sum Sq Mean Sq F value Pr(>F)
Height     1    308   308.3    9.04 0.0076 **
Residuals 18    614    34.1
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

```
anova(model2)
```

```
Analysis of Variance Table

Response: Weight
          Df Sum Sq Mean Sq F value Pr(>F)
Age        1      3     3.3    0.06    0.8
Residuals 18    919    51.0
```

```
anova(model3)
```

```
Analysis of Variance Table

Response: Weight
```

```
              Df Sum Sq Mean Sq F value  Pr(>F)
Circumference  1    467     467    18.5 0.00043 ***
Residuals     18    455      25
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

- Which model has the smallest error variance estimate?

Model 3 has the smallest error variance estimate. We can also obtain the error variance estimate using the "Residual standard error" from the summary output since, $MSE = s^2$.

Multiple Linear Regression and Prediction

- Fit a model 4 with both `Height` and `Circumference` as predictors.

```
model4 <- lm(Weight ~ Height + Circumference, data = bodytrain)
summary(model4)
```

```
Call:
lm(formula = Weight ~ Height + Circumference, data = bodytrain)

Residuals:
   Min     1Q Median     3Q    Max
-5.319 -3.536 -0.782  2.803  6.397

Coefficients:
              Estimate Std. Error t value Pr(>|t|)
(Intercept)    -70.820     28.452   -2.49  0.02346 *
Height           0.473      0.157    3.02  0.00770 **
Circumference    0.778      0.182    4.27  0.00051 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

s: 4.17 on 17 degrees of freedom
Multiple R-squared: 0.679,
Adjusted R-squared: 0.641
```

```
F-statistic:   18 on 2 and 17 DF,  p-value: 0.0000638
```

- Get test observations for prediction: (*Make a test data set called bodytest containing observations 21:40 (Hint: Check how we made `bodytrain` above)*)

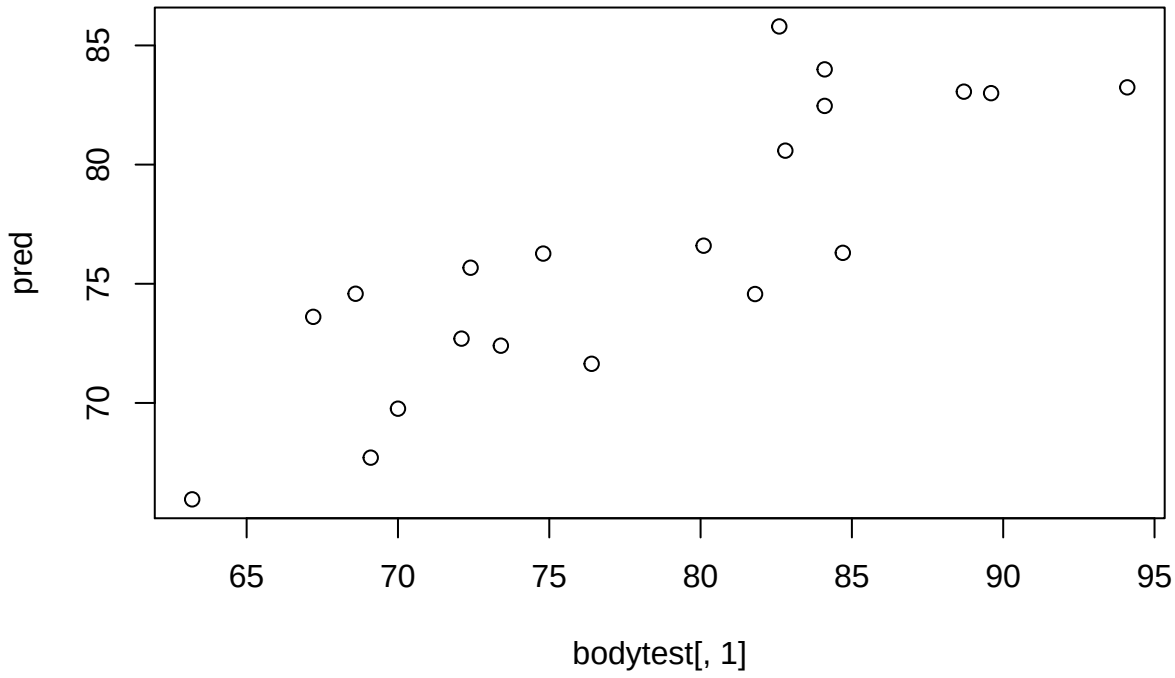
```
bodytest <- bodydata[21:40, ]
```

- Use `model4` to predict the Weights of the testdata.

```
pred <- predict(model4, newdata = bodytest)
```

- Make a scatter plot of the actually observed weights of the test data and the predicted weights.

```
plot(bodytest[ , 1], pred)
```



- Compute the squared correlation between the actually observed Weights and the predicted weights.

```
cor(pred, bodytest[ , 1]) ^ 2
```

```
[1] 0.714
```

What you get here is a so-called "prediction R-squared" of this model.

- Compare with the R-squared of `model4`

The prediction R-squared is close to the R-squared of model4 (0.679) which indicates that the results from model4 generalize well to new observations.

Extra on R-squared

In statistics we aim at finding models which fit the data well. However, the R-squared may easily lead to overfitting of models, that is by including too many variables.

- Fit a model with all three predictors to the bodytrain data:

```
model5 <- lm(Weight ~ Height + Circumference + Age, data = bodytrain)
summary(model5)
```

```
Call:
lm(formula = Weight ~ Height + Circumference + Age, data = bodytrain)

Residuals:
   Min     1Q Median     3Q    Max
-5.409 -3.390 -0.912  3.040  6.983

Coefficients:
              Estimate Std. Error t value Pr(>|t|)
(Intercept)    -66.579     30.010   -2.22  0.04133 *
Height           0.477      0.160    2.98  0.00883 **
Circumference    0.777      0.186    4.18  0.00071 ***
Age             -0.209      0.373   -0.56  0.58235
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

s: 4.26 on 16 degrees of freedom
Multiple R-squared: 0.685,
Adjusted R-squared: 0.626
F-statistic: 11.6 on 3 and 16 DF,  p-value: 0.000273
```

- Lets add some randomly generated junk from a normal distribution

```
Junk1 <- rnorm(n = 20, mean = 0, sd = 10)
Junk2 <- rnorm(20, 0, 10)
Junk3 <- rnorm(20, 0, 10)
model6 <- lm(Weight ~ Height + Circumference + Age +
               Junk1 + Junk2 + Junk3, data = bodytrain)
summary(model6)
```

```
Call:
lm(formula = Weight ~ Height + Circumference + Age + Junk1 +
    Junk2 + Junk3, data = bodytrain)

Residuals:
   Min     1Q Median     3Q    Max
 -4.90  -2.94  -1.18   2.96   6.47

Coefficients:
              Estimate Std. Error t value Pr(>|t|)
(Intercept)   -45.2110    34.4211   -1.31   0.2117
Height          0.3716     0.1850    2.01   0.0659 .
Circumference   0.7785     0.2384    3.27   0.0061 **
Age            -0.3277     0.4102   -0.80   0.4387
Junk1          -0.1569     0.1394   -1.13   0.2808
Junk2           0.1641     0.1367    1.20   0.2512
Junk3          -0.0771     0.1361   -0.57   0.5807
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

s: 4.34 on 13 degrees of freedom
Multiple R-squared: 0.734,
Adjusted R-squared: 0.611
F-statistic: 5.98 on 6 and 13 DF,  p-value: 0.00346
```

Exercises

- Compare models 5 and 6. What happens to the R-squared? (*Compare also the adjusted*

R-squared values for models 5 and 6.)

The results will vary from time to time since we sample random junk, but in general we will observe that R-squared increase, whereas the adjuste R-squared decrease as we add more junk variables.

- Try to add 3 more junk variables, `Junk4`, `Junk5` and `Junk6`.

```
Junk4 <- rnorm(n = 20, mean = 0, sd = 10)
Junk5 <- rnorm(20, 0, 10)
Junk6 <- rnorm(20, 0, 10)
model6 <- lm(Weight ~ Height + Circumference + Age + Junk1 + Junk2 + Junk3 +
               Junk4 + Junk5 + Junk6, data = bodytrain)
summary(model6)
```

```
Call:
lm(formula = Weight ~ Height + Circumference + Age + Junk1 +
    Junk2 + Junk3 + Junk4 + Junk5 + Junk6, data = bodytrain)

Residuals:
   Min     1Q Median     3Q    Max
 -4.47  -2.07   1.04   1.92   4.34

Coefficients:
             Estimate Std. Error t value Pr(>|t|)
(Intercept)   -94.5392    34.6101   -2.73   0.0211 *
Height          0.6117     0.1901    3.22   0.0092 **
Circumference   0.7818     0.2005    3.90   0.0030 **
Age            -0.0701     0.3488   -0.20   0.8448
Junk1           0.0822     0.1653    0.50   0.6295
Junk2          -0.0209     0.1469   -0.14   0.8897
Junk3           0.0488     0.1323    0.37   0.7197
Junk4          -0.2964     0.1181   -2.51   0.0309 *
Junk5           0.1626     0.1280    1.27   0.2326
Junk6          -0.0469     0.0826   -0.57   0.5822
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

```
s: 3.55 on 10 degrees of freedom
Multiple R-squared: 0.863,
Adjusted R-squared: 0.74
F-statistic: 7.01 on 9 and 10 DF,  p-value: 0.00269
```

- Observe the R-squared values (*What is the lesson to be learned here?*)

Adding variables and only observing R-squared may be misleading. We should at least also keep in mind that a simple model is better. Hence, if adding more variables does not increase R-squared very much, we should keep the simpler model. If in addition the difference between the R-squared and the adjusted R-squared starts to get large, it is a clear indicator of overfitting.

Dataset: mtcars

We will use an old data set from 1974 on gasoline consumption for various cars which is part of the `datasets` package in R.

```
head(mtcars)
```

```
                   mpg cyl disp  hp drat   wt qsec vs am gear carb
Mazda RX4         21.0   6  160 110 3.90 2.62 16.5  0  1    4    4
Mazda RX4 Wag     21.0   6  160 110 3.90 2.88 17.0  0  1    4    4
Datsun 710        22.8   4  108  93 3.85 2.32 18.6  1  1    4    1
Hornet 4 Drive    21.4   6  258 110 3.08 3.21 19.4  1  0    3    1
Hornet Sportabout 18.7   8  360 175 3.15 3.44 17.0  0  0    3    2
Valiant           18.1   6  225 105 2.76 3.46 20.2  1  0    3    1
```

As you can see there are multiple variables. If you have the datasets package you may look at the help file for the data by:

```
?datasets::mtcars
```

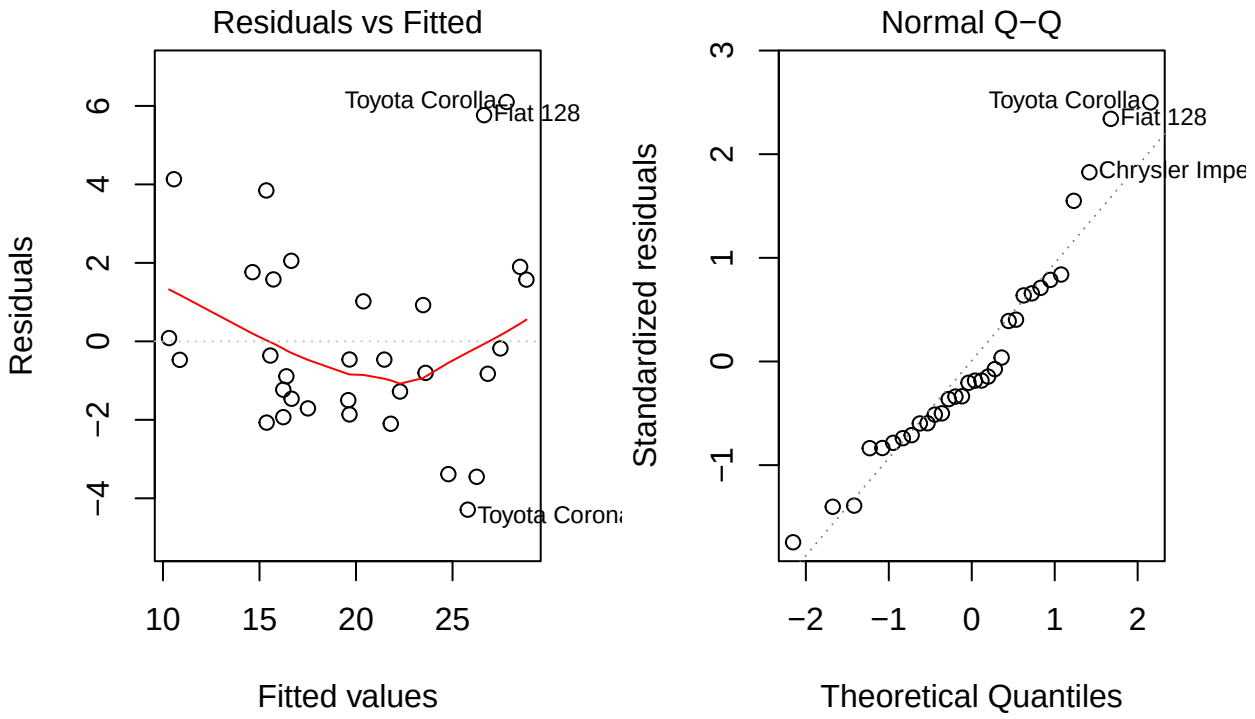
Ex-1: Model Fitting

- Fit a multiple linear regression model with mpg (Miles/Gallon) as response variable and `wt` (Weight) and `cyl` (Number of cylinders) as predictors. Call the model object "`cars1`".

```
cars1 <- lm(mpg ~ cyl + wt, data = mtcars)
```

- Check the model assumptions by residual analysis.

```
par(mfrow = c(1,2)) #This creates a layout for plots, one row and two columns
plot(cars1, which = c(1,2)) #Only the two first residual plots
```



- Give a summary of the results and compute the ANOVA-table.

```
summary(cars1)
```

```
Call:
lm(formula = mpg ~ cyl + wt, data = mtcars)
```

```
Residuals:
   Min     1Q Median     3Q    Max
-4.289 -1.551 -0.468  1.574  6.100

Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept)   39.686      1.715   23.14  < 2e-16 ***
cyl           -1.508      0.415   -3.64  0.00106 **
wt            -3.191      0.757   -4.22  0.00022 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

s: 2.57 on 29 degrees of freedom
Multiple R-squared: 0.83,
Adjusted R-squared: 0.819
F-statistic: 70.9 on 2 and 29 DF,  p-value: 0.00000000000681
```

```
anova(cars1)
```

```
Analysis of Variance Table

Response: mpg
          Df Sum Sq Mean Sq F value          Pr(>F)
cyl        1    818     818   124.0 0.0000000000054 ***
wt         1    117     117    17.8         0.00022 ***
Residuals 29    191       7
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

- Give a short report on the results.

Both `cyl` and `wt` appears to be highly significant predictors for `mpg`. The estimated effects are negative implying that the mileage decreases as both weight and cylinder numbers increase, which is a reasonable result. The R^2 is 0.83, hence, about 83% of the variability in mileage is explained by the linear relationship with `cyl` and `wt`. The residual plot of fitted values versus residuals gives an indication of a non-linear relationship, which may be a result of non-linear dependencies or missing explanatory variable(s). The normal

probability plot is more or less OK.

Ex-2: Indicator variable

The `am` variable is an indicator variable for transmission system of the cars, `0=automatic`, `1=manual`. Run the following model in R:

```
cars2 <- lm(mpg ~ cyl + wt*am, data = mtcars)
```

- Write up the assumed model which has been run here. Also write up the estimated models for automatic and manual transmission, respectively.

The model is:

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_4 x_2 \cdot x_3 + \epsilon$$

where $y =$ `mpg`, $x_1 =$ `cyl`, $x_2 =$ `wt`, $x_3 =$ `am` and $\epsilon \sim N(0, \sigma^2)$.

The fitted model from R is:

```
summary(cars2)
```

```
Call:
lm(formula = mpg ~ cyl + wt * am, data = mtcars)

Residuals:
   Min     1Q Median     3Q    Max
-3.462 -1.491 -0.788  1.396  5.350

Coefficients:
            Estimate Std. Error t value        Pr(>|t|)
(Intercept)   34.283      2.796   12.26 0.0000000000015 ***
cyl           -1.181      0.380   -3.11          0.0044 **
wt            -2.369      0.824   -2.87          0.0078 **
am            11.939      3.845    3.10          0.0044 **
wt:am         -4.197      1.312   -3.20          0.0035 **
```

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

s: 2.26 on 27 degrees of freedom
Multiple R-squared: 0.877,
Adjusted R-squared: 0.859
F-statistic: 48.1 on 4 and 27 DF,  p-value: 0.00000000000664
```

For automatic transmission (am=x_3=0) we have the estimated model:

$$\hat{y} = 34.28 - 1.18x_1 - 2.37x_2$$

For manual transmission (am=x_3=1) we have

$$\hat{y} = 34.28 - 1.18x_1 - 2.37x_2 + 11.94 \cdot 1 - 4.20x_2 \cdot 1$$

$$= 46.22 - 1.18x_1 - 6.57x_2$$

We observe that the negative effect of weight on mileage is larger for manual transmission than for automatic.

Ex-3: Comparing models - Partial F-test

From the p-values we observe that transmission gives a significant addition to the intercept and to the effect of weight, respectively. These p-values correspond to testing each effect GIVEN that all other variables are included in the model. Sometimes we would rather like to test several effects jointly. For instance, should we add both transmission (am) AND the interaction betwen transmission and weight (wt:am) to the model? This is a joint test of the significance of transmission in the model. To accomplish this we may compare the fits of cars2 (a full model) with cars1 (a reduced model) since the difference between these models are exactly the transmission effects. This is called a partial F-test (Fisher test) were we test whether the SSE has decreased significantly as we go from the reduced model to the full model. The partial F-test may be run in RStudio by:

```
anova(cars1, cars2)
```

```
Analysis of Variance Table

Model 1: mpg ~ cyl + wt
Model 2: mpg ~ cyl + wt * am
  Res.Df RSS Df Sum of Sq    F Pr(>F)
1     29 191
2     27 138  2      52.7 5.13  0.013 *
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

- From the output we see that the test statistic is an F-statistic. Is there a significant effect of transmission do you think?

A lengthy answer:

We are here really testing the hypotheses:

$$H_0 : \beta_3 = \beta_4 = 0$$

versus the alternative that at least one of them is different from zero.

We reject the null-hypothesis at test-level α if

$$F = \frac{(SSE_{\text{red.mod}} - SSE_{\text{full.mod}})/r}{MSE_{\text{full.mod}}}$$

is larger than $F_{\alpha,r,n-p}$, where r is the difference in the degrees of freedom for SSE for the two models (here $r = 2$), and $n - p$ are the degrees of freedom for SSE of the full model (here $n - p = 27$).

From the output we have (note RSS = SSE):

$$F = \frac{(191.17 - 138.51)/2}{138.51/27} = 5.13$$

We reject at level $\alpha = 0.05$ if this observed F is larger than $F_{0.05,2,27}$. At this point we could look this up in a Fisher-table, or alternatively compute this quantile of the Fisher distribution by:

```
qf(0.05, 2, 27, lower.tail = FALSE)
```

```
[1] 3.35
```

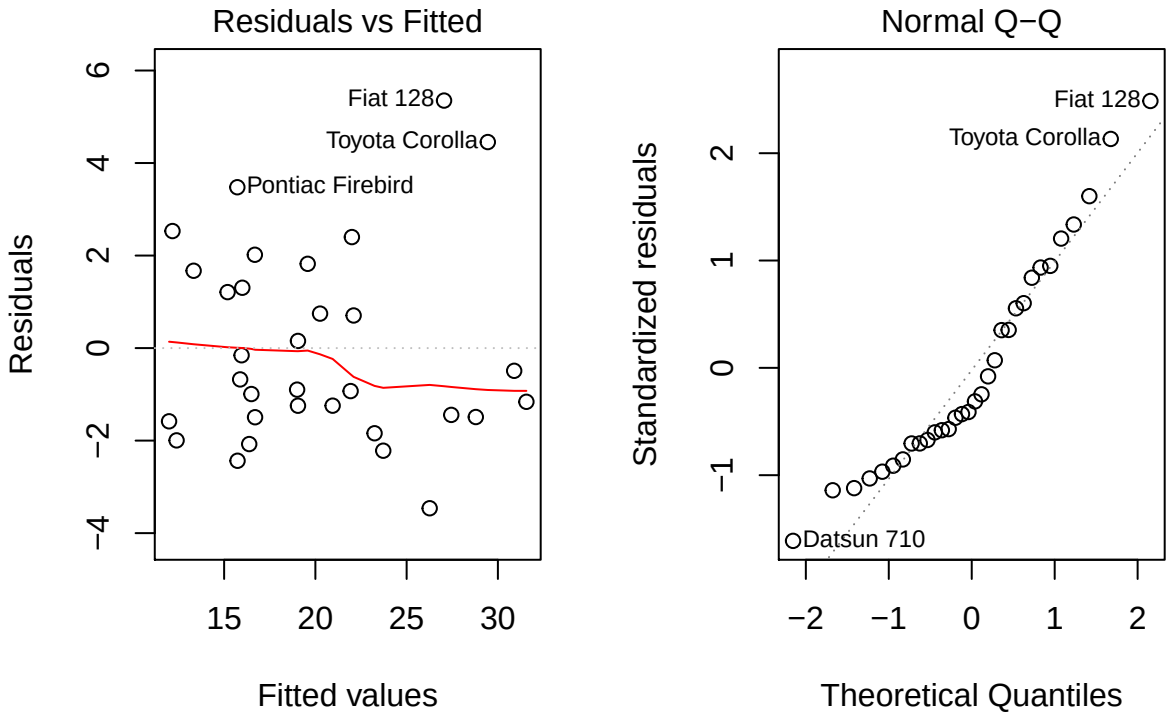
See `?FDist` for help-file for the Fisher distribution.

We reject the null-hypothesis.

Alternatively we reject since the p-value from the output is smaller than 0.05.

- Perform a residual analysis of the `cars2` model.

```
par(mfrow = c(1,2))
plot(cars2, which = c(1,2))
```



The linearity has improved, but maybe there is an increasing variance with increasing fitted value (estimated mileage). The normality looks good.

Ex-4: Influential measurements

- Use the `influence.measures()` function to compute the Cook's distances and the leverage (hat) values for all observations accoring to the `cars2` model. Are there any influential observations according to these measures?

```
summary(influence.measures(cars2))
```

```
Potentially influential observations of
     lm(formula = mpg ~ cyl + wt * am, data = mtcars) :

                   dfb.1_ dfb.cyl dfb.wt dfb.am dfb.wt:m dffit cov.r
Lincoln Continental  0.38   0.16   -0.52  -0.28   0.23    -0.59  1.57_*
Fiat 128             0.10  -0.31    0.17   0.25  -0.15     0.91  0.36_*
Ford Pantera L       0.01  -0.02    0.01   0.01  -0.02    -0.04  1.61_*
Maserati Bora       -0.03   0.09   -0.05  -0.35   0.49     0.73  1.64_*
                   cook.d hat
Lincoln Continental  0.07   0.33
Fiat 128             0.13   0.10
Ford Pantera L       0.00   0.25
Maserati Bora        0.11   0.38
```

Four observations are flagged by R, but none according to Cook's distance or leverage (hat).

Ex-5: Model selection

- Fit a third multiple linear regression model with mpg (Miles/Gallon) as response variable and `cyl`, `disp`, `hp`, `drat`, `wt` and `qsec` as predictor variables. Call the model object "`cars3`". Report a summary of the analysis.

```
cars3 <- lm(mpg ~ cyl + disp + hp + drat + wt + qsec, data = mtcars)
summary(cars3)
```

```
Call:
lm(formula = mpg ~ cyl + disp + hp + drat + wt + qsec, data = mtcars)

Residuals:
   Min     1Q Median     3Q    Max
-3.968 -1.580 -0.435  1.166  5.527
```

```
Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept)  26.3074    14.6299    1.80   0.0842 .
cyl          -0.8186     0.8116   -1.01   0.3228
disp          0.0132     0.0120    1.10   0.2831
hp           -0.0179     0.0155   -1.16   0.2585
drat          1.3204     1.4795    0.89   0.3806
wt           -4.1908     1.2579   -3.33   0.0027 **
qsec          0.4015     0.5166    0.78   0.4444
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

s: 2.56 on 25 degrees of freedom
Multiple R-squared: 0.855,
Adjusted R-squared: 0.82
F-statistic: 24.5 on 6 and 25 DF,  p-value: 0.00000000245
```

Apparently only wt is significant, but having many variables in a model may lead to inflated Std. Errors of the estimates due to correlation between predictors, and problems finding truly significant variables.

We would like to check various sub-models of this model by combining different variables. Install and load the '`mixlm`' package. The package contains a function called `best.subsets()` which can help us find a good model.

```
best.subsets(cars3)
```

```
         cyl disp hp drat wt qsec RSS    R2 R2adj    Cp
1  ( 1 )                  *      278 0.753 0.745 14.56
1  ( 2 )   *                     308 0.726 0.717 19.15
1  ( 3 )       *                 317 0.718 0.709 20.50
1  ( 4 )          *              448 0.602 0.589 40.46
1  ( 5 )               *         604 0.464 0.446 64.30
2  ( 1 )   *              *      191 0.830 0.819  3.24
2  ( 2 )          *       *      195 0.827 0.815  3.83
2  ( 3 )                  *    * 195 0.826 0.814  3.89
2  ( 4 )       *          *      247 0.781 0.766 11.72
2  ( 5 )               *  *      269 0.761 0.744 15.17
```

```
3  ( 1 )   *       *       *       177 0.843 0.826  3.01
3  ( 2 )   *               *     * 181 0.840 0.822  3.62
3  ( 3 )                 *   *     * 184 0.837 0.820  4.07
3  ( 4 )           *     *   *       184 0.837 0.819  4.09
3  ( 5 )           *         *     * 186 0.835 0.817  4.45
4  ( 1 )   *     *   *       *       170 0.849 0.826  4.07
4  ( 2 )           *     *   *     * 174 0.845 0.822  4.63
4  ( 3 )   *       *     *   *       174 0.845 0.822  4.67
4  ( 4 )   *       *         *     * 175 0.844 0.821  4.80
4  ( 5 )   *     *           *     * 176 0.844 0.821  4.86
5  ( 1 )   *     *   *     *   *       167 0.851 0.823  5.60
5  ( 2 )   *     *   *         *     * 169 0.850 0.821  5.80
5  ( 3 )         *   *     *   *     * 170 0.849 0.820  6.02
5  ( 4 )   *       *     *   *     * 171 0.848 0.819  6.20
5  ( 5 )   *     *         *   *     * 172 0.847 0.818  6.34
6  ( 1 )   *     *   *     *   *     * 163 0.855 0.820  7.00
```

The function reports by default the 5 best models for each model size (number of predictors). The model size is given in the first column. Column two is the rank within model size, then comes a column for each variable with a star indicating that a given variable is part of the model. Finally comes the residual sum of squares (RSS or SSE), R^2, R^2-adjusted and finally a diagnostic called Mallow's Cp.

- Which sub-model would you say is the best fitting model according to the R^2-adjusted?

A couple of models are quite similar, but the largest R^2-adjusted is obtained with a model with predictors `cyl`, `hp` and `wt`. This is also a quite simple model with few predictors. We should always strive for simple models and choose the simpler model in cases where the fit appears to be more or less equal for several models.

Ex-6: Model validation

On canvas you find a file called "`CV.R`" containing two functions `CV()` and `Kfold()`. Download this file and open it in RStudio and press the "source" button up to the right in the script window. This will run the file and create these functions. You can also scource the file as,

```
source('_functions/CV.R')
```

A fitted model should ideally be validated on a test set of new and un-touched data. We could predict the new samples using our best choice model and evaluate the prediction performance. If the model predicts well, we probably have a good model!

If we don't have a test set, we may perform Cross-validation. The most common version is the Leave-One-Out Cross-validation where we successively remove one observation from the data and fit the model to the remaining observations. The fitted model is used to predict the left out observation. After fitting a model, the left out observation is put back, and another is left out. In ttoal we then fit n models, and perform n predictions.

- Use the `CV()` function to perform a Leave-One-Out CV using the `cars2` model fit by:

```
res <- CV(cars2)
```

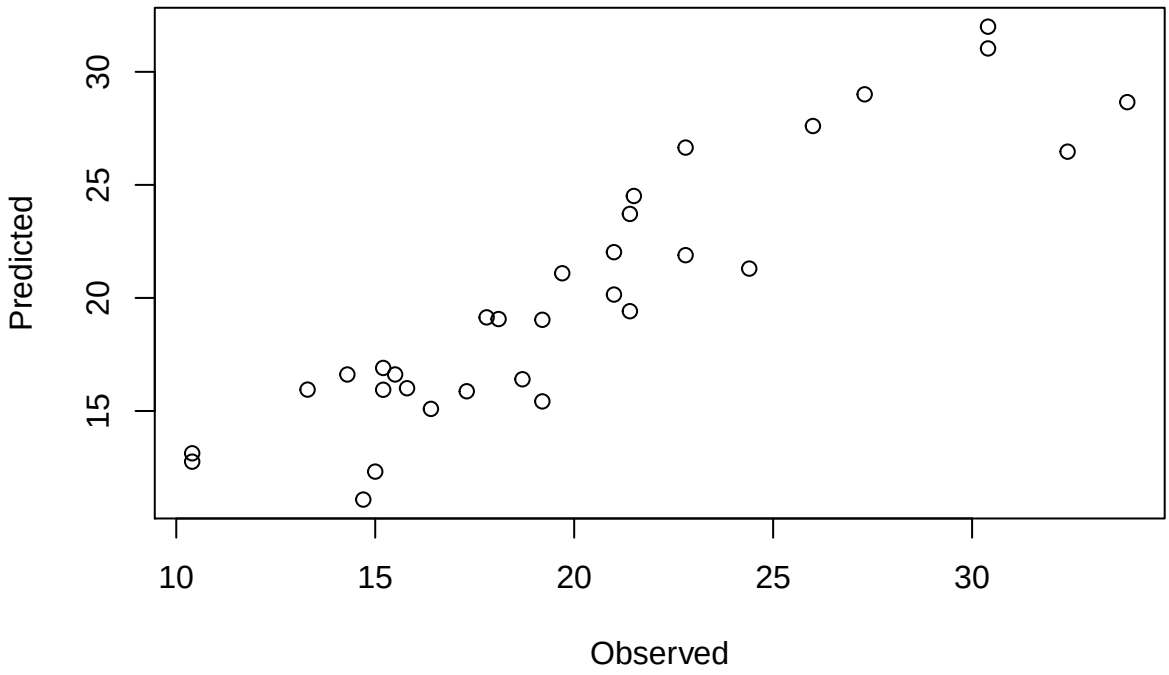
```
print(res)
```

```
$pred
 [1] 22.0 20.1 26.6 19.4 16.4 19.1 16.6 21.3 21.9 19.0 19.1 15.1 15.9 15.9
[15] 13.1 12.8 11.1 26.5 31.0 28.7 24.5 16.6 16.9 15.9 15.4 29.0 27.6 32.0
[29] 16.0 21.1 12.3 23.7

$msep
[1] 6.09

$r.squared.pred
[1] 0.828
```

The `CV()` returns a list with three elements, the predictions, the Mean Square Error of Prediction and and R^2-predicted.

- Make a plot of the observed mpg versus the cross-validation predictions.

```
plot(mtcars$mpg, res$pred, xlab = "Observed", ylab = "Predicted")
```



- Is the best model from the previous exercise, identified by the `best.subsets()`, a better model in terms of prediction error (MSEP)? The MSEP is defined by:

$$\text{MSEP} = \frac{1}{n}\sum_{i=1}^{n}\left(y_i - \hat{y}_{(i)}\right)^2$$

where $\hat{y}_{(i)}$ is the prediction of y_i using a model where observation i was left out from the model estimation. A small value implies better prediction.

```
cars4 <- lm(mpg ~ cyl + hp + wt, data = mtcars)
CV(cars4)
```

```
$pred
 [1] 22.97 22.08 26.26 20.91 16.98 20.41 15.65 23.65 23.38 20.03 20.10
[12] 14.97 16.05 16.07 11.02 10.09  8.74 26.32 28.71 27.35 25.83 17.69
[23] 18.09 14.79 15.57 27.70 26.62 27.72 16.58 21.28 12.89 24.61

$msep
[1] 7.19

$r.squared.pred
[1] 0.797
```

No, this model does not predict better than cars2.

- Leave-One-out CV is known to have large uncertainty, and using a K-fold CV is an alternative. Then the data are divided into K subsets (folds) of approximately equal sizes, and a leave-one-fold-out CV is performed instead. A K=10 is often recommended. Here, since n=32 a K=8 is better, since this gives subsets of equal sizes. Create K=8 random folds by

```
myfolds <- Kfold(n = 32, K = 8, random = TRUE)
```

```
print(myfolds)
```

```
[[1]]
[1] 11 22 14 10

[[2]]
[1]  8  6  4 21

[[3]]
[1] 17 25  9 16

[[4]]
[1] 29 26  5  3

[[5]]
[1]  1 24 19 30

[[6]]
[1] 32 15 28 31

[[7]]
[1]  2 27 20 23

[[8]]
[1] 13 18  7 12
```

Since the folds are sampled randomly, we get r different folds each time we run `Kfold()`.

As you see, myfolds is a list of 8 random subsets of observation numbers. Re-run the

validation of cars2 by

```
CV(cars2, folds = myfolds)
```

```
$pred
 [1] 22.3 20.1 27.0 19.5 16.2 18.8 16.6 21.7 21.9 19.2 19.2 15.3 16.1 16.1
[15] 13.2 10.8 11.0 26.5 31.2 28.8 23.5 16.8 16.8 16.0 15.3 29.4 26.9 32.4
[29] 16.0 21.3 12.3 23.2

$msep
[1] 5.83

$r.squared.pred
[1] 0.837
```

Note that the result now will vary if you repeat the creation of random K-folds for the cross-validation. Try to make a new myfolds and run the CV again.

Chapter 4

Analysis of variance

We will use following datasets for this exercise:

```
load("_data/city.rdata")
load("_data/nsr.rdata")
load("_data/barley.rdata")
```

R-package we will use in this exercises

```
# load the library
library(mixlm)
library(effects)
```

Chlorine levels in cities

Independent measurements of chlorine (ppm parts per million) were taken from 3 large cities:

```
city
```

```
   City1 City2 City3
1   0.46  1.21  0.44
2   0.92 10.86  0.71
3   0.86  2.09  2.87
4   0.33  6.76  0.81
```

```
5   0.53  3.20  7.34
6   5.13  2.02  2.21
7   1.51  2.16  9.00
8   1.00  0.44 17.20
9   0.70  7.80  2.76
10  1.89  1.20  1.07
11  0.68  1.39  2.07
12  0.71  2.42  1.70
13  0.41  1.62  7.89
14  0.78 10.78  0.79
15  0.11  3.25  0.24
16  2.70  0.41  4.44
17  0.41  0.52 15.40
18  0.75  3.71  4.21
19  0.81  5.20  8.63
20  0.35 13.89  3.90
```

- Load the `city.rdata` which is available on Canvas.

Before analyzing the data it is best to "stack" the data into two columns, a response column `y` and a city factor column `city`. By using the `stack()` function in R you can restructure the city data by

```
citydata <- stack(city)
```

- Use the `colnames()` function to rename the variables as `y` and `city`.

```
colnames(citydata) <- c("y", "city")
```

- Assume an ANOVA-model with chlorine as response and city as a factor. What assumptions do you make?

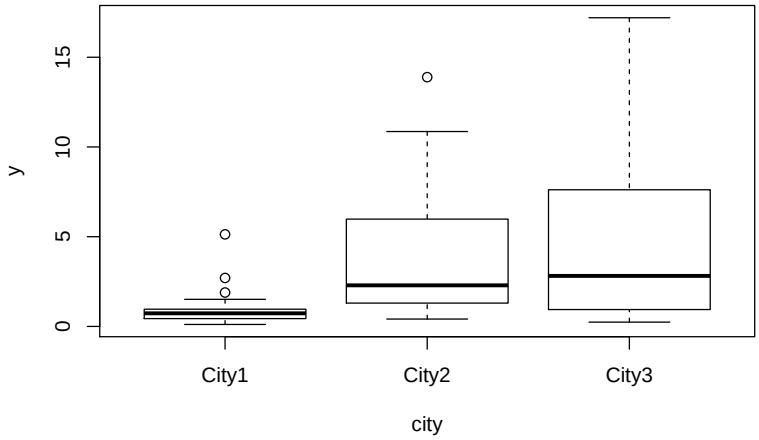
The model assumptions are:

$$y_{ij} = \mu_i + \epsilon_{ij}$$

where the error terms are assumed independent and identically distributed $\epsilon_{ij} \sim N(0, \sigma^2)$. Further μ_i is the expected chlorine level in city i.

- Make a box-plot of the data. Describe the variabilities between cities and within cities.

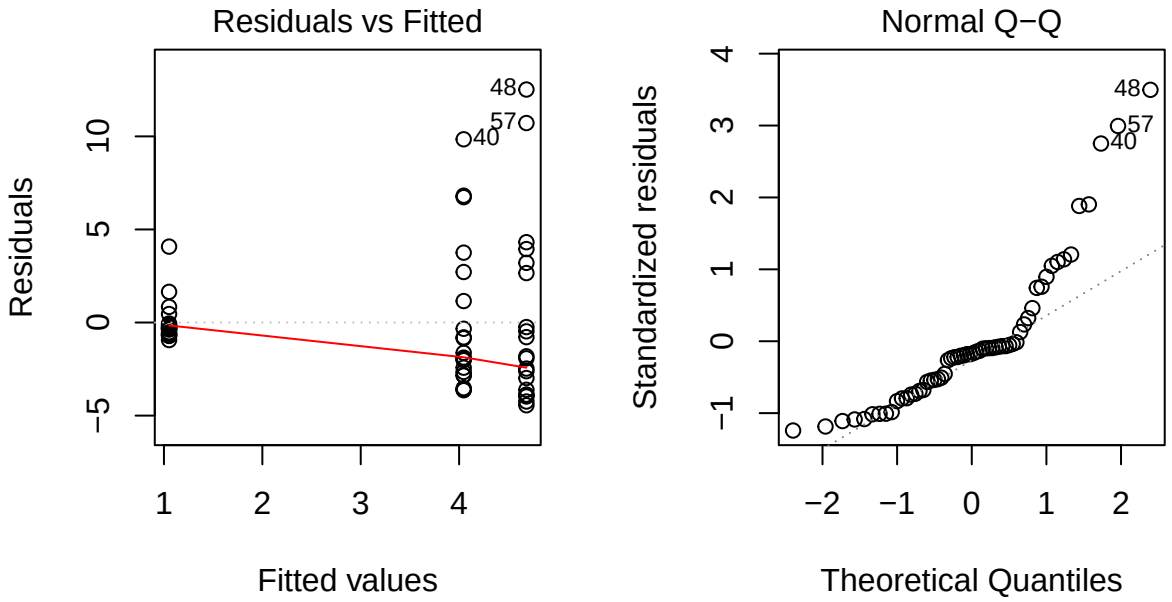
```
plot(y ~ city, data = citydata)
```



City 1 seems to have both the lowest average chlorine levels and the smallest variability in the measurements. Cities 2 and 3 are quite similar with both higher means and variability.

- Fit the model and perform a residual analysis. Comment on the model fit.

```
options(contrasts=c("contr.treatment", "contr.poly"))
citymod1 <- lm(y ~ city, data = citydata)
par(mfrow = c(1, 2))
plot(citymod1, which = c(1, 2))
```



The residual analysis reveals two problems: 1) Non-constant variability, which was also

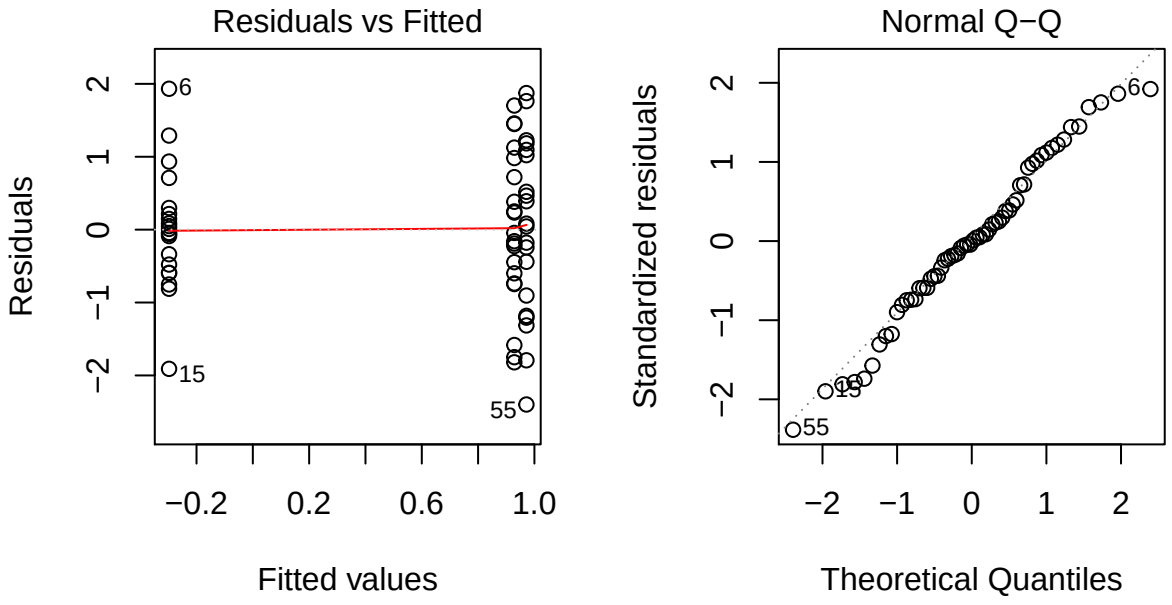
observed in the boxplot, and 2) A skeewed and non-normal distribution for the residuals with a heavy tail to the right.

- Make a log-transformation of y to create the variable `logy`, and add the new variable to your data set by:

```
citydata$logy <- log(citydata$y)
```

- Fit a new model with `logy` as response and check the model fit again.

```
citymod2 <- lm(logy~city, data = citydata)
par(mfrow = c(1,2))
plot(citymod2, which = c(1,2))
```



Both problems from the previous model appear to be corrected. We continue with this model.

- Estimate all model parameters from the latter model. Explain what the parameters measure given the parameterization of your choice (See lecture notes for parameterization).

The ANOVA analysis using contr.treatment parametrization:

```
summary(citymod2)
```

```
Call:
```

```
lm(formula = logy ~ city, data = citydata)

Residuals:
    Min      1Q  Median      3Q     Max
-2.3987 -0.5954 -0.0175  0.7122  1.9326

Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept)   -0.297      0.231   -1.29  0.20266
city(City2)    1.226      0.326    3.76  0.00041 ***
city(City3)    1.269      0.326    3.89  0.00027 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

s: 1.03 on 57 degrees of freedom
Multiple R-squared: 0.255,
Adjusted R-squared: 0.229
F-statistic: 9.75 on 2 and 57 DF,  p-value: 0.000228
```

```
Anova(citymod2)
```

```
Anova Table (Type II tests)

Response: logy
          Sum Sq Df F value  Pr(>F)
city        20.8  2    9.75 0.00023 ***
Residuals   60.7 57
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

```
coefs <- citymod2$coefficients
```

We observe that $R^2 = 0.25$ indicating that there is still a lot of unexplained variability in the response. We get the following estimates for the city means of log(chlorine)-levels using this parametrization (city 1 is reference city):

$\mu_1 = \mu =$ -0.3

$\mu_2 = \mu + \alpha_2 = 0.93$

$\mu_3 = \mu + \alpha_3 = 0.97$

The estimate of the error variance is $\hat{\sigma}^2 = MSE = SSE/(N-3) = 60.724/57 = 1.065$.

As we see from above, the "intercept" μ is the expected log-chlorine level for city 1. The α_2 is the difference between city 1 and city 2, and α_3 is the difference between city 1 and city 3. The σ^2 is the variance for log-chlorine levels measured in the same city.

- State the hypotheses for testing whether the expected chlorine levels differ between the cities, choose a test level α and perform the test. What is the conclusion?

The hypotheses are:

$$H_0 : \mu_1 = \mu_2 = \mu_3$$

versus

$$H_1 : \mu_i \neq \mu_{i'}$$

for at least two different cities i and i'.

Note:This is by the chosen parametrization equivalent to testing

$$H_0 : \alpha_2 = \alpha_3 = 0$$

versus

$$H_1 : \alpha_i \neq 0$$

for at least one $i \in \{2, 3\}$.

For test-level $\alpha = 0.05$ we reject the null-hypothesis if $F > F_{\alpha,2,57}$ or if the p-value is smaller than 0.05. Here we observe a very small p-value and reject the null-hypothesis. We claim that the expected log-chlorine levels differ between at least two of the cities, and from the observed means we know that cities 1 and 3 are significantly different since they have the largest observed difference in means. There may also be a significant difference between cities 1 and 2, and 2 and 3, but this should be checked by a pair-wise contrast.

Data from the NSR education test

The Norwegian Centre for Science Recruitment (NSR) has an online "education test" where youths may answer a questionnaire to check their so-called cognitive types, their science interest, their preferred learning methods and their interest to various science subjects. The test suggests different ares within the STEM (Science, Technology, Engineering and Mathematics) within which the youth may find suitable work.

We have an excerpt of these data which can be downloaded from Canvas as the `nsr.rdata` file. The data.frame `NSRdata` contains two variables, Science and Age:

```
head(NSRdata,5)
```

```
    Science Age
101     4.2  16
102     4.2  16
103     4.2  16
104     3.0  19
105     2.8  16
```

`Science` is an average liking score (scale 1-6) to various STEM-subjects, and `Age` is a factor indicating different age-groups:

a) 1: 1-12 yrs
b) 13: 13-15 yrs
c) 16: 16-19 yrs
d) 19: 19-29 yrs
e) 30: 30 + yrs

- Perform an analysis of the NSR data to check whether Age influences the liking to STEM subjects. State the model, fit the model, check model assumptions, test hypotheses, and give model critique. Write a short summary of the results.

Answer will come later.

- Follow up the previous exercise by performing a Tukey test for all pair wise comparisons with overall (family-wise) error rate 5%. Give a summary of the results.

```
NSRmod <- lm(Science ~ Age, data = NSRdata)
Anova(NSRmod, type = "III")
```

```
Anova Table (Type III tests)

Response: Science
            Sum Sq   Df F value Pr(>F)
(Intercept)   1601    1  1557.6 <2e-16 ***
Age            225    4    54.7 <2e-16 ***
Residuals    10270 9995
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

```r
pt <- simple.glht(NSRmod, "Age", corr = c("Tukey"),level = 0.95)
print(pt)
```

```
     Simultaneous Confidence Intervals and Tests for General Linear Hypotheses

Multiple Comparisons of Means: Tukey Contrasts


Fit: lm(formula = Science ~ Age, data = NSRdata)

Quantile = 2.73
Minimum significant difference = 0.157
95% confidence level

Linear Hypotheses:
        Lower  Center   Upper Std.Err t value      P(>t)
1-13   0.0455  0.2021  0.3588  0.0574    3.52     0.0040 **
1-16  -0.0183  0.1384  0.2951  0.0574    2.41     0.1126
1-19   0.1079  0.2646  0.4212  0.0574    4.61 0.00004063 ***
1-30  -0.3466 -0.1899 -0.0333  0.0574   -3.31     0.0084 **
13-16 -0.2204 -0.0637  0.0929  0.0574   -1.11     0.8015
13-19 -0.0942  0.0624  0.2191  0.0574    1.09     0.8132
13-30 -0.5487 -0.3921 -0.2354  0.0574   -6.83    < 2e-16 ***
16-19 -0.0305  0.1262  0.2828  0.0574    2.20     0.1808
16-30 -0.4850 -0.3283 -0.1717  0.0574   -5.72 0.00000011 ***
19-30 -0.6112 -0.4545 -0.2978  0.0574   -7.91    < 2e-16 ***
```

```
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
(Adjusted p values reported -- single-step method)


WARNING: Unbalanced data may lead to poor estimates
```

The anova table indicates a clear significance of Age-group with regard to the interest level to Science subjects. hence, at least two age-groups are have significantly different expected means. We can use the Tukey test to identify pairwise differences.

The Tukey output provides differences in mean (column "center") between all pairs of groups, and at the top of output the minimum difference yielding a significant difference in means is given to be 0.157. That is, all age-groups with a difference in averages of more than 0.157 are significantly different, according to Tukey. From the p-values we observe that 6 out of 10 pairs are significantly different, and the largest difference is found between age groups 30+ and 19-29.

```
cld(pt)
```

```
Tukey's HSD
Alpha: 0.05

   Mean G1 G2 G3
30 3.33  A
1  3.14     B
16 3.00     B  C
13 2.94        C
19 2.88        C
```

The compact letter display gives a grouping of the similar levels, and there are three groups of levels that are internaly non-significantly different. 30+ is different from all other levels, whereas 1-12 and 16-19 are similar and 16-19, 13-15 and 19-29 are also similar.

Barley Data

In `barley.rdata` are results from an experiment where the response is yield of barley pr 1000 square meter, and the factors sorts of barley, soil types, types of fertilizers. In addition was the experiment done in two different geographical areas (sites).

- Assume a two factor model including the main effects of `sort` and `soil` and their interaction. State the model and explain all parameters under a sum-to-zero parametrization.

The model can be written as:

$$y_{ijk} = \mu + \alpha_i + \beta_j + (\alpha\beta)_{ij} + \epsilon_{ijk}$$

where, $\epsilon \sim N(0, \sigma^2)$

The parametrization restrictions for "sum-to-zero"" are:

$$\sum_i \alpha_i = 0, \sum_j \beta_j = 0, \quad \sum_i (\alpha\beta)_{ij} = 0 \text{ and } \sum_j (\alpha\beta)_{ij} = 0$$

- Fit the model in R and estimate all parameters

```
options(contrasts = c("contr.sum", "contr.poly"))
mod1 <- lm(Yield ~ sort * soil, data = Barley)
summod1 <- summary(mod1)
summod1$coef
```

```
                Estimate Std. Error t value Pr(>|t|)
(Intercept)        380.9       10.1   37.55 1.70e-25
sort(1)            -23.6       10.1   -2.33 2.73e-02
soil(1)            -43.1       10.1   -4.25 2.14e-04
sort(1):soil(1)     13.8       10.1    1.36 1.84e-01
```

```
summod1$sigma ^ 2
```

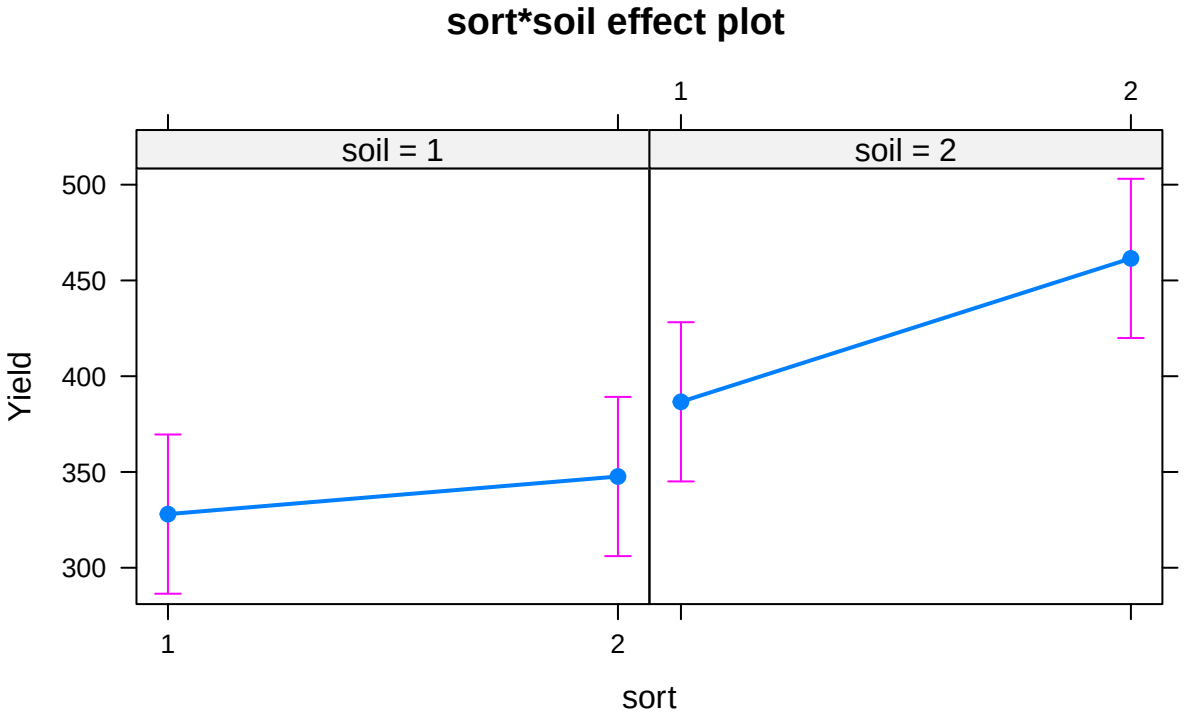
```
[1] 3293
```

From the model summaries we find the estimated parameters to be:

1. The estimated overall mean yield: $\hat{\mu} = 380.94$
2. The estimated effects of sort 1 and 2: $\hat{\alpha}_1$ = -23.625, $\hat{\alpha}_2 = -\hat{\alpha}_1 = 23.625$
3. The estimated effects of soil 1 and 2: $\hat{\beta}_1$ = -43.125, $\hat{\beta}_2 = -\hat{\beta}_1 = 43.125$
4. The estimated interaction effects of sort and soil: $\hat{\alpha\beta}_{11} = 13.812$, $\hat{\alpha\beta}_{12} = -\hat{\alpha\beta}_{11}$ -13.812, $\hat{\alpha\beta}_{21} = -\hat{\alpha\beta}_{11}$ -13.812, $\hat{\alpha\beta}_{22} = -\hat{\alpha\beta}_{21} = -\hat{\alpha\beta}_{12} = 13.812$
5. The estimated within `sort:soil` levels unexplained variability: $\hat{\sigma}^2 = MSE = 3293.21$

- Make an interaction plot and try to conclude about the presence of interaction from the plot. How would you explain interaction effect in this example for a person with experience in agriculture, but minimal statistical experience?

```
plot(allEffects(mod1,confidence.level = .95))
```



From the plot, it seems that a farmer can expect an increase in yield when using sort 2 instead of sort 1 for both types of soil, and there may be a higher gain of sort 2 over sort 1 for soil-type 2 than for soil type 1. If this is so, there is a so-called interaction effect of sort and soil on yield.

- Perform a hypothesis test for the interaction effect. Conclusion?

```
Anova(mod1, type = "III")
```

```
Anova Table (Type III tests)
```

```
Response: Yield
             Sum Sq Df F value  Pr(>F)
(Intercept) 4643628  1 1410.06 < 2e-16 ***
sort          17861  1    5.42 0.02731 *
soil          59513  1   18.07 0.00021 ***
sort:soil      6105  1    1.85 0.18419
Residuals     92210 28
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

The interaction between `soil` and `sort` is insignificant (high p-value). This result indicates that the slight non-parallel tendency of the lines in the interaction plot may be due to random errors. More data would be needed to verify any interaction effect.

- Fit a four factor model with sort, soil, fert and site as factors and with all possible 2-factor, 3-factor and 4-factor interactions. Use `Anova()` from the car-package with argument `type="III"` to produce an ANOVA table. Type III means that all factors are tested as if they were the last factor to be added to the model. Are there any higher order significant effects? Compare the R-squared and the adjusted R-squared values. What can you conclude from these?

```
mod2 <- lm(Yield ~ sort * soil * fert * site, data = Barley)
Anova(mod2, type = "III")
```

```
Anova Table (Type III tests)

Response: Yield
                     Sum Sq Df F value    Pr(>F)
(Intercept)         4643628  1 4503.19   < 2e-16 ***
sort                  17861  1   17.32   0.00073 ***
soil                  59512  1   57.71 0.0000011 ***
fert                   2813  1    2.73   0.11812
site                   1458  1    1.41   0.25176
sort:soil              6105  1    5.92   0.02707 *
sort:fert              2080  1    2.02   0.17472
soil:fert             33930  1   32.90 0.0000306 ***
sort:site             23220  1   22.52   0.00022 ***
```

```
soil:site               595  1    0.58   0.45849
fert:site               105  1    0.10   0.75364
sort:soil:fert         2245  1    2.18   0.15953
sort:soil:site         1405  1    1.36   0.26029
sort:fert:site         7442  1    7.22   0.01622 *
soil:fert:site           12  1    0.01   0.91370
sort:soil:fert:site     406  1    0.39   0.53914
Residuals             16499 16
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

```
summary(mod2)$r.squared
```

```
[1] 0.906
```

```
summary(mod2)$adj.r.squared
```

```
[1] 0.818
```

There is only one interaction effect significant at 5% levels, namely the `sort:fert:site` interaction. However, the least squares estimator is prone to inflated variance estimates and difficulties in finding significance when the number of variables `k` rises compared to the number of observations `N` and if variables are highy correlated. To many variables to estimate from a limited number of observations leaves few degrees of freedom to SSE, and tests with low power. Lack of significance may be an over-fitting problem. By removing some of the least significant variables, the problem is reduced, and a reduced model with significant effects may be identified.

The large difference between R^2 and R^2_{adj} is also an indication of an over-fitted model.

- Fit also a reduced model without site, but all other effects up to 3rd order interactions. Perform a partial F-test with the `anova()` function to test whether site (and all its interactions with the others) should be excluded from the model (See also Exercise set 3 and Ex-3).

```
mod3 <- lm(Yield ~ sort * soil * fert, data = Barley)
anova(mod2, mod3)
```

```
Analysis of Variance Table
```

```
Model 1: Yield ~ sort * soil * fert * site
Model 2: Yield ~ sort * soil * fert
  Res.Df   RSS Df Sum of Sq   F Pr(>F)
1     16 16499
2     24 51142 -8    -34644 4.2 0.0071 **
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

The `anova` result for partial F-test shows that site is needed to a certain degree in the model. The low p-value reject the hypothesis that there is no effect of `site` on `Yield`.

- In the `mixlm`-package there are convenient functions for performing automatic model selection by either `backward()` elimination of factors from a "full-model, by `forward()` addition of factors from a minimal model with only intercept, or a combined `stepwise()` function which combines both forward and backward addition/elimination.

For the backward function the least significant factor is removed from the model in each step if the p-value is larger than testlevel `alpha`. If all factors are significant at any step, the procedure stops. The elimination obeys the so-called marginality principle (hierarchy of factors) which states that any lower order effect or interaction should not be removed from the model if it is part of a higher order significant interaction. This is a good principle for practical data analysis.

Try to run the `backward()` function on the model object you created above with all four factors and interactions. Use `alpha=0.05` as test level. Use the Step-information from the output to explain which factors being excluded at each step. What is the final reduced model?

```
mod4 <- backward(mod2, alpha = 0.05)
```

```
Backward elimination, alpha-to-remove: 0.05

Full model: Yield ~ sort * soil * fert * site
<environment: 0x7f9dc63dac28>

                    Step   RSS AIC R2pred   Cp F value Pr(>F)
sort:soil:fert:site    1 16905 231   0.659 14.4    0.39   0.54
soil:fert:site         2 16918 229   0.696 12.4    0.01   0.91
```

```
sort:soil:site         3 18322 229  0.704 11.8    1.49   0.24
soil:site              4 18917 228  0.724 10.3    0.62   0.44
sort:soil:fert         5 21162 230  0.720 10.5    2.37   0.14
```

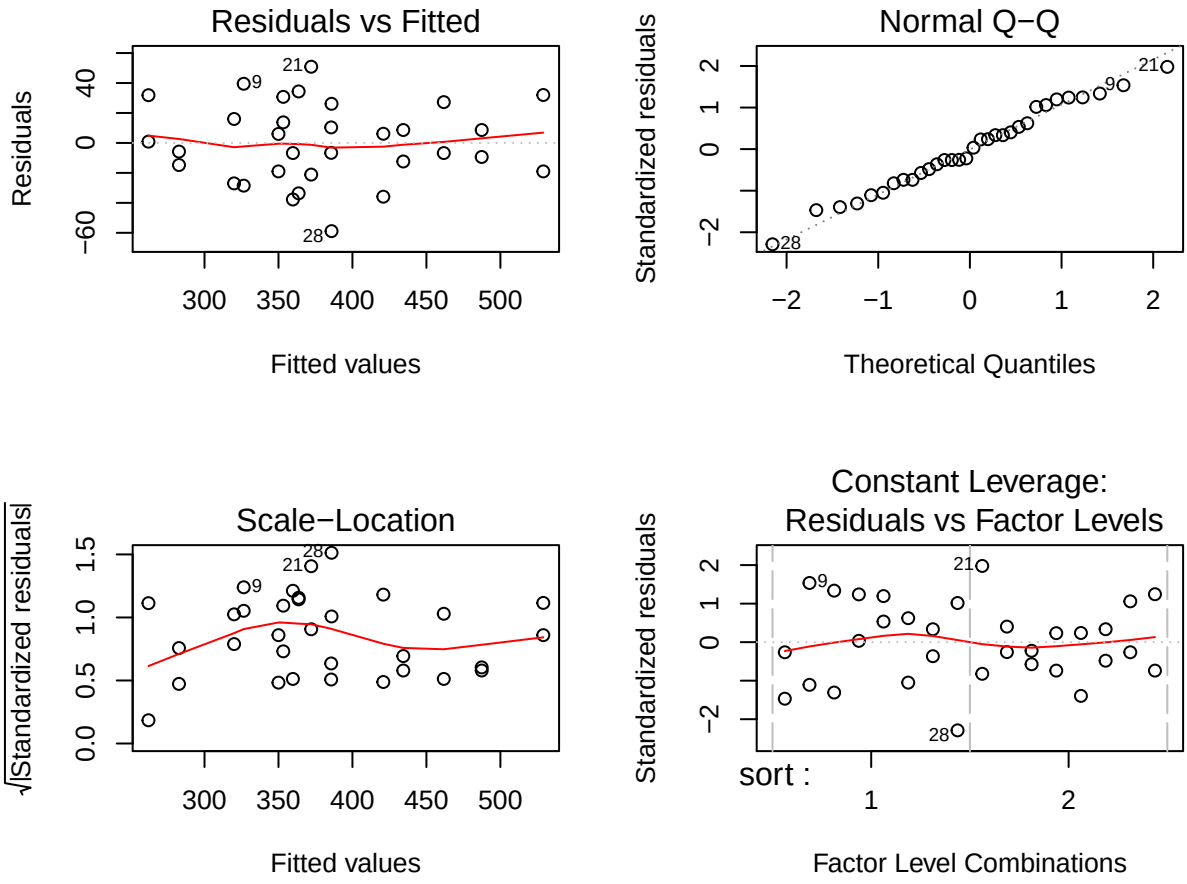
In the first step, the 4th order interaction is removed. In 2nd, 3rd and 4th step some 3rd order and a 2nd order interactions are removed. After removing interaction between `sort`,`soil` and `site` in the 5th step, the resulting model is,

```
Yield ~ sort + soil + fert + site + sort:soil + sort:fert + soil:fert +
    sort:site + fert:site + sort:fert:site
```

- Fit the reduced model and perform a model check using residual analysis.

The `backward` function has fitted the reduced model (her named `mod4`):

```
mod4 <- lm(Yield ~ sort + soil + fert + site + sort:soil +
     sort:fert + soil:fert + sort:site + fert:site + sort:fert:site,
     data = Barley)

par(mfrow = c(2,2))
plot(mod4)
```

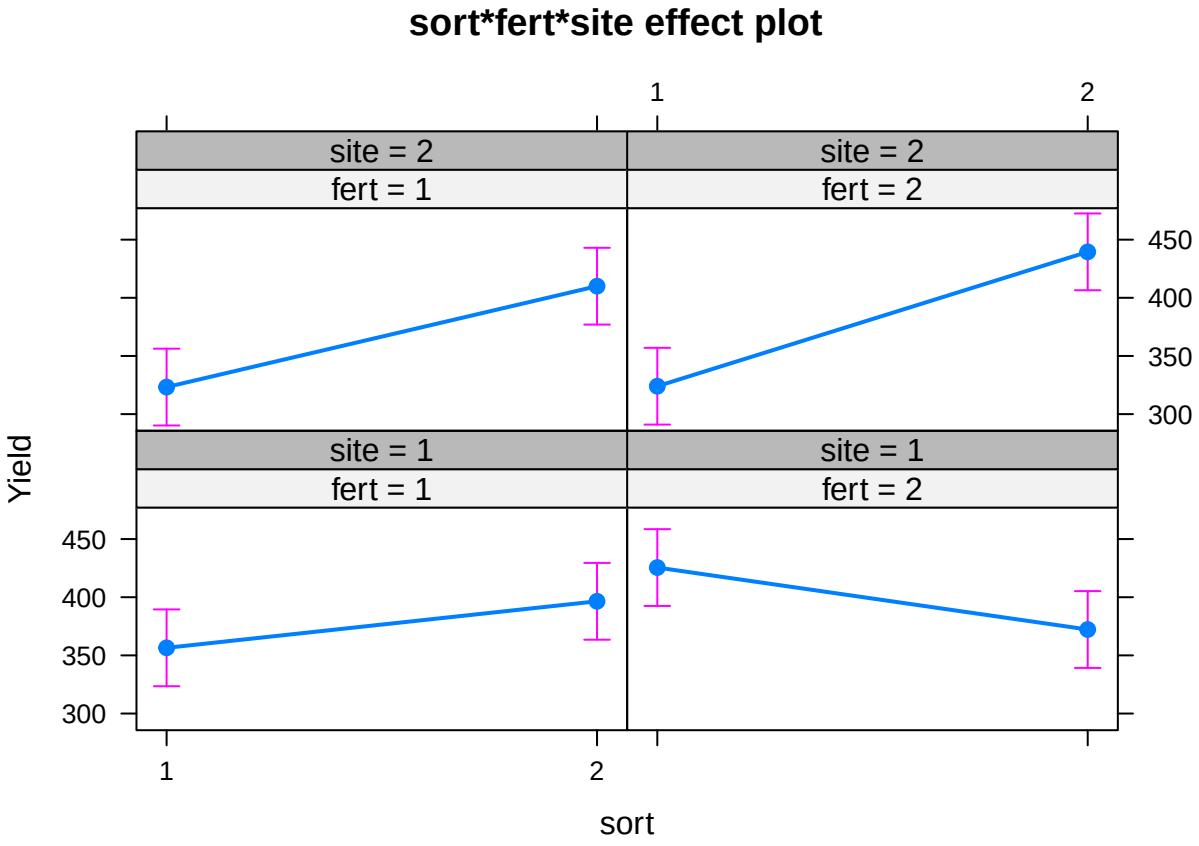


The residual plots give no evidence of any problems with the model assumptions.

- Make an interaction effects plot using the following code:

```
eff <- allEffects(mod4, confidence.level = .95)
plot(eff[3])
```


```
eff <- allEffects(mod4, confidence.level = .95)
plot(eff[3])
```



Try to explain the plot. Why do you think the interaction between sort, fertilizer and site was significant?

The plot shows that, when changing sort from 1 to 2, a farmer can expect different change in average Yield for `site:1` and `site:2` and the difference is not same when using `fertilizer:1` and `fertilizer:2`.

Chapter 5

Multivariate Analysis (PCA)

We will use `trackfieldrecord.rdata` in this exercise

```
load("_data/trackfieldrecords.rdata")
```

We need to load following R package

```
library(mixlm)
```

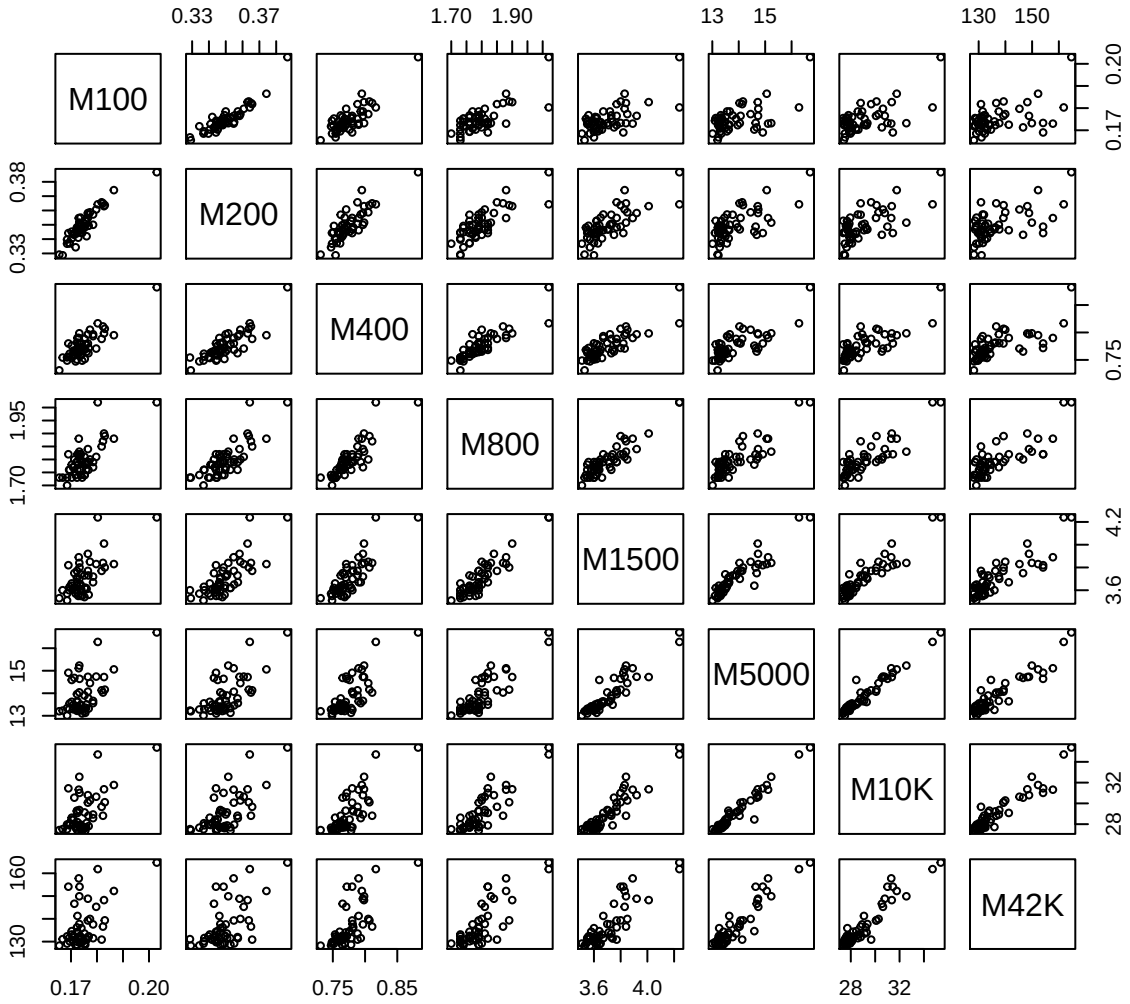
Track and Field data

Load the `trackfieldrecords.rdata` file with the objects `runMen` and `runWomen`containing national records (a few years ago...) for several track and field events like 100m, 200m and so on up to marathon.

- Explore the data for both men and women using the `pairs()` - plotting function (you must exclude the Nation variable since this is non-numeric). Which events appear to be most correlated with each other? Check by using the `cor()` - function.

For dataset: `runMen`

```
pairs(runMen[,-9], cex = 0.7)
```



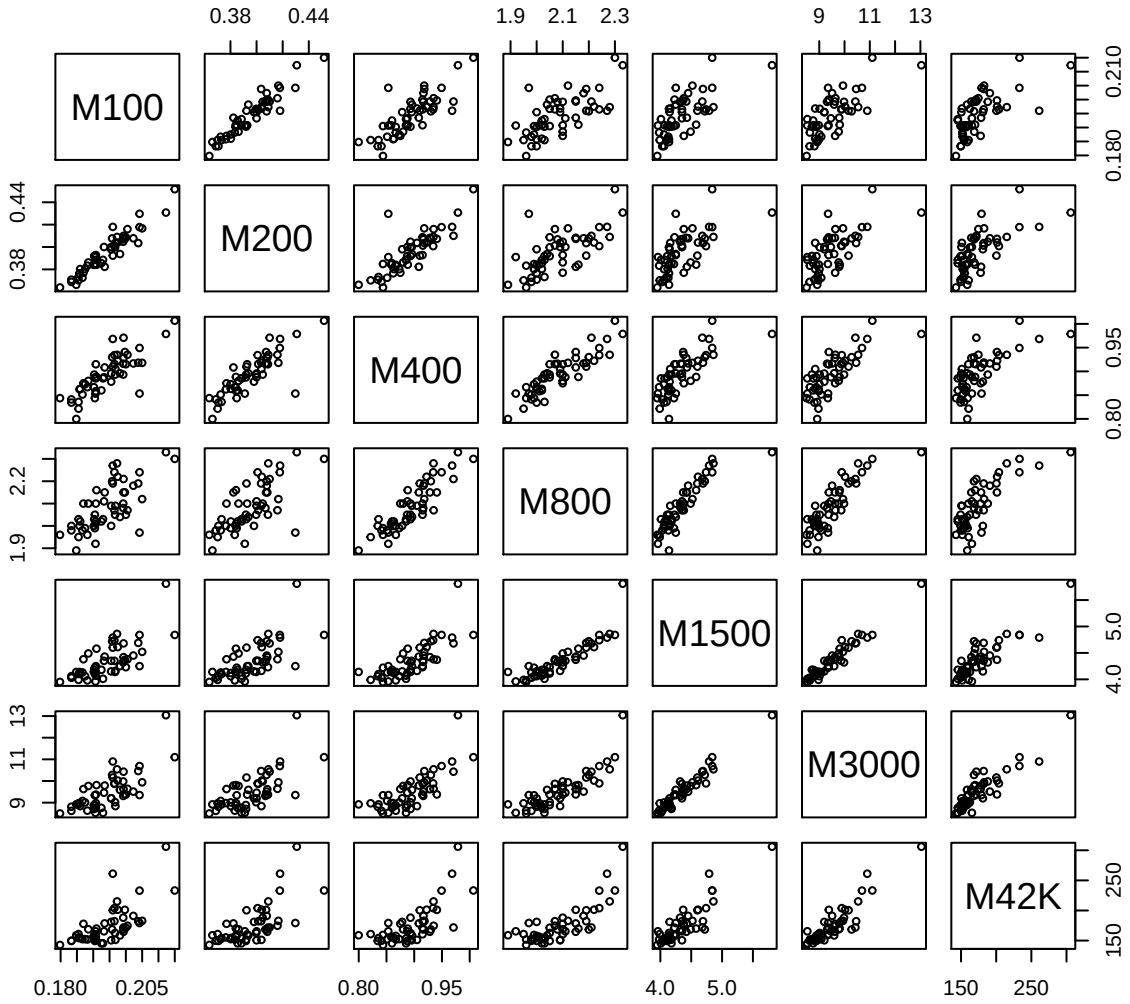

```
cor(runMen[,-9])
```

```
       M100  M200  M400  M800 M1500 M5000  M10K  M42K
M100  1.000 0.918 0.831 0.744 0.686 0.601 0.615 0.504
M200  0.918 1.000 0.840 0.800 0.767 0.682 0.683 0.585
M400  0.831 0.840 1.000 0.866 0.828 0.770 0.779 0.701
M800  0.744 0.800 0.866 1.000 0.914 0.858 0.864 0.803
M1500 0.686 0.767 0.828 0.914 1.000 0.926 0.933 0.865
M5000 0.601 0.682 0.770 0.858 0.926 1.000 0.974 0.931
M10K  0.615 0.683 0.779 0.864 0.933 0.974 1.000 0.943
M42K  0.504 0.585 0.701 0.803 0.865 0.931 0.943 1.000
```

Mens running 5000m have the highest correlation (0.974) with the mens running 10000m.

For dataset: `runWomen`

```
pairs(runWomen[,-8], cex = 0.7)
```




```
cor(runWomen[,-8])
```

```
        M100  M200  M400  M800 M1500 M3000  M42K
M100   1.000 0.947 0.808 0.693 0.704 0.724 0.683
M200   0.947 1.000 0.836 0.690 0.671 0.690 0.682
M400   0.808 0.836 1.000 0.887 0.771 0.767 0.710
M800   0.693 0.690 0.887 1.000 0.894 0.856 0.782
M1500  0.704 0.671 0.771 0.894 1.000 0.968 0.879
M3000  0.724 0.690 0.767 0.856 0.968 1.000 0.899
M42K   0.683 0.682 0.710 0.782 0.879 0.899 1.000
```

Womens running 3000m and 1500m have highest correlation (0.968)

- Run the following command and inspect the results:

```
cor(runWomen[,-8], runMen[,-9])
```

If you were going to "predict" a nation's record for women's M3000, which record among men would you use (rows in the table are women variables, columns are men)?

```
cor(runWomen[,-8], runMen[,-9])
```

```
       M100  M200  M400  M800 M1500 M5000  M10K  M42K
M100  0.650 0.760 0.777 0.804 0.784 0.718 0.713 0.651
M200  0.716 0.799 0.811 0.817 0.766 0.703 0.703 0.621
M400  0.645 0.715 0.792 0.778 0.770 0.738 0.731 0.691
M800  0.595 0.697 0.740 0.785 0.834 0.817 0.820 0.785
M1500 0.517 0.636 0.676 0.848 0.876 0.858 0.868 0.822
M3000 0.571 0.681 0.684 0.856 0.882 0.865 0.864 0.814
M42K  0.612 0.701 0.647 0.811 0.830 0.803 0.817 0.762
```

Men's M1500 shows the highest corrlation to women's M3000 and appears to be the best indicator, but in order to really check this we should run a regression analysis with cross-validation to see which predicts best.

- Run a PCA (with scale=FALSE) on the men's data and print out a summary and the weights (loadings) for the two first PC's. How many components is needed to explain at least 99% of the variation in the data? Try to give an interpretation of PC1, and explain why so few components explains so much of the total variability.

```
pr <- prcomp(runMen[,1:8], scale = FALSE)
summary(pr)
```

```
Importance of components:
                          PC1     PC2     PC3     PC4     PC5     PC6
Standard deviation     9.571 0.64469 0.16890 0.05837 0.02504 0.0117
Proportion of Variance 0.995 0.00451 0.00031 0.00004 0.00001 0.0000
Cumulative Proportion  0.995 0.99964 0.99995 0.99999 1.00000 1.0000
                           PC7     PC8
Standard deviation     0.00553 0.00191
Proportion of Variance 0.00000 0.00000
Cumulative Proportion  1.00000 1.00000
```

```
pr
```

```
Standard deviations (1, .., p=8):
[1] 9.57139 0.64469 0.16890 0.05837 0.02504 0.01174 0.00553 0.00191

Rotation (n x k) = (8 x 8):
           PC1      PC2       PC3      PC4        PC5       PC6       PC7
M100  0.000311  0.00379 -0.000446  0.03426  0.0692868  0.185797 -0.387429
M200  0.000656  0.00660 -0.004506  0.06800  0.0994247  0.274399 -0.850073
M400  0.001759  0.01308 -0.005035  0.13044  0.2647439  0.885091  0.355339
M800  0.005393  0.03175 -0.020469  0.38876  0.8602795 -0.326436  0.027660
M1500 0.014222  0.08536 -0.050540  0.90239 -0.4184781 -0.015186  0.015555
M5000 0.078990  0.37121 -0.921125 -0.08648  0.0031867  0.000642  0.000858
M10K  0.180437  0.90259  0.385347 -0.06522  0.0031326 -0.002815 -0.000183
M42K  0.980290 -0.19749  0.004152  0.00345 -0.0000589  0.000652 -0.000359
            PC8
M100   0.8996602
M200  -0.4330211
M400  -0.0551806
M800  -0.0018789
M1500  0.0073064
M5000  0.0012362
M10K  -0.0009295
M42K   0.0000788
```

Only one component is needed to explain more than 99% of the variation. From the loadings we see that the loading weight for M42K (Marathon) is totally dominating with a weight of 0.98. All other weights are small. PC1 is therefore more or less indentical to the Marathon variable.

PC1 is located in the direction of larget variability, and due to the large scale of marathon times, this variable totally dominates the PCA. In such cases it may be better to use standardized variables (which is equivalent to running the Eigenvalue decomposition on the correlation matrix instead of the covariance matrix of the variables).

- Re-run the PCA with option `scale=TRUE` in `prcomp()`. How many variables are needed to explain 99% of the variation in this case? How much is explained by the

two first components? How would you interprete the loadings of PC1, PC2 and PC3?

```
pr <- prcomp(runMen[,1:8], scale = TRUE)
summary(pr)
```

```
Importance of components:
                          PC1   PC2    PC3    PC4    PC5     PC6     PC7
Standard deviation     2.563 0.953 0.4076 0.3615 0.2859 0.26585 0.21933
Proportion of Variance 0.821 0.114 0.0208 0.0163 0.0102 0.00883 0.00601
Cumulative Proportion  0.821 0.935 0.9557 0.9720 0.9822 0.99106 0.99707
                           PC8
Standard deviation     0.15305
Proportion of Variance 0.00293
Cumulative Proportion  1.00000
```

```
pr
```

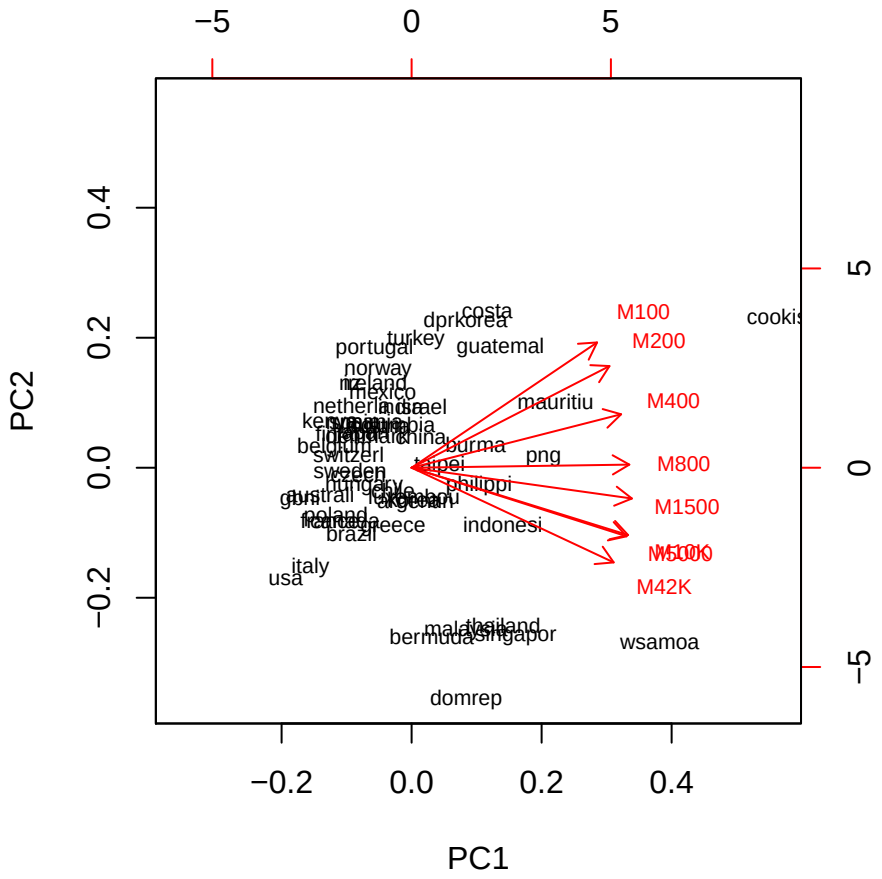
```
Standard deviations (1, .., p=8):
[1] 2.563 0.953 0.408 0.361 0.286 0.266 0.219 0.153

Rotation (n x k) = (8 x 8):
        PC1     PC2    PC3     PC4    PC5     PC6     PC7      PC8
M100  0.315  0.5716  0.322 -0.1783  0.269 -0.5781  0.1425 -0.10781
M200  0.336  0.4638  0.372  0.2485 -0.158  0.6498 -0.1218  0.09974
M400  0.356  0.2439 -0.615 -0.5946 -0.236  0.1619 -0.0119  0.00229
M800  0.369  0.0142 -0.496  0.5214  0.541 -0.0318 -0.2233  0.03623
M1500 0.374 -0.1404 -0.105  0.4103 -0.494 -0.1747  0.6048 -0.14352
M5000 0.365 -0.3129  0.194 -0.0463 -0.237 -0.1448 -0.5974 -0.54333
M10K  0.367 -0.3071  0.180 -0.0985 -0.120 -0.2202 -0.1728  0.79734
M42K  0.343 -0.4319  0.228 -0.3176  0.489  0.3413  0.4028 -0.15986
```

Now we need 6 components to achieve 99% explained variance. Two components explain about 93.5% of the total variance. The loadings for PC1 are almost identical for all variables, hence PC1 is close to identical to the average run record across all distances for each country. PC2 has weights ranging from highly negative for marathon to highly positive for M100. This PC therefore contrasts short versus long runs. PC3 is a component that contrasts medium long distances (400, 800 and 1500 m) and either short or long distances. This component appears to extract information about how these distances differ from both

sprint and endurance distances.

Make a biplot with the first two components. You may use the argument "xlabs" in biplot to indicate that "Nations" should be used to label the scores from each country. Give comments to how the nations cluster relative to the loadings.

```
biplot(pr, xlabs = runMen$Nation, cex = 0.7)
```



On the first axis (PC1) we observe that Cook's Islands and West Samoa have the largest weights, and they therefore have on average poor (long time) national records for all distance. At the other end we find USA and others with on average good national records. Along PC2 (vertically) we find those with relatively poor times on long distances, but relatively good times on short, at the bottom (Dom. Repub, Bermuda, Singapore, Malaysia, Thailand and West Samoa) whereas at the top we find countries with poor records on short distances compared to their long distance records (Costa Rica, North-Korea, Cook's Island and others).

- Let's try to predict the 3000M national records for women using the men's data. First use a least squares approach using the men's variables directly as predictor for

women's M3000. To accomplish this use `runWomen$M3000` as response in `lm()`. Are there any significant variables? What is the R^2 and the adjusted R^2 values?

```
lmmod <- lm(runWomen$M3000 ~ M100 + M200 + M400 + M800 + M1500 +
              M5000 + M10K + M42K, data = runMen)
(lm_sumry <- summary(lmmod))
```

```
Call:
lm(formula = runWomen$M3000 ~ M100 + M200 + M400 + M800 + M1500 +
    M5000 + M10K + M42K, data = runMen)

Residuals:
    Min      1Q  Median      3Q     Max
-0.7333 -0.2060 -0.0537  0.2496  0.7184

Coefficients:
             Estimate Std. Error t value Pr(>|t|)
(Intercept)  -6.09205    1.98465   -3.07   0.0037 **
M100        -23.17895   23.87260   -0.97   0.3370
M200         18.93566   13.76942    1.38   0.1762
M400        -11.69187    5.19182   -2.25   0.0295 *
M800          6.06528    2.25105    2.69   0.0100 *
M1500         1.70738    1.16573    1.46   0.1503
M5000         0.20068    0.28632    0.70   0.4871
M10K          0.08099    0.14783    0.55   0.5866
M42K         -0.00202    0.01715   -0.12   0.9070
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

s: 0.357 on 43 degrees of freedom
Multiple R-squared: 0.84,
Adjusted R-squared: 0.81
F-statistic: 28.2 on 8 and 43 DF,  p-value: 1e-14
```

```
lm_sumry[c("r.squared", "adj.r.squared")]
```

```
$r.squared
```

```
[1] 0.84

$adj.r.squared
[1] 0.81
```

Two variables are significant at 5% level in this fitted model, M800 and M400. The R^2-values indicate more than 80% explained variance. There is a slight difference between the adjusted and the non-adjusted R^2 indicating that there may be too many variables included in the model.

- Either perform a manual elimination of insignificant variables, or run `backward()` from the mixlm-package to find a reduced model with only significant effects (5% testlevel). Which variables do you end up having in your model?

```
red.mod <- backward(lmmod, alpha = 0.05)
```

```
Backward elimination, alpha-to-remove: 0.05

Full model: runWomen$M3000 ~ M100 + M200 + M400 + M800 + M1500 + M5000 +
    M10K + M42K
<environment: 0x7f9dc4481778>

      Step  RSS  AIC R2pred   Cp F value Pr(>F)
M42K     1 5.49 -101  0.644 7.01    0.01  0.907
M10K     2 5.53 -102  0.687 5.32    0.32  0.576
M100     3 5.64 -104  0.730 4.15    0.86  0.359
M200     4 5.75 -104  0.746 3.03    0.92  0.343
M5000    5 6.20 -103  0.755 4.55    3.67  0.061 .
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

```
summary(red.mod)
```

```

Call:
lm(formula = runWomen$M3000 ~ M400 + M800 + M1500, data = runMen)

Residuals:
    Min      1Q  Median      3Q     Max
```

```
-0.6139 -0.2798 -0.0541  0.2591  0.7221

Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept)   -6.930      1.687   -4.11  0.00015 ***
M400         -11.241      4.286   -2.62  0.01166 *
M800           6.661      2.211    3.01  0.00412 **
M1500          3.556      0.806    4.41 0.000058 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

s: 0.359 on 48 degrees of freedom
Multiple R-squared: 0.819,
Adjusted R-squared: 0.808
F-statistic: 72.6 on 3 and 48 DF,  p-value: <2e-16
```

In addition to M400 and M800 I find M1500 to be highly significant after removing other variables. This "covered" effect from the full model was because of the inflated variances due to multicollinear variables in the full model.

- Fit another model using all principal component scores from the men's data as predictors for women's M3000. The scores are stored in the principal component object as element names `x`. Which components are significant at a 5% test level? Compare the R^2 values with those from the full model using all original variables as predictors.

```
#You need to transform the scores into a data.frame first
PCdata <- as.data.frame(pr$x)
pcrmod <- lm(runWomen$M3000 ~ PC1 + PC2 + PC3 + PC4 + PC5 +
               PC6 + PC7 + PC8, data = PCdata)

summary(pcrmod)
```

```
Call:
lm(formula = runWomen$M3000 ~ PC1 + PC2 + PC3 + PC4 + PC5 + PC6 +
    PC7 + PC8, data = PCdata)
```

```
Residuals:
    Min      1Q  Median      3Q     Max
-0.7333 -0.2060 -0.0537  0.2496  0.7184

Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept)  9.49673    0.04956  191.61  < 2e-16 ***
PC1          0.27603    0.01952   14.14  < 2e-16 ***
PC2         -0.17201    0.05249   -3.28  0.00208 **
PC3          0.03614    0.12279    0.29  0.76990
PC4          0.53593    0.13844    3.87  0.00036 ***
PC5          0.00982    0.17503    0.06  0.95551
PC6          0.04261    0.18825    0.23  0.82201
PC7         -0.09547    0.22818   -0.42  0.67772
PC8          0.04242    0.32698    0.13  0.89737
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

s: 0.357 on 43 degrees of freedom
Multiple R-squared: 0.84,
Adjusted R-squared: 0.81
F-statistic: 28.2 on 8 and 43 DF,  p-value: 1e-14
```

Components 1,2 and 4 are highly significant, the others not. The R^2 values are identical to the full model on the orginal variables since we use all available components. The information content in PC1-PC8 is therefore the same as in the eight original variables.

- Perfom a model reduction also for the PCR-model by excluding Principal components until you have only PC's significant at 5% test level. Compare the estimated regression coefficients between the full and the reduced PCR-models. Why do you think the effects don't change for the variables retained in the model?

```
pcr.red.mod <- backward(pcrmod, alpha = 0.05)
```

```
Backward elimination, alpha-to-remove: 0.05

Full model: runWomen$M3000 ~ PC1 + PC2 + PC3 + PC4 + PC5 + PC6 + PC7 + PC8
<environment: 0x7f9dc56ea6e0>
```

```
    Step  RSS  AIC R2pred     Cp F value Pr(>F)
PC5    1 5.49 -101  0.632  7.003    0.00   0.96
PC8    2 5.50 -103  0.683  5.020    0.02   0.90
PC6    3 5.50 -105  0.733  3.071    0.05   0.82
PC3    4 5.51 -107  0.749  1.158    0.09   0.76
PC7    5 5.54 -108  0.763 -0.667    0.19   0.66
```

```
summary(pcr.red.mod)
```

```

Call:
lm(formula = runWomen$M3000 ~ PC1 + PC2 + PC4, data = PCdata)

Residuals:
    Min      1Q  Median      3Q     Max
-0.7232 -0.2207 -0.0461  0.2415  0.6907

Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept)   9.4967     0.0471  201.67  < 2e-16 ***
PC1           0.2760     0.0186   14.88  < 2e-16 ***
PC2          -0.1720     0.0499   -3.45  0.00118 **
PC4           0.5359     0.1315    4.07  0.00017 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

s: 0.34 on 48 degrees of freedom
Multiple R-squared: 0.839,
Adjusted R-squared: 0.829
F-statistic: 83.3 on 3 and 48 DF,  p-value: <2e-16
```

The reduced model has only PC1, PC2 and PC4 as predictors, and the R^2 is almost as high as for the full model. The estimated effects are identical due to the fact that the PC's are orthogonal to each other and explain independent variability.

- For special interested: Use the estimated effects (alphas from the lecture) from the reduced PCR-model to compute PCR-estimated regression coefficients (betas in

the lecture) for the original variables back back-rotation. Compare the estimated regression coefficients from the PCR-approach with Least squares estimates using original (BUT SCALED) variables.

```
#PCR-estimated betas using components 1,2 and 4. The %*% operator is the inner-product
#multiplier in R
PCRest <- pr$rotation[,c(1,2,4)] %*% (coef(pcr.red.mod)[-1])

#Scaling the original variables and re-running the least squares model:
runMen.scaled <- as.data.frame(scale(runMen[,-9]))
lmmod2 <- lm(runWomen$M3000 ~ M100 + M200 + M400 + M800 + M1500 +
               M5000 + M10K + M42K, data = runMen.scaled)

#Estimates without intercept.
Estimates <- cbind(coef(lmmod2)[-1],PCRest)
colnames(Estimates) <- c("Least Squares", "PCR")
Estimates
```

```
      Least Squares      PCR
M100        -0.1355 -0.10698
M200         0.2015  0.14607
M400        -0.2789 -0.26247
M800         0.3879  0.37900
M1500        0.2673  0.34725
M5000        0.1622  0.12968
M10K         0.1477  0.10142
M42K        -0.0189 -0.00125
```

For most of the variables the PCR-estimates are closer to zero (shrinkage effect) which induces a bias, but as lectured, the PCR-model may have smaller variance for the estimates due to avoidance of the multicollinearity problem. It seems like PCR has down-weighted the short and long distances compared to the Least Squares approach, which seems reasonable.

Chapter 6

Multivariate Analysis (PCR, PLS)

In this exercise we will study a data set used in the paper by Liland et al (2009) (`http://www.sciencedirect.com/science/article/pii/S0169743909001476`) were PLS-regression was used to predict the percentage of cow-milk in mixtures of cow, goat and ewe milk.

```
load("_data/maldidata.rdata")
```

An excerpt from the paper explains why this is interesting:

> "Quality assurance is an important issue in modern food production. The products are expected to have the right taste, smell, texture and appearance. In addition they should be safe, wholesome, authentic and have a composition that complies with regulations. As a practical example this paper will analyse data simulating milk adulteration. In real life such adulteration could occur where one type of milk is replaced by, or mixed with, another deliberately, by accident or because of failing routines.
>
> There are several reasons why detection of the concentrations of cow, goat and ewe milk is of importance. Pure products of goat milk may be used as a supplement of milk for humans who are born with allergic reactions towards cow milk. Some mixed milk products are produced with regard to specifications which specify the mixture of milk from cow, goat and/or ewe. Professionals and consumers want to control the origin of milk in order to be sure that they get products following specifications and labelling. Farmers producing more than one type of milk might be tempted to add cow milk to goat or ewe milk as

this would result in higher quantities of the better paid milk variants"

For the exercise we will need `pls` package.

```
library(pls)
```

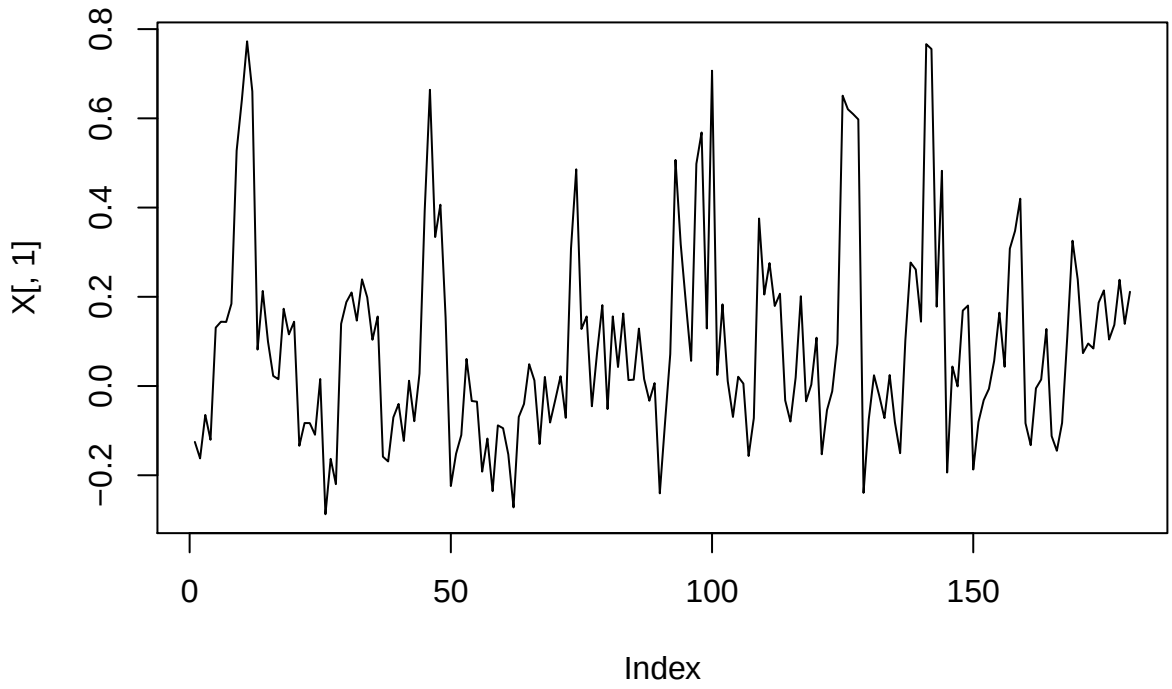
Prediction of cow milk percentage

In the data file "`maldidata.rdata`" you find four objects:

- `Y` : The percentage of cow-milk for 4 replicates of 45 different milk mixtures
- `X` : Mass Spectrometry data (`MALDI-TOF`) for the milk samples. The 6179 variables is a quantification of molecule "`size`" and "`charge`" in a sample. For simplicity we may say that the size of molecules increases from variable 1 to variable 6179. The measurements are then amounts of molecules of different sizes. The method is used to separate proteins, peptides and other ionizable compunds.
- `Ytest` : Cow-milk percentages for 45 extra test samples
- `Xtest` : The `MALDI-TOF` values for the test samples.

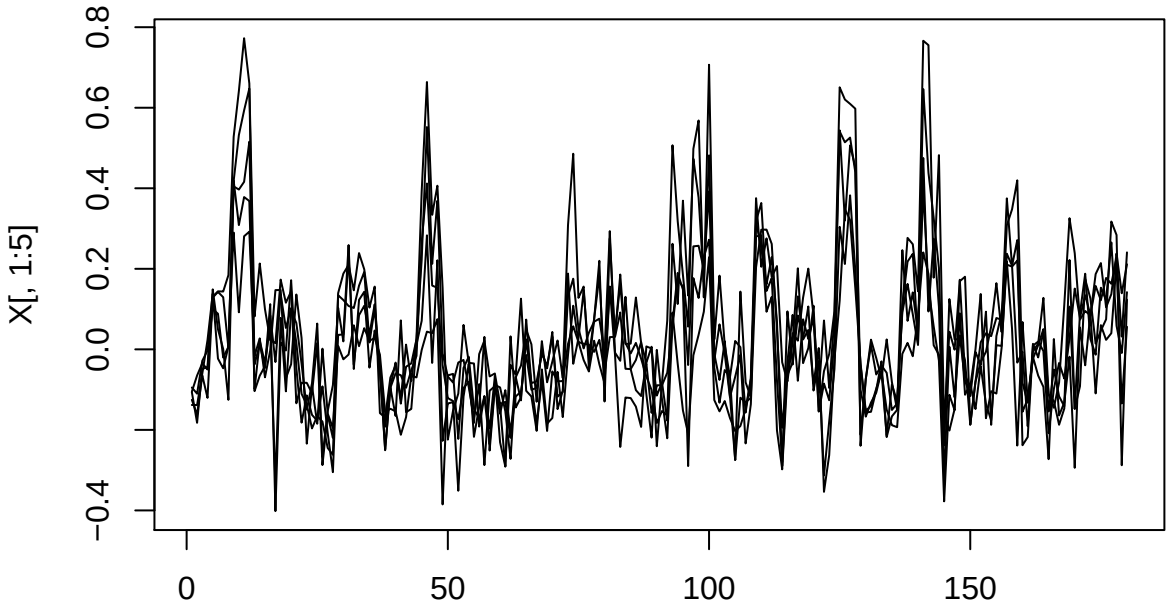
You may plot the spectra in `X` one-by-one as,:

```
plot(X[, 1], type = "l")
```



We can also plot multiple (all) spectra together, takes more time.

```
matplot(X[, 1:5], type = "l", lty = 1, col = "black")
```



The peaks show molecule sizes that are abundant in the sample.

- First run a PCA on `X`. How many components are needed to explain 80% and 90% of the variability in `X`?

```
pr <- prcomp(X)
summary(pr)$importance[, 1:14]
```

```
                            PC1    PC2    PC3    PC4    PC5    PC6     PC7
Standard deviation     12.502 4.4833 3.0218 2.5373 2.0112 1.7430 1.30637
Proportion of Variance  0.648 0.0833 0.0379 0.0267 0.0168 0.0126 0.00708
Cumulative Proportion   0.648 0.7313 0.7691 0.7958 0.8126 0.8252 0.83228
                            PC8     PC9    PC10    PC11    PC12    PC13
Standard deviation     1.0875 1.05133 0.96666 0.91363 0.84363 0.83145
Proportion of Variance 0.0049 0.00458 0.00387 0.00346 0.00295 0.00287
Cumulative Proportion  0.8372 0.84176 0.84564 0.84910 0.85205 0.85491
                           PC14
Standard deviation     0.81638
Proportion of Variance 0.00276
Cumulative Proportion  0.85768
```

We need 5 components to explain 80% and 36 to explain 90% (check yourself). Hopefully

we do not need to use all X-information to predict `Y`.

- Compute the correlations between Y and the principal components. How can you use this get an idea of how many components PLS-regression will require to make a good model for cow-milk prediction?

```
cor(Y, pr$x)
```

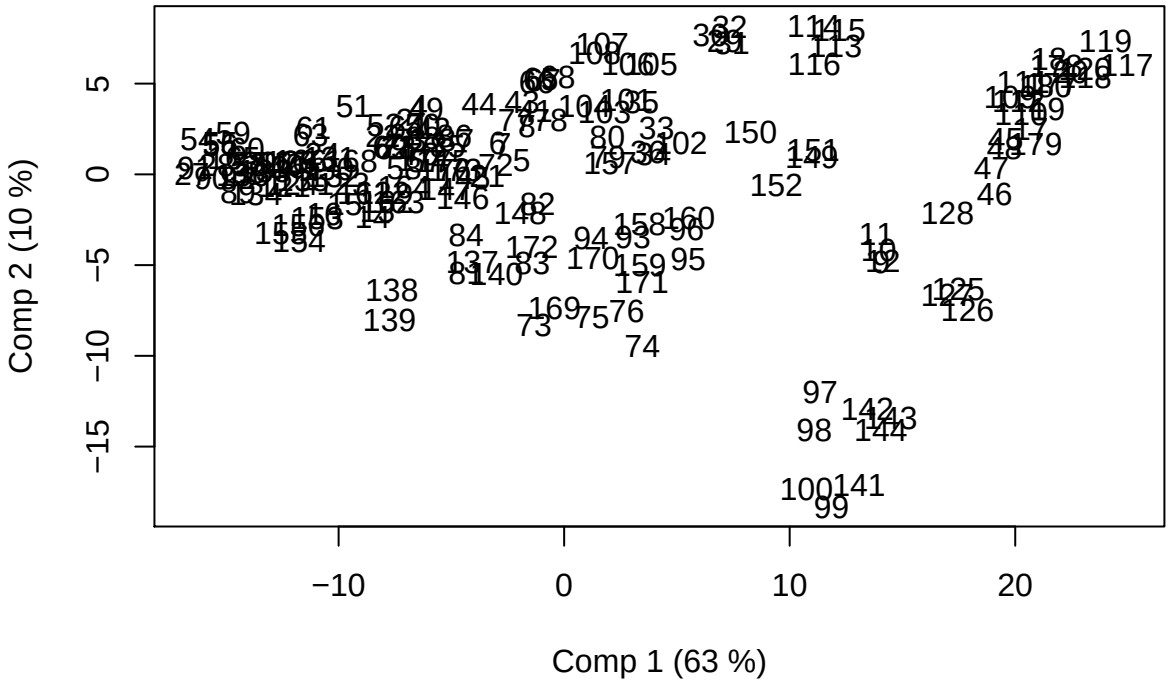
```
       PC1    PC2    PC3    PC4    PC5     PC6   PC7    PC8      PC9
[1,] 0.528 -0.754 0.0338 -0.225 0.0744 -0.0503 0.015 -0.166 -0.00757
       PC10   PC11    PC12   PC13   PC14    PC15    PC16   PC17    PC18
[1,] -0.0754 -0.137 -0.0432 0.0183 0.0167 -0.0155 -0.0263 0.0222 -0.0187
        PC19    PC20    PC21    PC22    PC23    PC24    PC25    PC26
[1,] -0.00495 -0.0413 0.00649 -0.0187 -0.0442 -0.0069 -0.0411 0.00412
       PC27  PC28    PC29   PC30     PC31   PC32    PC33   PC34     PC35
[1,] -0.0123 0.017 -0.0147 0.0387 0.000618 0.0185 -0.0213 0.0478 -0.00964
       PC36     PC37  PC38   PC39     PC40    PC41   PC42   PC43    PC44
[1,] -0.0106 -0.00503 0.021 -0.011 -0.00874 -0.0191 -0.014 0.0082 -0.0124
      PC45    PC46   PC47    PC48   PC49     PC50     PC51    PC52
[1,] 0.0176 0.00597 0.0141 -0.0193 0.0217 -0.00107 -0.00454 0.00781
       PC53    PC54   PC55     PC56    PC57    PC58     PC59      PC60
[1,] 0.00674 -0.0041 0.0027 -0.00404 -0.0269 0.00521 -0.00471 -0.000586
      PC61    PC62   PC63    PC64     PC65    PC66   PC67    PC68
[1,] 0.0124 -0.0142 0.0125 -0.0181 -0.00766 0.00276 0.0146 -0.0221
        PC69     PC70     PC71     PC72   PC73    PC74    PC75   PC76
[1,] -0.00245 -0.00385 -0.00334 -0.00403 -0.038 -0.0394 0.00702 0.0103
      PC77    PC78    PC79     PC80    PC81     PC82   PC83    PC84
[1,] -0.017 -0.0104 -0.0116 -0.00895 0.00664 -0.00716 0.0086 -0.0205
       PC85  PC86   PC87    PC88   PC89    PC90     PC91    PC92     PC93
[1,] -0.0217 0.018 0.0284 0.00673 0.0166 0.00445 -0.00696 -0.0109 -0.00113
      PC94   PC95    PC96     PC97   PC98     PC99    PC100    PC101
[1,] 0.0244 0.0304 -0.0186 -0.00388 0.0214 -0.00707 -0.00238 0.000283
     PC102    PC103   PC104   PC105  PC106  PC107   PC108   PC109  PC110
[1,] 0.0251 -0.00757 -0.0175 -0.0259 0.0244 -0.026 0.00272 -0.0157 0.0142
      PC111  PC112   PC113  PC114   PC115   PC116 PC117    PC118   PC119
[1,] -0.0115 -0.009 -0.0115 0.0299 0.00924 0.00246 -0.01 -0.00907 -0.0242
      PC120   PC121  PC122   PC123   PC124   PC125   PC126   PC127  PC128
```

```
[1,] 0.00516 -0.0066 0.0147 0.00467 -0.0254 -0.0224 -0.0124 0.00816 0.0101
       PC129   PC130    PC131   PC132    PC133   PC134    PC135  PC136
[1,] -0.0142 -0.0119 -0.00018 -0.0108 -0.00172 0.00275 -0.00635 0.0103
       PC137   PC138   PC139    PC140    PC141  PC142    PC143   PC144
[1,] -0.0087 0.00552 0.00742 -0.00805 -0.00327 0.0159 -0.00109 0.00291
        PC145    PC146    PC147    PC148   PC149    PC150  PC151   PC152
[1,] -0.00378 -0.00148 -0.00736 -0.00656 0.00354 -0.00579 0.0034 0.00252
      PC153    PC154   PC155  PC156  PC157    PC158    PC159   PC160
[1,] 0.0015 -0.00918 -0.0111 0.0232 0.0108 -0.00734 -0.00148 0.00503
        PC161    PC162    PC163   PC164    PC165   PC166   PC167   PC168
[1,] -0.00242 -0.00583 -0.00701 0.00558 -0.00344 0.00436 0.00368 0.00529
      PC169   PC170   PC171    PC172    PC173  PC174   PC175    PC176
[1,] -0.015 -0.0092 -0.0134 -0.00933 -0.00255 0.0113 0.00024 -0.000418
       PC177   PC178  PC179  PC180
[1,] -0.0057 -0.0103 0.0218 0.0288
```

Components 1, 2, 4 and perhaps 8 are moderately to highly correlated with `Y`. Supposedly 3 to 4 components will be necessary for PLSR.

- Fit a PLS-regression model using `Y` as response and `X` as predictor (You may simply write `Y ~ X` as your model call in `plsr`. Also use `ncomp=10` as extra argument to only fit 1 to 10 components). Use the `scoreplot()` function to make a scoreplot. Check the help-file for this function to see how you can chose the component numbers to plot, and how you can put labels to your observations. Plot component 1 against 2 and put observation numbers 1:180 as labels. If the noise level of the measurements is low, the replicates should group in clusters of size four (obs 1,2,3 and 4 are from the same mixture, and so on). Do you see any tendency to this?

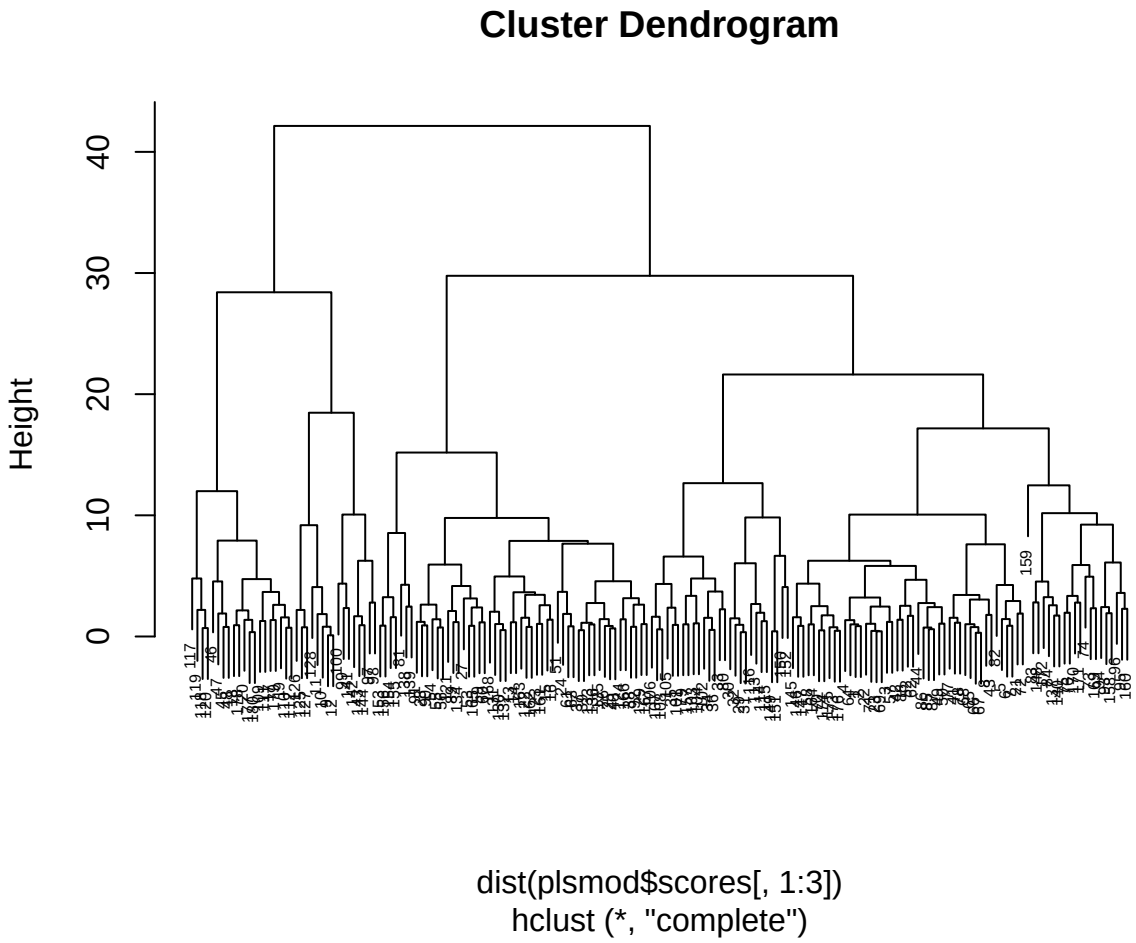
```
plsmod <- plsr(Y ~ X, ncomp = 10)
scoreplot(plsmod, comps = c(1,2), labels = 'names', pch = 0.7)
```



We observe that there are clusters of observations and that there is a tendency of successive numbers to be close in the scoreplot. Cluster sizes are difficult to determine.

- Perform hierarchical clustering of the samples using the 3 first PLS-component scores as input variables. Try both "complete" and "average" agglomeration method and make a dendrogram. Are the replicate clusters more apparent in the dendrogram than in the scoreplot? Is there any samples that are very different from all others?

```
clust1 <- hclust(dist(plsmod$scores[,1:3]), method = "complete")
plot(clust1, cex = 0.5)
```



From the dendrogram we observe several clusters of size four, and some of three with successive observation numbers. This implies that the replicates are more similar to each other than samples from different milk samples. Sample 159 seems to be an outlier, very different from all others.

- Use K-means clustering with K=45 on the three first PLS-component scores. How do the replicates cluster?

```
clust2 <- kmeans(plsmod$scores[,1:3], centers = 45)
clust2$cluster
```

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
39	39	39	39	13	13	13	44	20	20	20	20	31	31	31	31	38	15
19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36
38	15	13	1	1	40	25	25	14	17	2	2	2	2	22	32	22	32
37	38	39	40	41	42	43	44	45	46	47	48	49	50	51	52	53	54
25	17	25	25	44	23	9	34	3	3	3	3	11	11	19	23	17	24

```
 55  56  57  58  59  60  61  62  63  64  65  66  67  68  69  70  71  72
 24  24  30  30  14  14  40  23  40  39   9   9   9   9   1  30   1  13
 73  74  75  76  77  78  79  80  81  82  83  84  85  86  87  88  89  90
 12  45  45  45  44  44  33  22   5  13  12  35  34  34  34  23  14  17
 91  92  93  94  95  96  97  98  99 100 101 102 103 104 105 106 107 108
 17  17   6   6  28  28  42  42  42  42  22  32  43  43   7   7   7   7
109 110 111 112 113 114 115 116 117 118 119 120 121 122 123 124 125 126
 38  38  38  38   4   4   4   4  37  37  37  37  41   8   8  41  29  29
127 128 129 130 131 132 133 134 135 136 137 138 139 140 141 142 143 144
 29  26  25  16  16  16  25  41  25  25  35   5   5  35  42  42  42  42
145 146 147 148 149 150 151 152 153 154 155 156 157 158 159 160 161 162
 21  21  21  21  36  36  36  36  18  18  18  18  33   6  27  28   8   8
163 164 165 166 167 168 169 170 171 172 173 174 175 176 177 178 179 180
  8  30  14  41  41  16  12  45  45  35  10  30  10  10  15  15   3  15
```

Many replicates fall into the same clusters, but some clusters observations from more than one "true" cluster. E.g. cluster number 43 contains observations (97, 98, 99, 100) and (141, 142, 143, 144), which is a mixture of four true replica clusters. We conclude that the replicates are somewhat similar, but there is some noise in the `MALDI-TOF` data which makes similar milk mixtures hard to distinguish.

- We will use cross-validation to estimate the expected prediction error of PLSR and to choose the appropriate number of components. Instead of using Leave-One-Out Cross-validation we will exclude all four replicates in a "Leave-Four-Out" type of Cross-validation. Why is this smart?

Since the replicates are from the same mixture, they are not independent. If we use Leave-One-Out CV the three replicates still contained in the training set will make the model "too good" to predict the given mixture, and we will under-estimate the prediction error of new samples.

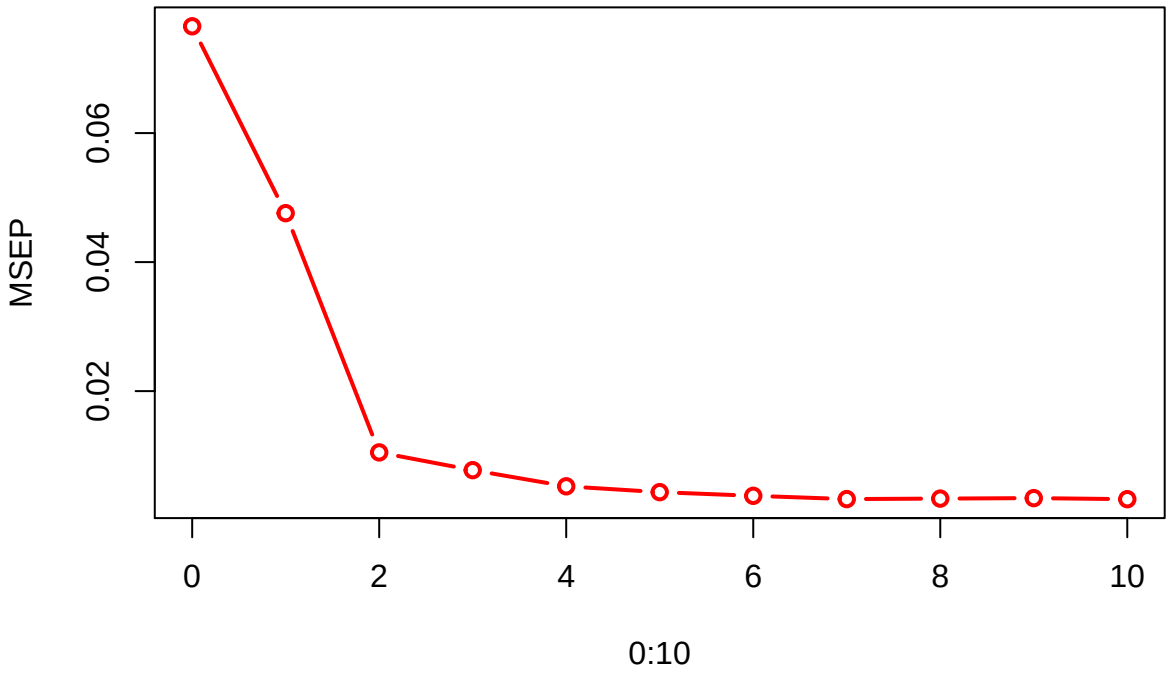
- Refit the plsmodel from exercise c. but add the arguments `validation="CV"`, `segments=45` and `segment.type="consecutive"` in the plsr-model call. This sets up the "Leave-Four-Out" CV to be performed.

```
plsmod <- plsr(Y ~ X, ncomp = 10, validation = "CV",
               segments = 45, segment.type = "consecutive")
```

- The sum of squared prediction errors (PRESS) for different number of components

is given in the `validation$PRESS` element of the fitted pls-model. The null-model PRESS (prediction using the mean-response) is given in the `validation$PRESS0` element. You find the MSEP-values (Mean Squared Error of Prediction) by dividing the PRESS by the number of observations (N=180). Make a prediction error plot of MSEP with 0 to 10 components. How many components do you think gives satisfying prediction of cow-milk content in new mixtures? Remember that simple models are often better than complex.

```
MSEP <- c(plsmod$validation$PRESS0, plsmod$validation$PRESS)/180
plot(0:10, MSEP, type = "b", col = 2, lwd = 2)
```



The prediction error is heavily reduced as we introduce components 1 and 2, but there is a small gain by adding components 3, 4 and 5. Simple models are usually more robust, so I would not go any further than 5 components here.

- Predict the cow-milk content of the test samples using `Xtest` as newdata in the `predict`-function and use the number of components you found as best from the previous exercise. Save the predictions into an object called `pred`. (See `?predict.mvr` for the help-file to predict for pls-objects.). The predict-function returns an array of dimension [45,1,1] of predictions. You can extract all predictions by `pred[,1,1]`.

```
pred <- predict(plsmod, newdata = Xtest, ncomp = 5)
```

Copy the folowing code into R and execute:

```
MSEPfunc <- function(y, yhat){
    mean((y - yhat) ^ 2)
}
```

- Use `MSEPfunc()` to compute the MSEP-value for the test-predictions using `Ytest` and the predicted values as inputs. Did the cross-validation under-estimate the prediction error?

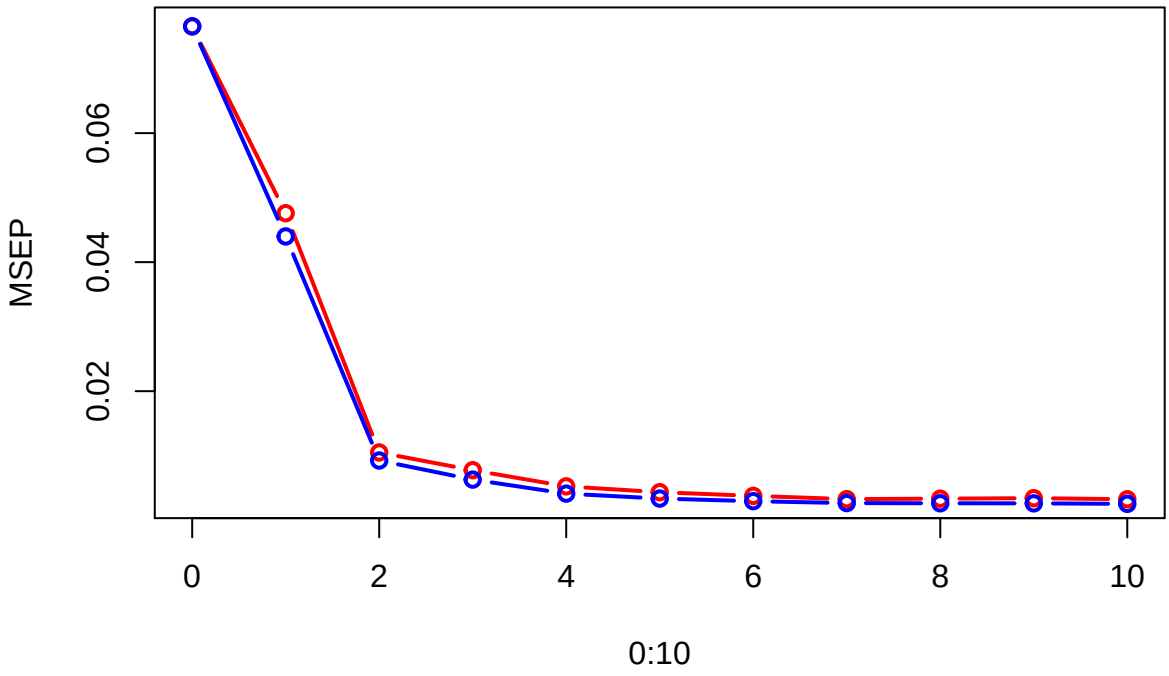
```
MSEPfunc(Ytest, pred[,1,1])
```

```
[1] 0.00692
```

The MSEP-value is slightly larger than the value found for five components using Cross-validation, but the order of magnitude is the same.

- EXTRA for those interested. Redo the exercises g. and h. with Leave-One-Out CV. (See also lecture notes Lesson 7.) Compare the MSEP-values you find with the previous CV-routine.

```
plsmod2 <- plsr(Y ~ X, ncomp = 10, validation = "LOO")
MSEP2 <- c(plsmod2$validation$PRESS0, plsmod2$validation$PRESS)/180
plot(0:10, MSEP, type = "b", col = 2, lwd = 2)
points(0:10, MSEP2, type = "b", col = 4, lwd = 2)
```



We see that LOO-CV underestimates the prediction error, as commented in exercise f.

Chapter 7

Discrimination and classification

Load the datasets,

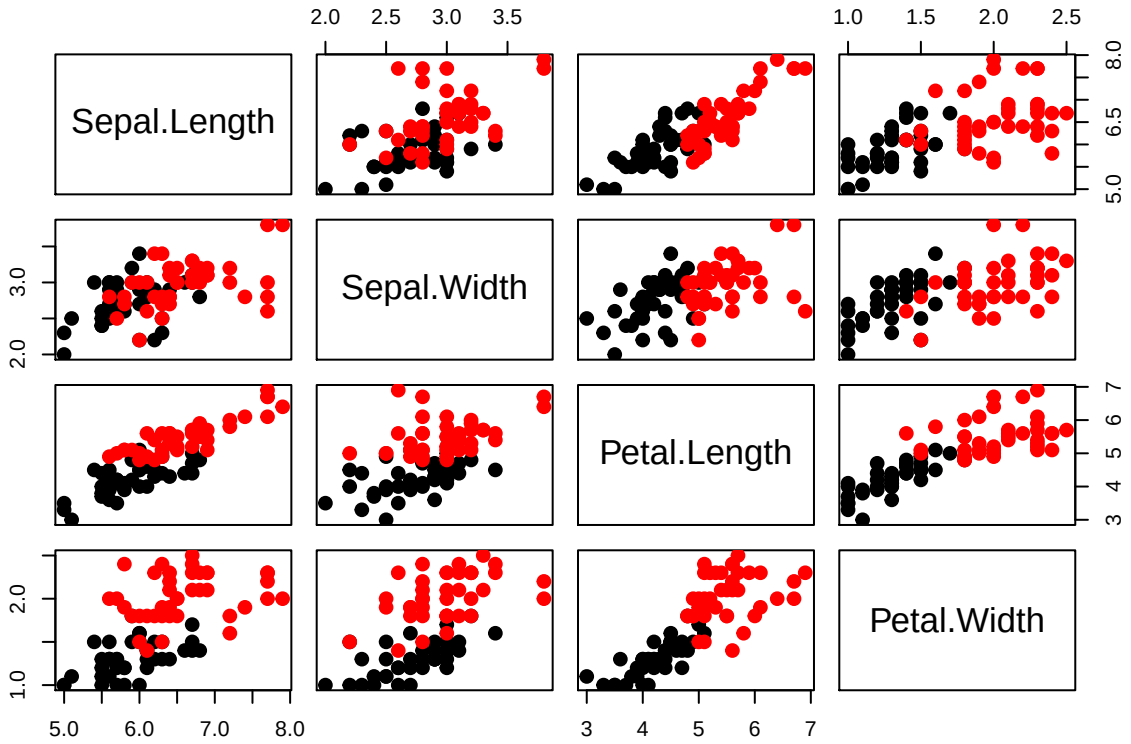
```
load("_data/iris.train.rdata")
load("_data/iris.test.rdata")
source("_functions/CV.class.R")
```

Load the packages,

```
library(MASS)
```

Iris Dataset

- a) Consider the famous iris data set `iris.train.rdata` as introduced in lesson 8. Reproduce the pairs plot for the four sepal and petal variables as given in lesson 8 slide 4. Which variable appears to be discriminating the species best? And which is worst?



The two classes are best separated from the point of view of Petal.Length. The Sepal.Width looks like the worst discriminator.

- b) Explain the difference between "discrimination" and "classification".

Discrimination corresponds to the model fitting process in statistical inference. We seek good variables for discriminating classes. Classification corresponds to the actual prediction of new samples, that is, to allocate new samples to classes using the presumably best "classifier"-model estimated from the training data.

- c) Explain what is meant by the assumption "We assume apriori that versicolor and virginica are equally likely".

This means that both species are equally probable if you sample a random plant from the population.

- d) Fit an LDA model to the iris data using Sepal.Length as the predictor. Assume equal prior probabilities for both species. Use the `print()`-function on you fitted model. What are the sample means of each species for this predictor variable?

```
mod1.lda <- lda(Species ~ Sepal.Length, data = iris.train, prior = c(0.5, 0.5))
mod1.lda
```

```
Call:
lda(Species ~ Sepal.Length, data = iris.train, prior = c(0.5,
    0.5))

Prior probabilities of groups:
versicolor  virginica
       0.5        0.5

Group means:
           Sepal.Length
versicolor         5.89
virginica          6.59

Coefficients of linear discriminants:
              LD1
Sepal.Length 1.89
```

The means are reported in the print output as `Group means`.

- e) Source in the `CV.class.R` file (open the fil in the script window and press the "Source" button to the upper right). Look at the `CV.class.examples.R`-file for reference. Perform a Leave-One-Out Cross-Validation of the model you fitted in the previous exercise. Report the confusion matrix, the accuracy and the cross-validated error rate.

```
cvres1 <- CV.class(mod1.lda, data = iris.train)
```

```
            True
Predicted    versicolor virginica
  versicolor         32        11
  virginica           8        29
  Total              40        40
  Correct            32        29

Proportions correct
versicolor  virginica
     0.800      0.725
```

```
N correct/N total = 61/80 = 0.762
```

The confusion matrix is given in the first part of the output. 32 out of 40 versicolor are correctly classified, whereas 29 out of 40 virginica are correct. In total 61 out of 80 are correctly classified giving an accuracy of 0.7625 as reported. The APER is 1-accuracy, hence APER=1-0.7625 = 0.2375. We typically seek classifiers that minimize the classification error rate.

- f) Use the scheme from exercises d. and e. to identify a good classifier for iris species. You may use either `lda` or `qda` and you may use one or several predictors. Report the cross-validated error for you "best choice".

Through some trial and error, and by looking at the pairs-plot from exercise a, my personal choice is the following model:

```
mymod <- qda(Species ~ Petal.Length + Petal.Width, data = iris.train, prior = c(0.5, 0.5
cvres2 <- CV.class(mymod, data = iris.train)
```

```
            True
Predicted    versicolor virginica
  versicolor         38         2
  virginica           2        38
  Total              40        40
  Correct            38        38

Proportions correct
versicolor  virginica
      0.95       0.95

N correct/N total = 76/80 = 0.95
```

This has an accuracy of 0.95 and, hence, an error of 0.05.

- g) What is the model assumption difference between an LDA and a QDA model?

In LDA we assume equal variance structure for all classes, whereas in QDA we assume different variance structures for all classes.

- h) Use the model of your choice to predict the samples in `iris.test.rdata`. Use the `confusion()`-function in the mixlm-library to evaluate the performance of

your classifier.

```
pred <- predict(mymod, newdata = iris.test)
confusion(iris.test$Species, pred$class)
```

```
            True
Predicted    versicolor virginica
  versicolor         10         0
  virginica           0        10
  Total              10        10
  Correct            10        10

Proportions correct
versicolor  virginica
         1          1

N correct/N total = 20/20 = 1
```

The model I found in f. gave a perfect classification, accuracy=1.0 and error=0.0.

- e. Use a logistic model of your choice (perhaps the same predictors as you used in your best choice classifier of Ex-1) to estimate the posterior probabilities of "virginica" for the samples of the `iris.test.Rdata` set. Allocate the samples to the most probable species class and use the `confusion()` function to evaluate the classification performance. (Hint: The posterior probabilies, say you name then `postprob`, should be classified into a factor variable by

```
predicted <- factor(ifelse(postprob > 0.5,"virginica","versicolor"))
```

```
mymod2 <- glm(Species ~ Petal.Length + Petal.Width, family = binomial, data = iris.train
postprob <- predict(mymod2, new = iris.test, type = "response")
predicted <- factor(ifelse(postprob > 0.5,"virginica","versicolor"))
confusion(iris.test$Species, predicted)
```

```
            True
Predicted    versicolor virginica
  versicolor         10         1
  virginica           0         9
  Total              10        10
```

```
  Correct            10         9

Proportions correct
versicolor  virginica
       1.0        0.9

N correct/N total = 19/20 = 0.95
```

With my chosen model I got one mis-classification and an error rate of 0.05.

–>

Chapter 8

Generalized Linear Model

For the exercises in this section, we require following package, data and functions. You can download them from canvas.

```
library(nnet)
load("_data/taxonomy.rdata")
load("_data/species.rdata")
source("_functions/CV.class.multinom.R")
```

Species Data

Consider the plant species count data used in lecture of Generalized linear model.

- a. Redo the analysis using the `Biomass` and `pH` variables as predictors for species counts (as in slide 9). Find separate expressions for the estimated linear predictors $\hat{\eta}_j$ for each `pH`-level j = "`low`","`medium`","`high`". Also find the estimated expected count for `Biomass = 2` and `pH = high`.

First we fit the model:

```
mod2.glm <- glm(Species ~ Biomass + pH, family = poisson, data = species)
summod2 <- summary(mod2.glm)
summod2$coefficients
```

```
            Estimate Std. Error z value Pr(>|z|)
```

```
(Intercept)    3.849     0.0528   72.89 0.00e+00
Biomass       -0.128     0.0101  -12.58 2.76e-36
pH(low)       -1.136     0.0672  -16.91 3.77e-64
pH(mid)       -0.445     0.0549   -8.11 4.88e-16
```

Then the estimated linear predictors are:

$$\eta_{\text{low}} = 3.85 - 0.128 \cdot \text{Biomass} - 1.14$$

$$\eta_{\text{medium}} = 3.85 - 0.128 \cdot \text{Biomass} - 0.45$$

$$\eta_{\text{high}} = 3.85 - 0.128 \cdot \text{Biomass}$$

For `Biomass = 2` and `pH = high` the estimated expected count is:

$$\hat{\lambda} = \exp(3.85 - 0.128 \cdot 2) = 36.4$$

Alternatively we could compute this in R by:

```
predict(mod2.glm, newdata = data.frame(Biomass = 2, pH = "high"), type = "response")
```

```
   1
36.4
```

- b. Fit the same model as in a. using the quasipoisson approach. Is there any evidence of overdisperion?

```
mod2q.glm <- glm(Species ~ Biomass + pH, family = quasipoisson, data = species)
summary(mod2q.glm)
```

```

Call:
glm(formula = Species ~ Biomass + pH, family = quasipoisson,
    data = species)

Deviance Residuals:
```

```
   Min      1Q  Median      3Q     Max
-2.596  -0.699  -0.074   0.665   3.560

Coefficients:
            Estimate Std. Error t value      Pr(>|t|)
(Intercept)   3.8489     0.0556   69.28       < 2e-16 ***
Biomass      -0.1276     0.0107  -11.96       < 2e-16 ***
pH(low)      -1.1364     0.0707  -16.07       < 2e-16 ***
pH(mid)      -0.4452     0.0577   -7.71 0.00000000002 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

(Dispersion parameter for quasipoisson family taken to be 1.11)

    Null deviance: 452.346  on 89  degrees of freedom
Residual deviance:  99.242  on 86  degrees of freedom
AIC: NA

Number of Fisher Scoring iterations: 4
```

The dispersion parameter is only marginally larger than 1. We conclude that over-disperion is not a problem here.

- c. Extend the model from a. by including an interaction between Biomass and pH. Test the significance of the interaction. Is there a significant difference between pH="high" and pH="medium" with regard to the effect of Biomass to the species count?

```
mod3.glm <- glm(Species ~ Biomass * pH, family = poisson, data = species)
summary(mod3.glm)
```

```
Call:
glm(formula = Species ~ Biomass * pH, family = poisson, data = species)

Deviance Residuals:
   Min      1Q  Median      3Q     Max
-2.498  -0.748  -0.040   0.557   3.230
```

```
Coefficients:
                Estimate Std. Error z value Pr(>|z|)
(Intercept)       3.7681     0.0615   61.24  < 2e-16 ***
Biomass          -0.1071     0.0125   -8.58  < 2e-16 ***
pH(low)          -0.8156     0.1028   -7.93  2.2e-15 ***
pH(mid)          -0.3315     0.0922   -3.60  0.00032 ***
Biomass:pH(low)  -0.1550     0.0400   -3.87  0.00011 ***
Biomass:pH(mid)  -0.0319     0.0231   -1.38  0.16695
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

(Dispersion parameter for poisson family taken to be 1)

    Null deviance: 452.346  on 89  degrees of freedom
Residual deviance:  83.201  on 84  degrees of freedom
AIC: 514.4

Number of Fisher Scoring iterations: 4
```

```r
anova(mod2.glm, mod3.glm, test = "Chi")
```

```
Analysis of Deviance Table

Model 1: Species ~ Biomass + pH
Model 2: Species ~ Biomass * pH
  Resid. Df Resid. Dev Df Deviance Pr(>Chi)
1        86       99.2
2        84       83.2  2       16  0.00033 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

The interaction term is highly significant with a p-value of 0.00033. The Wald tests (the approximate normal test) given in the summary output gave a p-value of 0.167 for the term `Biomass:pHmid` which really is the contrast between interactions `Biomass:pHhigh`and `Biomass:pHmedium` since `pHhigh` is the reference level in this model. The relatively large p-value says that there is no evidence that Biomass has different effect on counts for these

two pH-levels.

- d. Optional R-programming exercise for those interested: Reproduce the graph on slide 3 of lesson 10 and add curves visualizing the estimated expected counts as a function of Biomass and with separate curves for the pH-levels. The curves should be based on the fitted model with interaction between Biomass and pH-level.

Answers from students

Taxonomy Data

We return to the taxonomy data used in the lecture on cluster analysis. In the file `taxonomy.Rdata` you find seven variables measured on plants from four different taxa. We will use multinomial regression as means for classification of taxa. A code file for performing cross-validation of classifications based on multinomial regression is found in the file `CV.class.multinom.R` on Fronter. Throughout this exercise you may need to increase the number of iterations used in the Maximum Likelihood estimation procedure. The default is 100 iterations. For example, in exercise a. `maxit = 200` should suffice.

- a. Use multinomial regression to model the probabilities of the various taxa as a function of the variable `Sepal`. Save the model as an object called `mod1.multi`. Use summary to display the results.

```
mod1.multi <- multinom(Taxon ~ Sepal, data = taxonomy, maxit = 200)
```

```
# weights:  12 (6 variable)
initial  value 166.355323
iter  10 value 98.990404
iter  20 value 98.141917
iter  30 value 98.100674
iter  40 value 98.097605
iter  50 value 98.096106
iter  60 value 98.095900
iter  70 value 98.095310
iter  80 value 98.095057
```

```
iter  90 value 98.094619
iter 100 value 98.092238
final  value 98.092209
converged
```

```
summary(mod1.multi)
```

```
Call:
multinom(formula = Taxon ~ Sepal, data = taxonomy, maxit = 200)

Coefficients:
    (Intercept)  Sepal
II         1.49 -0.593
III        2.86 -1.148
IV       -48.04 13.738

Std. Errors:
    (Intercept)  Sepal
II         2.31  0.914
III        2.32  0.924
IV        84.93 24.439

Residual Deviance: 196
AIC: 208
```

- b. What are the estimated linear predictors η_j for each of the four taxa, $j = 1, 2, 3, 4$?

First we extract the estimated regression coefficients. Remember that for the reference level taxon the regression coefficients are assumed equal to zero. We therefore add a row of zeros for this taxon (here `taxon = 1`).

```
summod1.multi <- summary(mod1.multi)
co <- summod1.multi$coefficients
co <- rbind(c(0,0),co)
rownames(co)[1] <- "I"
co
```

```
    (Intercept)  Sepal
I          0.00  0.000
```

```
II         1.49 -0.593
III        2.86 -1.148
IV       -48.04 13.738
```

This gives the following linear predictors:

$$\eta_1 = 0 + 0 \cdot \text{Sepal} = 0$$

$$\eta_2 = 1.49 - 0.593 \cdot \text{Sepal}$$

$$\eta_3 = 2.86 - 1.15 \cdot \text{Sepal}$$

$$\eta_4 = -48.0 + 13.7 \cdot \text{Sepal}$$

- c. What is the most probable taxon according to this model for a plant with average value of `Sepal`? (Hint: If your coefficients are stored in a matrix called `co` you may compute the probabilities for each taxon by using the code `probs <- exp(co[,1]+co[,2]*x)/sum(exp(co[,1]+co[,2]*x))` where `x`is the value of interest for `Sepal`.

```
x <- mean(taxonomy$Sepal)
probs <- exp(co[ ,1] + co[ ,2] * x) / sum(exp(co[ ,1] + co[ ,2] * x))
probs
```

```
       I       II      III       IV
0.433455 0.324557 0.241505 0.000483
```

```
maxp <- which.max(probs)
maxp
```

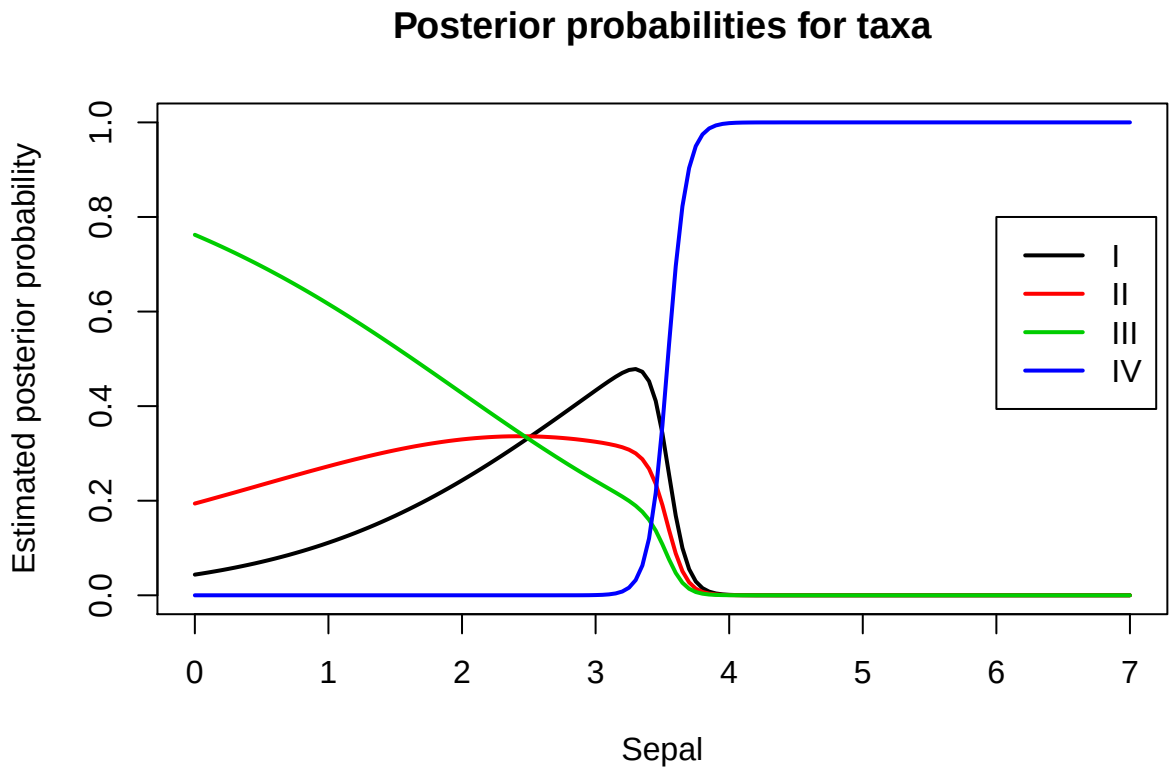
```
I
1
```

We see that taxon I is the most probable with a probability equal to 0.433.

Extra: The following figure shows the probabilities of each taxon for various values of

Sepal. Remember that these probabilities are the posterior probability estimates for the class in a classification terminology. We classify to the most probable class given the observed predictor values.

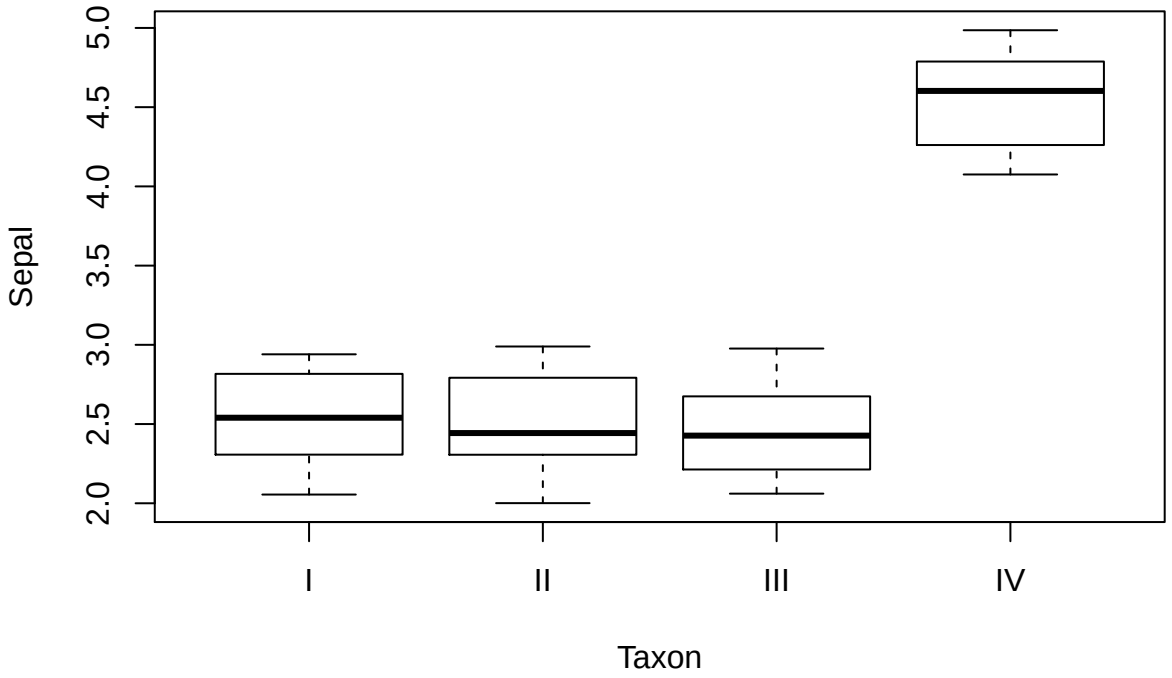
```
xvector <- seq(0,7, by = 0.05)
probfunc <- function(x){
    exp(co[ ,1] + co[ ,2] * x) / sum(exp(co[ ,1] + co[ ,2] * x))
}
probmat <- t(sapply(xvector, probfunc))
matplot(xvector, probmat, lty = 1, type = "l", lwd = 2,
        main = "Posterior probabilities for taxa",
        xlab = "Sepal", ylab = "Estimated posterior probability")
legend(6, 0.8, legend = c("I", "II", "III", "IV"), lty = 1, col = 1:4, lwd = 2)
```



We observe that taxon III is the most probable for Sepal<2.5, taxon I for 2.5 < Sepal < 3.5 and taxon IV for Sepal >= 3.5. Taxon 2 is the most probable taxon only for Sepal $\approx$ 2.5.

- d. Execute the following plot command: plot(Sepal ~ Taxon, data=taxonomy). Use the figure to explain the result from exercise c.

```
plot(Sepal ~ Taxon, data = taxonomy)
```



We see that taxon I has the median (and probably also the mean) closest to the average Sepal length which is 3.0. Taxa II and III are very similar, but slightly further away, hence their probabilities are a bit smaller. Taxa IV has Sepal lengths much larger than the average and is thus the least probable taxon.

- e. Repeat the taxon classification of exercise c. by means of the `predict()` - function.

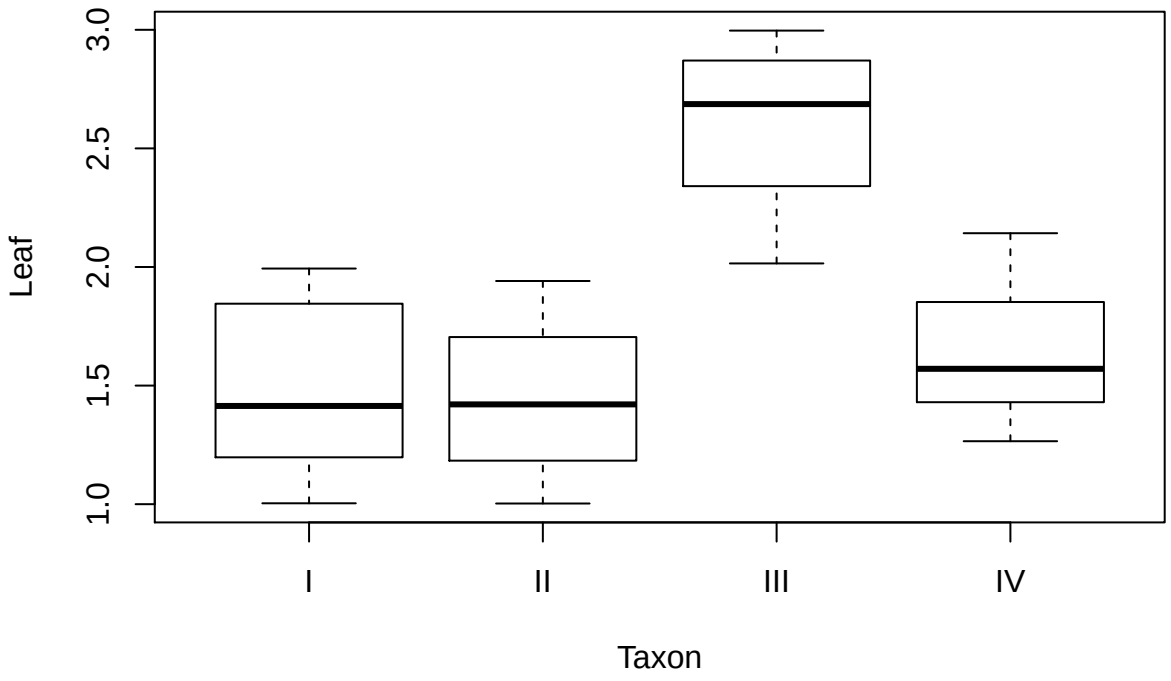
```
predict(mod1.multi,newdata = data.frame(Sepal = mean(taxonomy$Sepal)))
```

```
[1] I
Levels: I II III IV
```

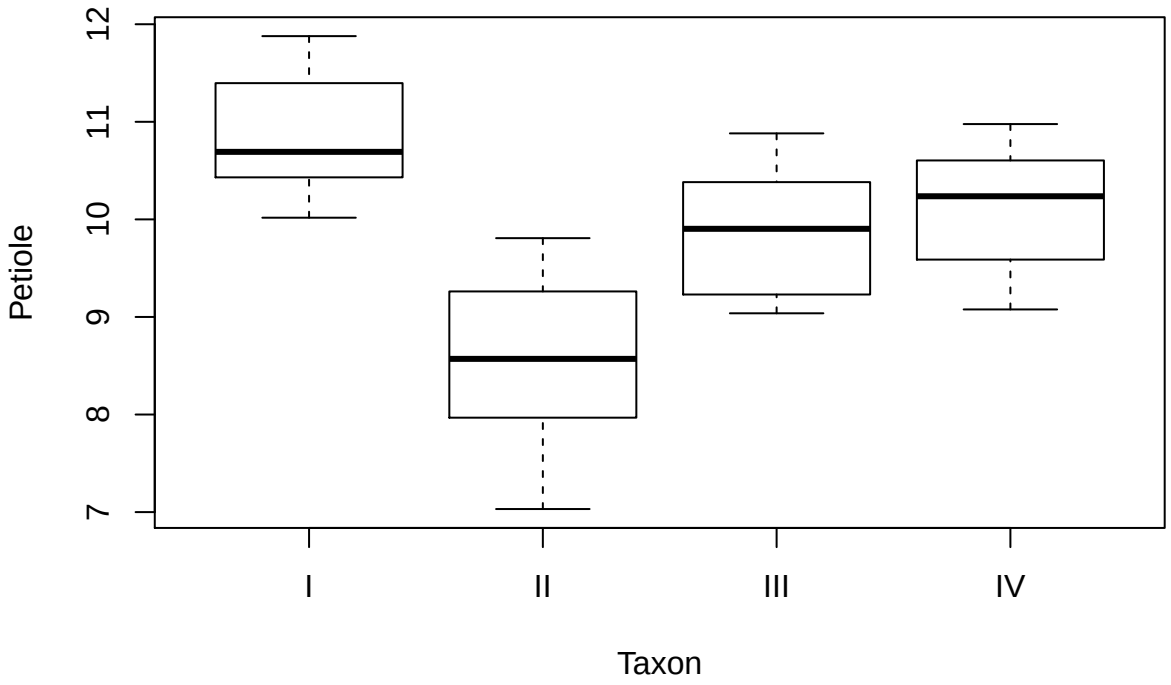
- f. Use similar plots like in d. to identify other variables which are promising with regard to separating taxa I, II and III (Sepal is already a good variable to distinguish taxon IV from the others). Fit an extended model with the variables you have chosen and save the model as an object called `mod2.multi`.

I have found two variables which are promising; `Leaf` and `Petiole`, as shown in the figures below.

```
plot(Leaf ~ Taxon, data = taxonomy)
```




```
plot(Petiole ~ Taxon, data = taxonomy)
```



`Leaf` seems to distinguish taxon III from the others, and `Petiole` may separate taxa I and II.

I therefore fit a model with `Sepal`, `Leaf` and `Petiole` as predictors for taxa. This model

requires many iterations in the estimation process. I set `maxit = 5000` to be sure. (`trace =FALSE` supresses a long list of convergence details)

```
mod2.multi <- multinom(Taxon ~ Sepal + Leaf + Petiole , data = taxonomy,
                       maxit = 5000, trace = FALSE)
summary(mod2.multi)
```

```
Call:
multinom(formula = Taxon ~ Sepal + Leaf + Petiole, data = taxonomy,
    maxit = 5000, trace = FALSE)

Coefficients:
    (Intercept) Sepal  Leaf Petiole
II        554.9  23.1  12.8   -64.6
III       -67.1 -73.5 371.7   -51.6
IV        -68.1  63.3   6.4   -14.4

Std. Errors:
    (Intercept) Sepal Leaf Petiole
II       3631.9   574  387     465
III      9508.8  5686 3115     456
IV         21.5  4054 7258     848

Residual Deviance: 0.00067
AIC: 24
```

- Use a Chis-square test to test the joint significance of the extra variables you added as you extended `mod1.multi` to `mod2.multi`.

We test whether the difference in deviances between the two models is significant.

```
dev.diff <- -2 * (logLik(mod1.multi) - logLik(mod2.multi))
pchisq(dev.diff, 6, lower = FALSE)
```

```
'log Lik.' 1.23e-39 (df=6)
```

The p-value indicates that `Leaf` and `Petiole` are highly significant in addition to `Sepal` as predictors in the model.

- h. Use the `predict()`function on `mod2.multi` with `newdata=taxonomy` to classify

all plants in the dataset to taxa. Then apply the `confusion()` function in the `mixlm`- package to compute the classification performance of the multinomial model. What is the accuracy and apparent classification error?

```
pred.all <- predict(mod2.multi, newdata = taxonomy)
mixlm::confusion(taxonomy$Taxon, pred.all)
```

```
          True
Predicted  I II III IV
  I       30  0   0  0
  II       0 30   0  0
  III      0  0  30  0
  IV       0  0   0 30
  Total   30 30  30 30
  Correct 30 30  30 30

Proportions correct
  I  II III  IV
  1   1   1   1

N correct/N total = 120/120 = 1
```

I get an accuracy of 1 and an apparent classification error (APER) of 0. That is, a perfect "fit" to the data. (Note the R-code `mixlm::` for extracting the confusion function from mixlm without loading the entire package).

- i. We should watch out for over-fitting. Use the `CV.class.multinom()` function to run a Leave-One-Out Cross-validation to validate the `mod2.multi` model.

```
#source("CV.class.multinom.R")
CVres <- CV.class.multinom(mod2.multi,data = taxonomy, trace = FALSE)
```

```
          True
Predicted  I II III IV
  I       28  1   1  0
  II       1 29   1  0
  III      1  0  28  0
  IV       0  0   0 30
  Total   30 30  30 30
```

```
  Correct 28 29  28 30

Proportions correct
    I    II   III    IV
0.933 0.967 0.933 1.000

N correct/N total = 115/120 = 0.958
```

The cross-validation gave 5 mis-classifications. Taxon IV is perfectly classified, but there are some mix-up's between taxa I, II and III. The accuracy is still high (0.96) and the total classification error is correspondingly small (0.04).