Lesson 10: Functions in R

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2022-11-09

Contents

Wellcome & Disclaimer

This site contains the materials for the *Coding tools for Biochemistry & Molecular Biology* (Herramientas de Programación para Bioquímica y Biología Molecular) course of fall 2022 in the Bachelor's Degree in Biochemistry @UAM. This materials are the basis for GitHub-pages-based website that can be accessed here. Detailed academic information about the course contents, dates and assessment only can be found at the UAM Moodle site.

R packages

As you already know, R is a 'GNU Software' with a GPL license. As a a freely available language it has a great community of users from diverse background and interests. This community have developed a myriad of applications for R, called ***R Packages***. Packages are the fundamental units of reproducible R code. They include reusable R functions, the documentation that describes how to use them, and sample data. The idea behind R packages is that the chances are that someone has already solved a problem that you're working on, and you can benefit from their work by downloading their package.

Packages can be installed from one of the public R repositories. In this course we will use two R repos, **CRAN** and **Bioconductor**. The name CRAN stands for "The Comprehensive R Archive Network", and it contains a huge variety of packages free to use. On the other hand, as we will see later on, Bioconductor is a repository of software devoted to bioinformatics or computational biology applications. As for August 2022, the CRAN package repository features 18,558 available packages whereas Bioconductor release 3.15 contains 2,140 packages.

A full list of CRAN packages can be found here and a list by topic here.

Installing and use R packages

As an example, we are going to install and use `xlsx`, a handy package to import/export tables in MS Excel format. You may also check related packages, such as `readxl` or `pzfx`.

```
# install the package you may require other packages,add
# dependencies=TRUE if this example doesn't work
install.packages("xlsx")
```

```
## Error in contrib.url(repos, "source"): trying to use CRAN without setting a mirror
```

```
# load
library(xlsx)
require(xlsx)

# trick to install package only if not installed
if (!require(xlsx)) {
    install.packages("xlsx")
    library(xlsx)
}
```

Try to read again the file coli_genomes_renamed.csv that we saved in the previous lesson and save it ready for MS Excel.

```
# open it again
coli_genomes <- read.csv2(file = "data/coli_genomes_renamed.csv")
# save
write.xlsx(coli_genomes, "data/coli_genomes.xlsx")
```

In the above code we have used `require()` and `library()` functions to call for package loading. Those are very similar functions, often interchangeable. The main difference is that if you use `require()`, you will get a warning (see below for *warning* use), but not an error. Thus, your code will continue to run if possible.

```
library(uam)
```

```
## Error in library(uam): there is no package called 'uam'
```

```
require(uam)
```

```
## Loading required package: uam
```

```
## Warning in library(package, lib.loc = lib.loc, character.only = TRUE,
## logical.return = TRUE, : there is no package called 'uam'
```

Many packages in CRAN also contain a reference manual and some of them also a *vignette*. A vignette is practical guide to each package. You can see all the installed vignettes with `browseVignettes()`. You can find a bunch of tutorials and tricks about how to use popular packages, but the *vignette* is an official and complete reference that is always helpful.

```
browseVignettes("xlsx")
```

```
## starting httpd help server ... done
```

```
browseVignettes("seqinr")
```

```
## No vignettes found by browseVignettes("seqinr")
```

```
browseVignettes("ggplot2")
```

Sometimes, you can come into two different namesake functions from independent packages. Also, to reduce the memory load you may want to use a function without loading the package. In those cases, as in the examples below, there is a trick to call a specific function, the prefix `package::`. However, it should be noted that in some packages the syntax is complex and you need to call more than one function to actually use a major function. In the example 2 below, you will see that `ggplot()` function can be used if you specify the package with the prefix `ggplot::` for all the required functions (see Lesson 13).

```
# example1, package getwiki
install.packages("getwiki")
```

```
## Error in contrib.url(repos, "source"): trying to use CRAN without setting a mirror
```

```
vignette("getwiki")
DNA <- getwiki::search_wiki("DNA")
str(DNA)
```

```
## 'data.frame':    20 obs. of  2 variables:
##  $ titles : chr  "A-DNA" "Circular DNA" "DNA" "DNA (disambiguation)" ...
##  $ content: chr  "A-DNA is one of the possible double helical structures which DNA can adopt. A-DNA i
```

```
DNA$titles
```

```
##  [1] "A-DNA"                 "Circular DNA"          "DNA"
##  [4] "DNA (disambiguation)"  "DNA Films"             "DNA extraction"
##  [7] "DNA ligase"            "DNA methylation"       "DNA polymerase"
## [10] "DNA profiling"         "DNA repair"            "DNA replication"
## [13] "DNA sequencing"        "DNA virus"             "DNA²"
## [16] "DNA-DNA hybridization" "DnaA"                  "Extrachromosomal DNA"
## [19] "Mitochondrial DNA"     "Recombinant DNA"
```

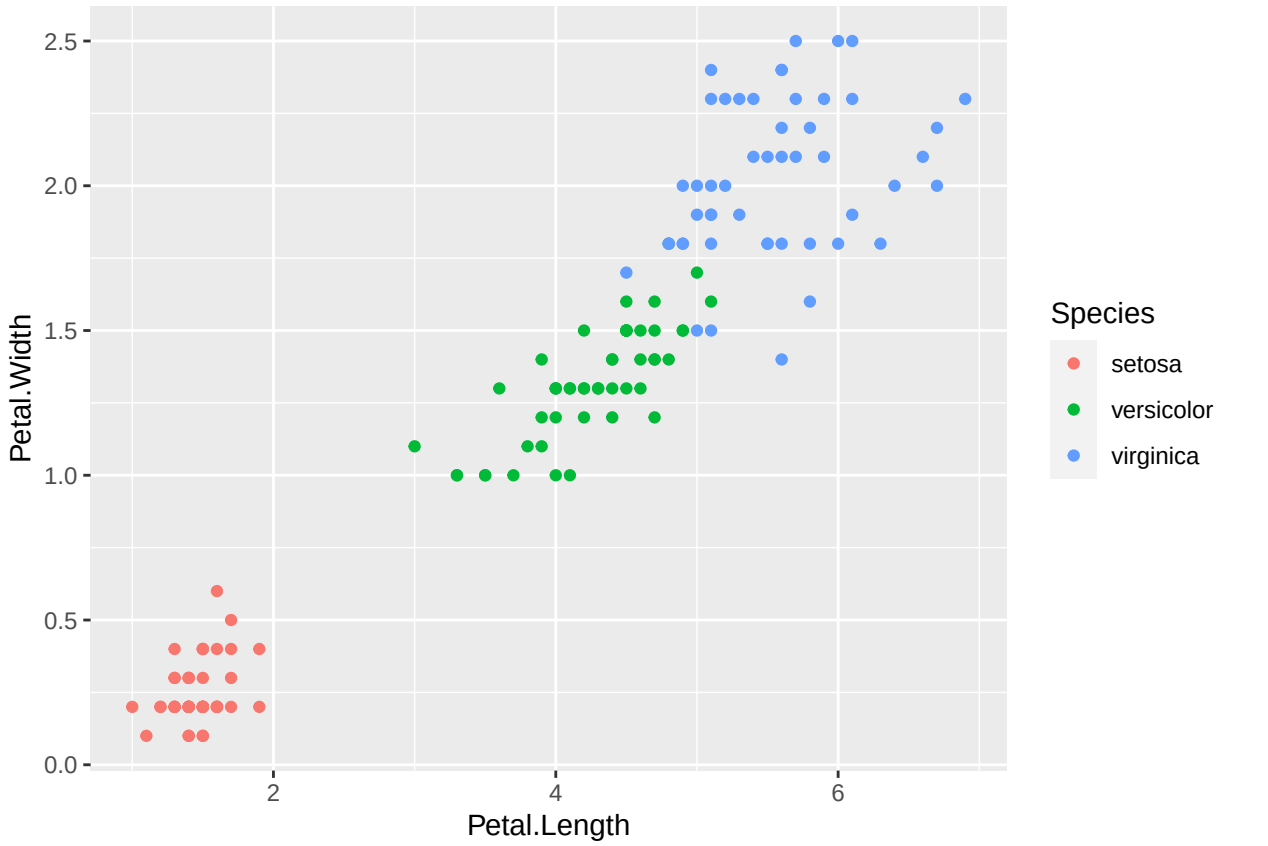
```
# example2, package ggplot2
ggplot(iris, aes(Petal.Length, Petal.Width, colour = Species)) +
    geom_point()
```

```
## Error in ggplot(iris, aes(Petal.Length, Petal.Width, colour = Species)): no se pudo encontrar la fun
```

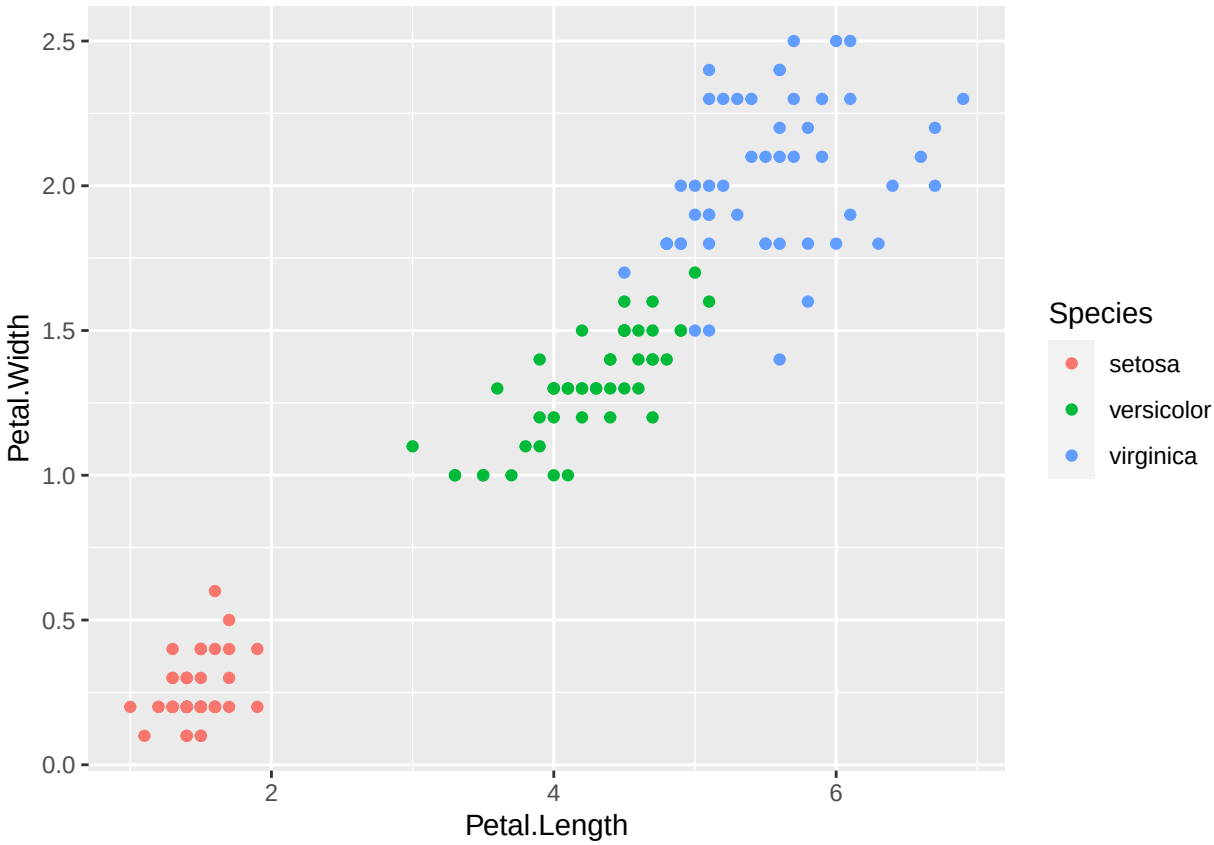
```
ggplot2::ggplot(iris, aes(Petal.Length, Petal.Width, colour = Species)) +
    geom_point()
```

```
## Error in aes(Petal.Length, Petal.Width, colour = Species): no se pudo encontrar la función "aes"
```

```
ggplot2::ggplot(iris, ggplot2::aes(Petal.Length, Petal.Width,
    colour = Species)) + ggplot2::geom_point()
```




```
library(ggplot2)
ggplot(iris, aes(Petal.Length, Petal.Width, colour = Species)) +
    geom_point()
```



R has some built-in datasets that can be used as examples. You can check them using the function `data()`. Note that in the example we have plotted some data from the dataset named iris.

Create user-written functions

Why? How?

We have discussed throughout the last lectures how R can help you if you to save time when you need to analyze and plot the data from your experiment. However, many times, particularly in Bioinformatics, you won't have the data from one single experiment but from many of them.

Creating you own function will be very useful for automation of repetitive analyses or to encapsulate a sequence of expressions that need to be executed numerous times, perhaps under slightly different conditions. Functions are also often written when code must be shared with others or the public.

In R, functions are also considered as objects. That means that (1) they can be nested, so you can define a function inside another function and (2) you can use functions as arguments to other functions. We will see very useful examples of this latter feature in Lesson 12, using custom functions as arguments for `lapply()` or `sapply()`.

The overall scheme of an R function is the following:

```
my_function <- function(argument1, argument2,...){
  statements
  return(object)
  }
```

My first simple functions

We are going to learn with some examples from a good online tutorial. First, a quite simple function can simply help with calculations:

```
# my first function
myFunction <- function(x) {
    f <- x^2 * 4 + x/3
    return(f)
}
# we try it
myFunction(4)
```

```
## [1] 65.33333
```

```
myFunction(0)
```

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

```
myFunction(22)
```

```
## [1] 1943.333
```

```
myFunction(3)
```

```
## [1] 37
```

We can include conditions, loops... Another example can be a function to identify even/odd numbers:

```
# A simple R function to check whether x is even or odd
evenOdd <- function(x) {
    if (x%%2 == 0) {
        return("even")
    } else {
        return("odd")
    }
}
# test
evenOdd(4)
```

```
## [1] "even"
```

```
evenOdd(3)
```

```
## [1] "odd"
```

```
# note that simple ifs within a function does not need the
# curly braces!
evenOdd2 <- function(x) {
    if (x%%2 == 0)
        return("even") else return("odd")
}
evenOdd2(4)
```

```
## [1] "even"
```

```
evenOdd2(3)
```

```
## [1] "odd"
```

```
evenOdd2(7)
```

```
## [1] "odd"
```

```
evenOdd2(8)
```

```
## [1] "even"
```

In the above example, we found out that curly braces can be omitted sometimes in *if* statements or loops (see https://www.learnbyexample.org/r-for-loop/#for-loop-without-curly-braces). This modification makes the code handier, but also riskier, use it carefully. Remember, a great power entails a great responsibility. The same applies to functions. Thus, sometimes when creating an R script, you want to create a small function and use it just once. That happens usually when you want to use your own functions to parse data within an `apply` family function (see Lesson 12). To deal with those situations, you can use the *inline* function. To create an inline function you have to use the function command with the argument x and then the expression of the function.

Example:

```
# inline functions
f <- function(x) x^2 * 4 + x/3

f(4)
```

```
## [1] 65.33333
```

```
f(0)
```

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

```
f(22)
```

```
## [1] 1943.333
```

Functions with multiple arguments

Now, we will create a function in R Language that will take multiple inputs and gives us one output.

```
# A simple R function to calculate area and perimeter of a
# rectangle

area <- function(length, width) {
    area = length * width
    # you may format the output
    print(paste("The area of the rectangle is", length, "x",
        width, "=", area, "cm²"))
}

area(2, 3)  # call the function
```

```
## [1] "The area of the rectangle is 2 x 3 = 6 cm²"
```

Notice that the output also can be a vector or a list:

```
# Now we calculate area and perimeter of a rectangle


Rectangle <- function(length, width) {
    area = length * width
    perimeter = 2 * (length + width)

    # create an object called result which is a list of
```

```
    # area and perimeter
    result = list(Area = area, Perimeter = perimeter)
    return(result)
}

Rectangle(2, 3)
```

```
## $Area
## [1] 6
##
## $Perimeter
## [1] 10
```

Like in any R function, you can call the arguments by position or by name. Thus, if add the names of the variables when calling the function you can switch the order of the arguments. Also, you can add some default values when you define the function.

```
# A simple R program to demonstrate passing arguments to a
# function

Rectangle <- function(length = 5, width = 4) {
    area = length * width
    return(area)
}
for (x in 0:4) print(x^2)
```

```
## [1] 0
## [1] 1
## [1] 4
## [1] 9
## [1] 16
```

```
# Case 1:
Rectangle(2, 3)
```

```
## [1] 6
```

```
# Case 2: If you do not want to follow any order, you can
# include the name of the arguments
Rectangle(width = 8, length = 4)
```

```
## [1] 32
```

```
# Case 3: default's values
Rectangle()
```

```
## [1] 20
```

Including checkpoints

Now we are going to try a longer code.

Example

Your laboratory provides PCR service for detection of Covid19, according to fares detailed in the table.
The **normal** price rises 15% for a **priority** order (result in <72h) and it is doubled for an **urgent** request (24h).

Samples	Price/sample
1-9	19€
10-49	14€
>50	10€

Create a function `price_calculator()` that uses the previous loop for this problem.

How many arguments should have this function?
How would you take into account possible mistyping errors?

```
# we need to arguments
price_calculator <- function(samples, category) {
    categories <- c(1, 1.15, 2)
    names(categories) = c("normal", "priority", "urgent")
    if (samples < 10) {
        price <- 19 * samples * which(names(categories) == category)
    } else if (samples < 50) {
        price <- 14 * samples * which(names(categories) == category)
    } else if (samples >= 50) {
        price <- 10 * samples * which(names(categories) == category)
    } else {
        # if we cannot calculate the price we return a
        # message
        price <- paste("No se ha podido calcular el precio. Revise los datos introducidos")
    }
    paste(price)
}

# new version with checkpoints
price_calculator <- function(samples, category = "normal" | "priority" |
    "urgent") {
    category <- switch(category, normal = 1, priority = 1.5,
        urgent = 2)
    if (samples < 10) {
        price <- 19 * samples * category
    } else if (samples < 50) {
        price <- 14 * samples * category
    } else if (samples >= 50) {
        price <- 10 * samples * category
    }
    ifelse(length(price) > 0, return(price), stop("Prioridad incorecta. No se ha podido calcular el pre
}
price_calculator(5.3, "normal")
```

```
## [1] 100.7
```

```
# WTF?
```

We just noticed that the function calculated the price for 5.3 samples, which is nonsense. We should then

introduce a checkpoint for the format of the introduced value for the variable samples.

```
# alternative with checkpoint for number of samples
price_calculator <- function(samples, category = "normal" | "priority" |
    "urgent") {
    category <- switch(category, normal = 1, priority = 1.5,
        urgent = 2)
    if (abs(floor(samples)) != samples) {
        # check that number of samples is an integer number
        stop("Número de muestras incorrecto")
    }
    if (samples < 10) {
        price <- 19 * samples * category
    } else if (samples < 50) {
        price <- 14 * samples * category
    } else if (samples >= 50) {
        price <- 10 * samples * category
    }
    ifelse(length(price) > 0, return(price), stop("Prioridad incorecta. No se ha podido calcular el pre
}

# test again
price_calculator(50, "urgente")
```

```
## Error in ifelse(length(price) > 0, return(price), stop("Prioridad incorecta. No se ha podido calcula
```

```
price_calculator(50, "urgent")
```

```
## [1] 1000
```

```
price_calculator(-5, "normal")
```

```
## Error in price_calculator(-5, "normal"): Número de muestras incorrecto
```

```
price_calculator(5.2, "normal")
```

```
## Error in price_calculator(5.2, "normal"): Número de muestras incorrecto
```

In-class exercise

When creating functions, you can include any R functionality, including reading external data. Let's check the following example, within the context of molecular biology. It makes a short function that convert R into a molecular biology dogma interpreter. It takes as input a nucleic acid sequence codon and returns its encoded amino acid in IUPAC one letter code.

```
# the molecular biology dogma with R

codon2aa <- function(inputCodon) {
    aa <- c()
    code <- read.csv2("data/genetic_code.csv", stringsAsFactors = FALSE)
    aa <- code$AA[code$Codon == inputCodon]
    return(aa)
}

# now let's try it
codon2aa("ATG")
```

```
## [1] "M"
```

```
codon2aa("TAA")
```

```
## [1] "*"
```

```
codon2aa("CAT")
```

```
## [1] "H"
```

```
codon2aa("AXG")
```

```
## character(0)
```

```
# Can you check the value of the variable 'aa'
aa
```

```
## Error in eval(expr, envir, enclos): objeto 'aa' no encontrado
```

What just happened? There are a few things worth to comment here:

1. When writing a function, we need to define a vector before assigning it a value.
2. If the function cannot find the right value to return, the output is empty: `character(0)`
3. The variable `aa` seems nonexistent! Variables defined in a function are only **local variables** and cannot be called outside the function.

However, proteins are made up of more than one amino acid, so it'd be great if the input could be a vector of several codons instead a single codon.

Additionally, we can customize how R handles the empty returns. This allow us helping the user to use our code and preventing errors.

```
# version 2

codon2aa_2 <- function(codons) {
    aa <- c()
    code <- read.csv2("data/genetic_code.csv", stringsAsFactors = FALSE)
    for (i in 1:length(codons)) {
        # loop over all the elements of the vector 'codons'
        # check for correct values
        if (codons[i] %in% code$Codon) {
            aa[i] <- code$AA[code$Codon == codons[i]]
        } else {
            stop("Uno o más de los codones no es correcto. No se ha podido traducir.")
            # break and message in case of empty return
        }
    }
    return(aa)
}

# let's try it
codon2aa_2(c("ATG", "TGA"))
```

```
## [1] "M" "*"
```

```
codon2aa_2(c("ARG", "TGA"))
```

```
## Error in codon2aa_2(c("ARG", "TGA")): Uno o más de los codones no es correcto. No se ha podido tradu
```

```
codon2aa_2(c("ATG", "CAT", "CAT", "AAA", "TAA"))
```

```
## [1] "M" "H" "H" "K" "*"
```

References

- *R packages*, https://r-pkgs.org/index.html
- *R programming for data science,* https://bookdown.org/rdpeng/rprogdatascience/
- Creating functions in *Programming in R* Swcarpentry, http://swcarpentry.github.io/r-novice-inflammation/02-func-R/index.html
- Functions in R programming in *GeeksforGeeks*: https://www.geeksforgeeks.org/functions-in-r-programming/
- Learn R by examples: https://www.learnbyexample.org/

Short exercises

1. Install the package `report` and check its *vignette* and the info at the package site: https://easystats.github.io/report/

2. R has some built-in datasets that can be used as example. You can check them using the function `data()`. Use the function `report()` with some of the R built-in datasets, like *DNase.* Explore the dataset and try to use the report to answer some question, like normal distribution or correlation between two variables.

3. Write a function called micro() that transforms concentrations units: molar (M) into micromolar (µM)

4. Write a function that transform mass into concentration (in µM and with four decimal digits). For simplicity, we can consider that the units of mass, molecular weight and volume are µg, kg/mol and µL, respectively.

5. Write a function that calculate your approximate age in months. Check the functions `date()`, `Sys.Date()`, `as.Date()`, and `difftime()`. See some examples here or here.

More exercises...

https://www.r-bloggers.com/2016/02/functions-exercises/

http://mathcenter.oxford.emory.edu/site/math117/probSetRFunctions/

Challenge

Write a function that translate any nucleotide sequence into a protein sequence. Hints:

1. You may need to check for the number of nucleotides (i) and the number of codons (j=i/3) in the sequence.
2. You may use the function `substr()` (check the help) to divide the sequence into codons. To do so, you may use a loop that split the nucleotides in groups of three.
3. You would add a `warning()` call when 1-2 nucleotides at the end of the sequence are not used.
4. Use the function `readLines()` to read the file *lacz.fa,* which contains the nucleotide sequence of *E. coli* lacZ gene in fasta format, and obtain the translated sequence.

Session Info

```
sessionInfo()
```

```
## R version 4.2.2 (2022-10-31)
## Platform: x86_64-apple-darwin17.0 (64-bit)
## Running under: macOS Big Sur ... 10.16
##
## Matrix products: default
## BLAS:   /Library/Frameworks/R.framework/Versions/4.2/Resources/lib/libRblas.0.dylib
## LAPACK: /Library/Frameworks/R.framework/Versions/4.2/Resources/lib/libRlapack.dylib
##
## locale:
## [1] es_ES.UTF-8/es_ES.UTF-8/es_ES.UTF-8/C/es_ES.UTF-8/es_ES.UTF-8
##
## attached base packages:
## [1] stats     graphics  grDevices utils     datasets  methods   base
##
## other attached packages:
## [1] ggplot2_3.3.6 xlsx_0.6.5    formatR_1.12  knitr_1.40
##
## loaded via a namespace (and not attached):
##  [1] highr_0.9        compiler_4.2.2   pillar_1.8.1     tools_4.2.2
##  [5] digest_0.6.30    jsonlite_1.8.3   evaluate_0.17    lifecycle_1.0.3
##  [9] tibble_3.1.8     gtable_0.3.1     pkgconfig_2.0.3  rlang_1.0.6
## [13] cli_3.4.1        rstudioapi_0.14  getwiki_0.9.0    yaml_2.3.6
## [17] xfun_0.34        fastmap_1.1.0    rJava_1.0-6      withr_2.5.0
## [21] stringr_1.4.1    dplyr_1.0.10     generics_0.1.3   xlsxjars_0.6.1
## [25] vctrs_0.5.0      tidyselect_1.2.0 grid_4.2.2       glue_1.6.2
## [29] R6_2.5.1         fansi_1.0.3      rmarkdown_2.17   farver_2.1.1
## [33] magrittr_2.0.3   scales_1.2.1     htmltools_0.5.3  colorspace_2.0-3
## [37] labeling_0.4.2   utf8_1.2.2       stringi_1.7.8    munsell_0.5.0
```

Course home