Introduction to Programming in R

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Organization

Slides and exercises are available online:
https://www.costalab.org/bioinformatics-in-r-2020/

Daily Schedule:

9:30 - 12:00 - Theory and practices via zoom
13:00 - 17:00 - Exercises (see webpage) via discord

Important: M.Sc. and B.Sc. students need to send scripts with solutions for all mandatory exercises by the end of the day to courses@costalab.org

Programming, Language & Algorithms

What is an algorithm?

- finite set of well defined and unambiguous commands to solve a task.

Programming language

- vocabulary and set of instructions to command a computer

Algorithm Example - “Cake baking”

- Prepare a cake pan by spraying with baking spray or buttering and lightly flouring. Next, combine flour, baking powder, baking soda, and salt in a large bowl and set the mix aside. Add 3 eggs, one at a time, and mix just until combined. Add flour mixture and buttermilk, alternately, beginning and ending with flour. Preheat oven to 200 C. Pour the dough in a pan and bake it for 25-30 minutes until edges turn loose from pan and toothpick inserted into middle of cake comes out clean. Remove from the oven and allow to cool for about 10 minutes.

Algorithm Analysis

Algorithm Example - “Cake baking”

- Prepare a cake pan by spraying with baking spray or buttering and lightly flouring. Next, combine flour, baking powder, baking soda, and salt in a large bowl and set the mix aside. Add 3 eggs, one at a time, and mix just until combined. Add flour mixture and buttermilk, alternately, beginning and ending with flour. Preheat oven to 350º F, pour the dough in a pan and bake it for 25-30 minutes until edges turn loose from pan and toothpick inserted into middle of cake comes out clean. Remove from the oven and allow to cool for about 10 minutes.

Task - back a cake

Language - English

Algorithm Analysis

Algorithm Example - “Cake baking”

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Task - back a cake

Language - English

Exact - ???

Well defined - ???

Algorithm Analysis

Algorithm Example - “Cake baking”

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Task - back a cake

Language - English

Exact - ???

Well defined - ???

Language & Algorithms

Computer Language

- well defined commands.
- tests to decide the next steps (if-else command)
- tests for repeating commands until a condition is satisfied (while or repeat)

My first algorithm- “Cake baking”

```
1. If baking spray is available then
           prepare cake pan by spraying
   else
         prepare pan by buttering and lightly flouring.
2. While mixture is not creamy
     1. Combine flour, baking powder, baking soda, and salt in a large  bowl
3. Repeat 3 times
     1. Add an egg
     2. While mixture not homogeneous
          1. Mix dough.
4. Pour the dough in a pan.
5. Turn oven on.
6. Wait until temperature is 200 C.
7. Put pan into oven
8. While “not” edges turn loose from pan or 30 minutes have passed.
     1. Wait 1 minute.
9. Remove from the oven
10. Wait for 10 minutes.
```

Algorithms

1. **Exercise:**
    1. Describe how to change a tire using “if” and “else” and while.

R Language

- Script based Programming language
- Focus of statistical data analysis
- Open source
- Contributing packages
  - Bioconductor (bioinformatics functions)
  - ggplot2 (plotting functions)
  - …

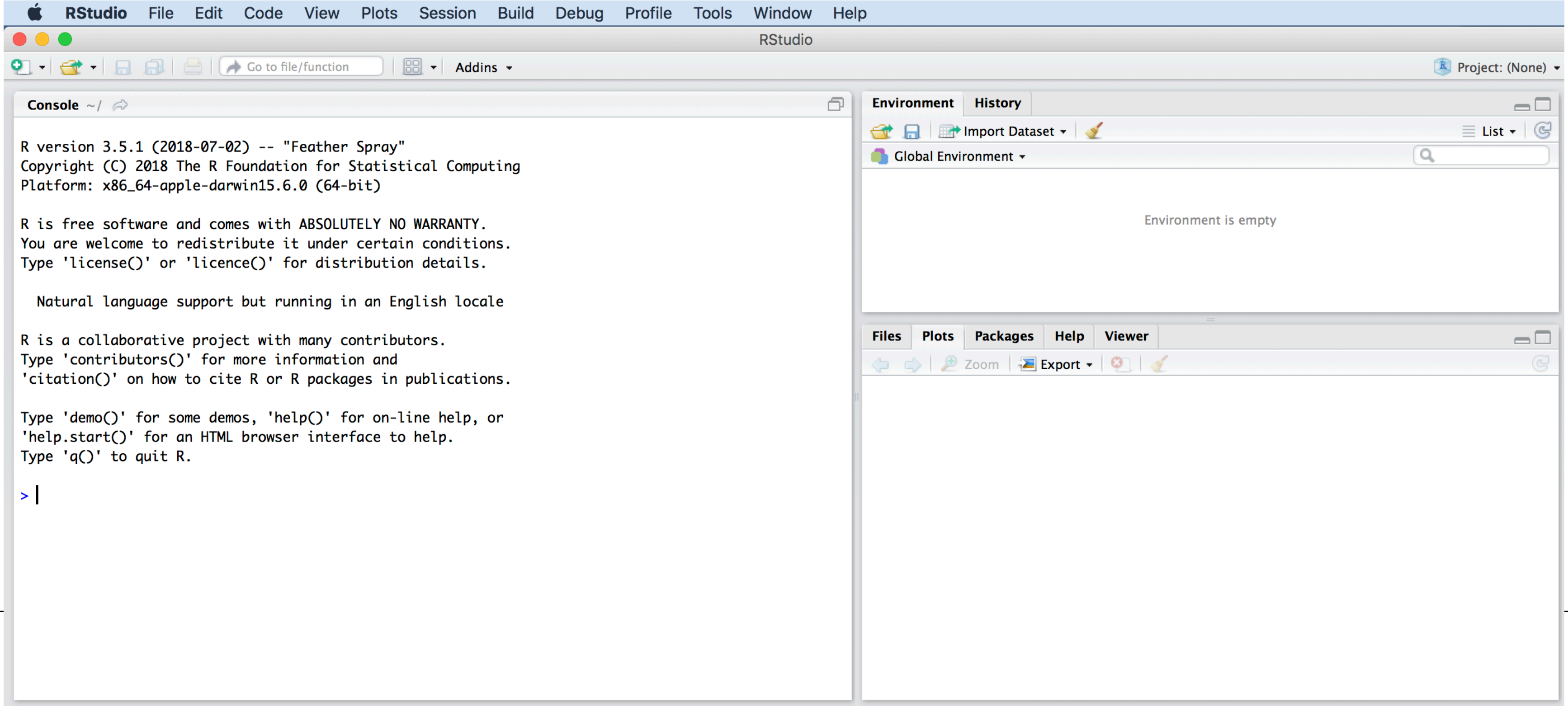
http://www.r-project.org/

RStudio - Getting Started

- Install RStudio

  https://www.rstudio.com

- Run RStudio



```
R version 3.5.1 (2018-07-02) -- "Feather Spray"
Copyright (C) 2018 The R Foundation for Statistical Computing
Platform: x86_64-apple-darwin15.6.0 (64-bit)

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>
```
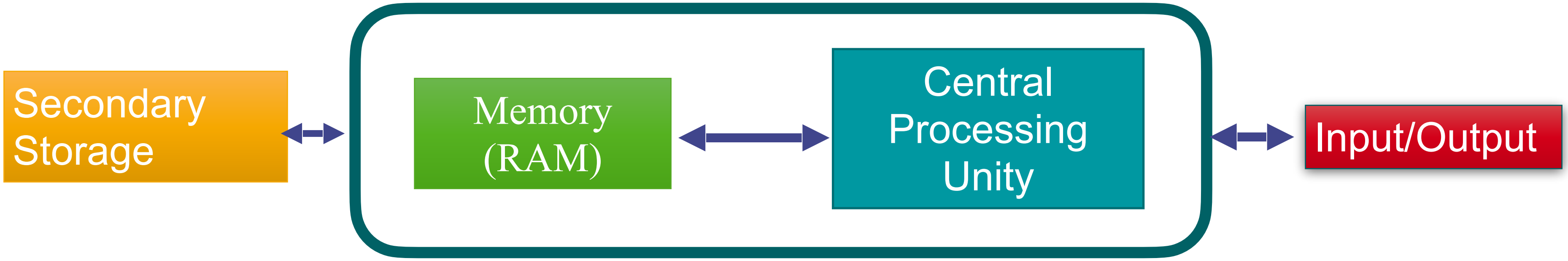

Computer Architecture



- **Central Processing Unity (CPU)**
  - execute mathematical operations
- **Memory (RAM)**
  - stores (limited) data for CPU (4-32 Gigabytes)
  - fast access but not permanent
- **Permanent Storage**
  - Slow access / large capacity (1.000 Gigabytes)
  - Permanent storage of files
- **Input/output**
  - monitor/keyboard/network card

Memory (RAM)

- A **computer memory** is like a large cabinet
- Each drawer can be used to keep information
  - i.e. names, telephones
- Each drawer holds a particular type of information
  - i.e. **strings**, **numbers**
- Computer knows the location of a particular drawer

Variables

- Each drawer is called a **variable** (and we can give it a name)

Variables

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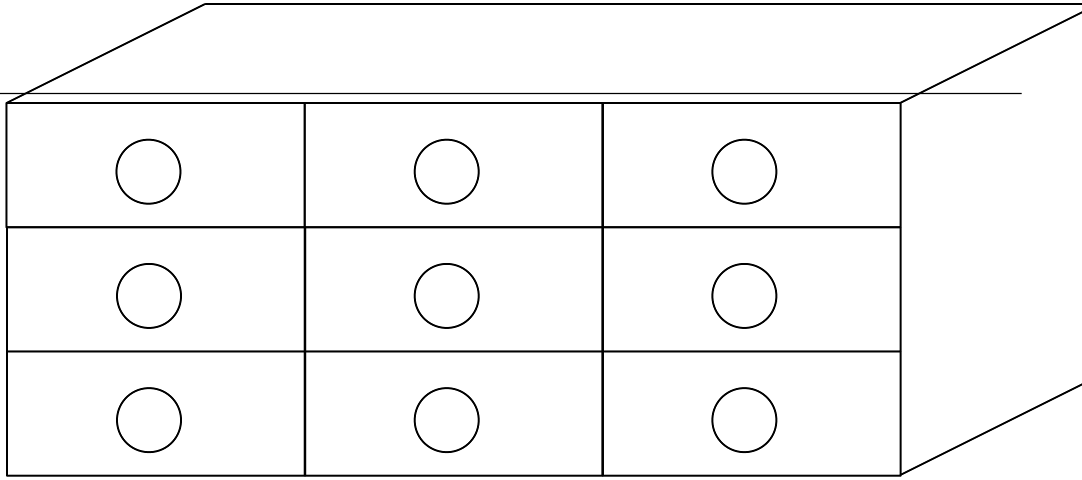
- Each drawer has a **type**

Variables



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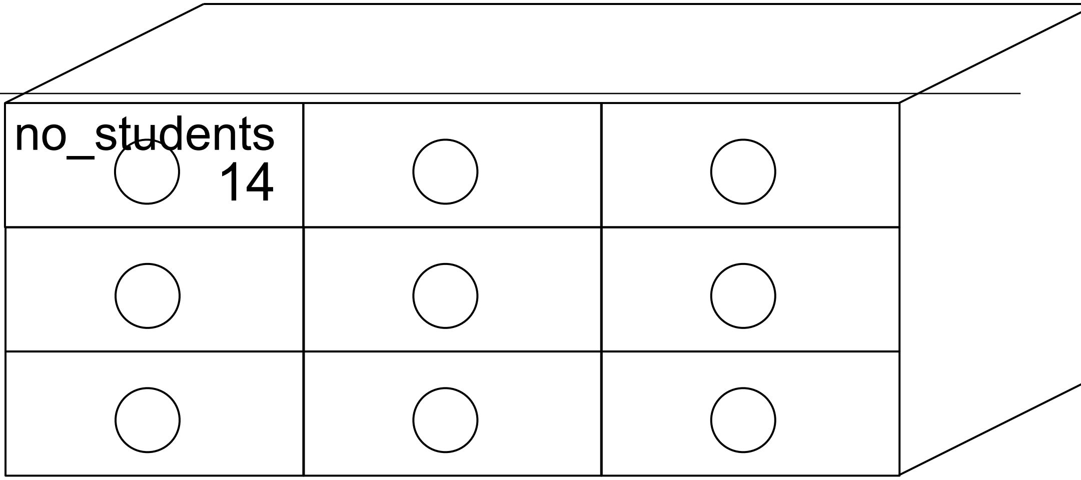
Variables



- Each drawer is called a **variable** (and we can give it a name)
- Each drawer has a **type**
- In R, we have the following **types:**
  - **numeric:** no_students = 14
  -

Variables

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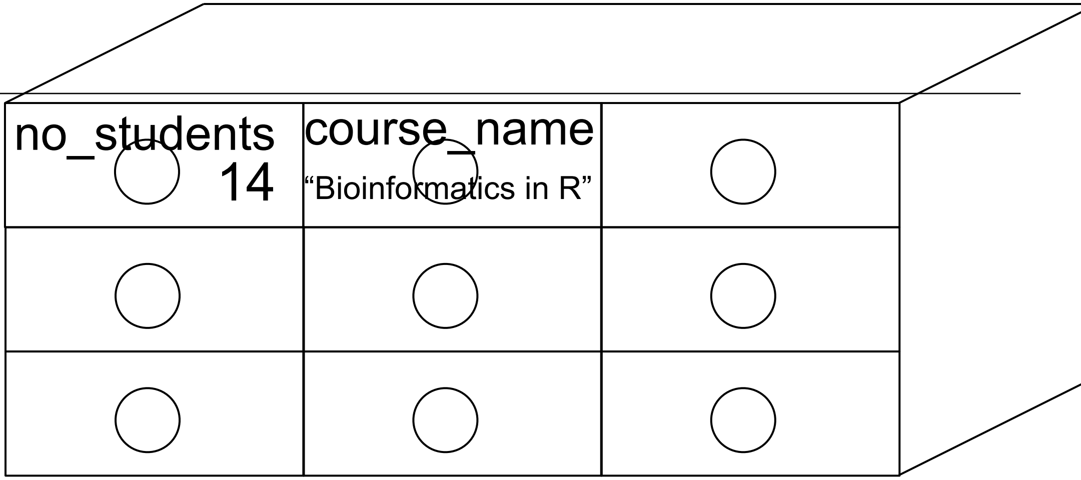
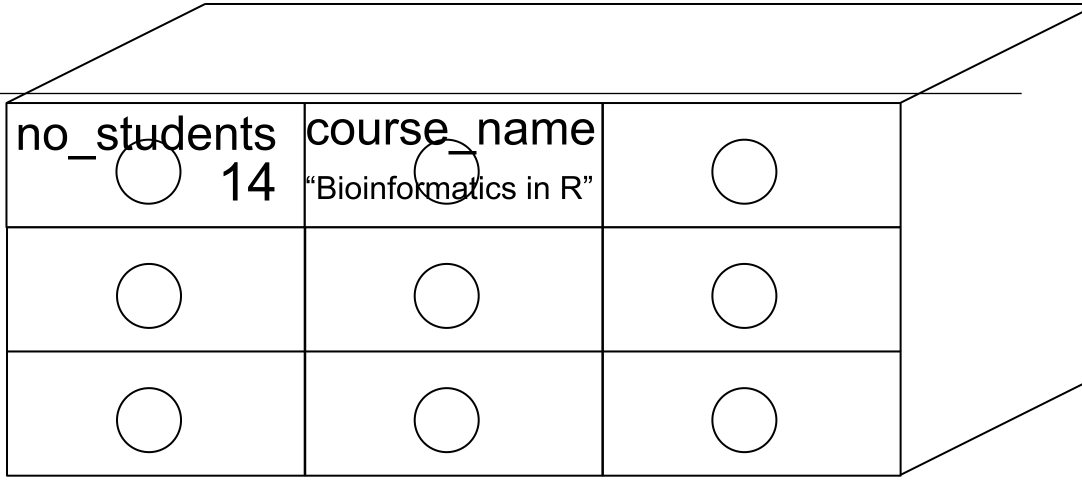


- Each drawer has a **type**
- In R, we have the following **types:**
  - **numeric:** no_students = 14
  - **character:** course_name **=** “Bioinformatics in R”

Variables



- Each drawer is called a **variable** (and we can give it a name)
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  - **character:** course_name **=** “Bioinformatics in R”
  - **boolean:** graduate_level = True

Variables

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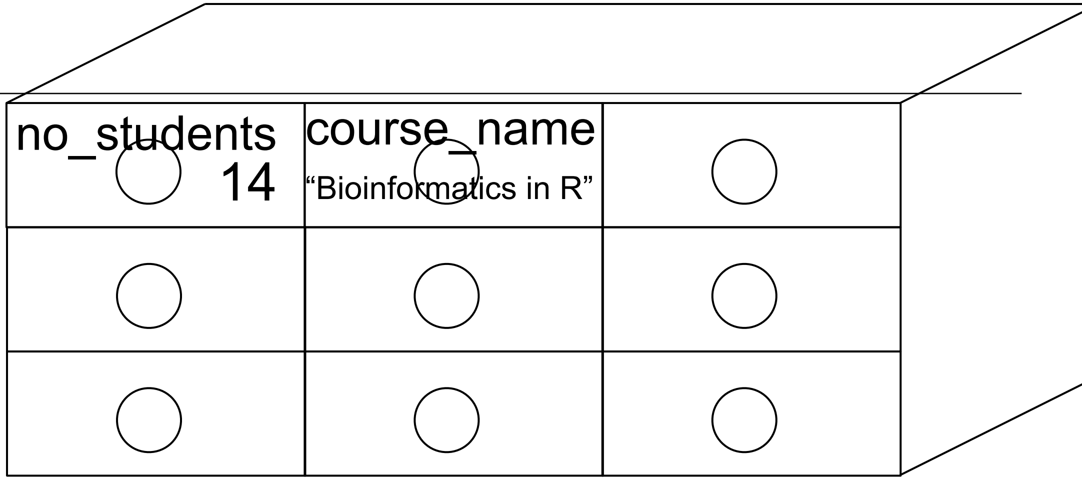
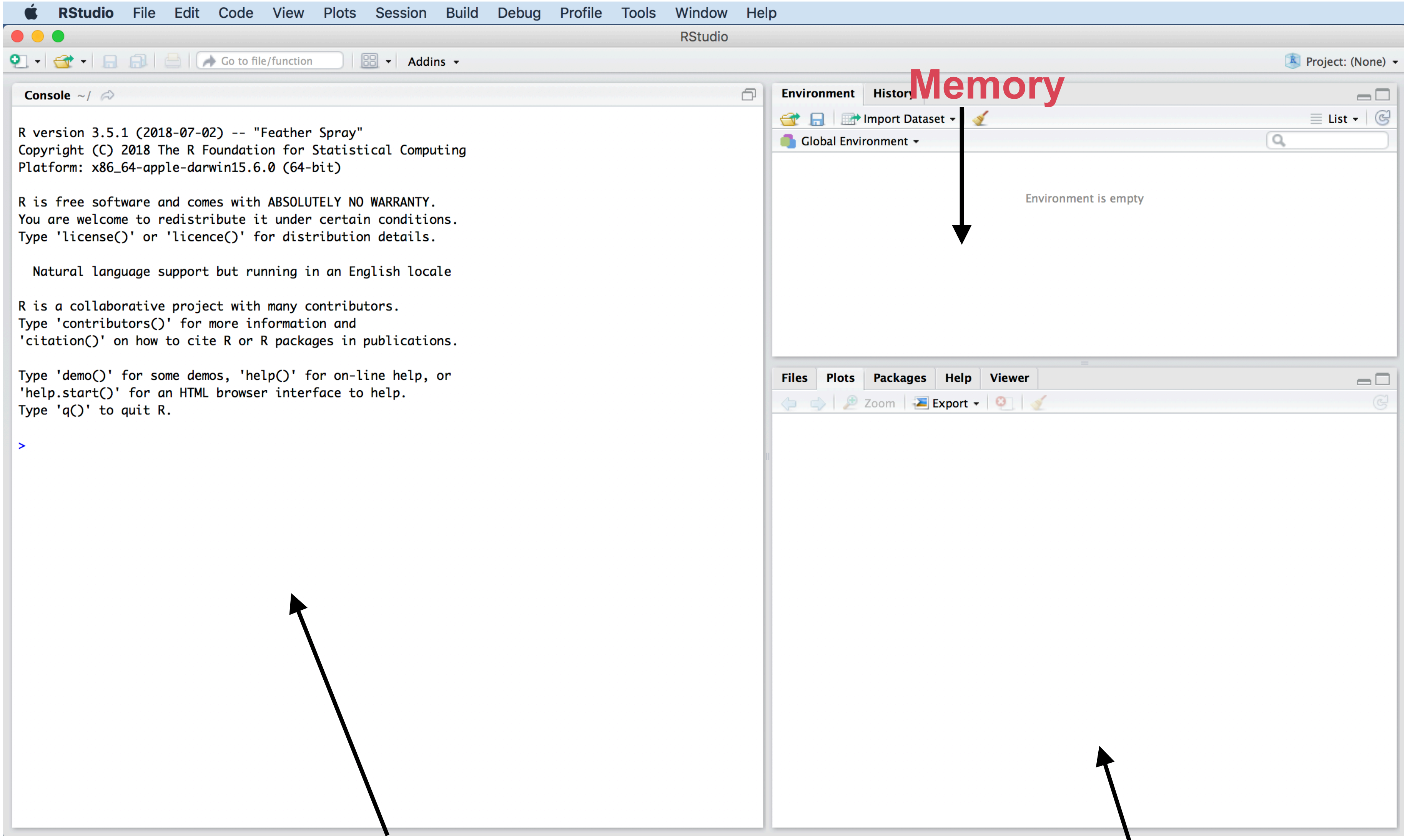


- Each drawer has a **type**
- In R, we have the following **types:**
  - **numeric:** no_students = 14
  - **character:** course_name **=** “Bioinformatics in R”
  - **boolean:** graduate_level = True
  - **vectors:** (combination of several variables of same type): instructors = c(“Ivan”,”Tiago”,”Fabio”)
  - **Matrices:** …

RStudio & Memory



```
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>
```

R console: local to provide commands!

Graphs (not now)

Variables and Data Types

Single data can be stored in variables

- Data Types: “numeric”, ”character”, “logical”, …

R console

```
x = 3; <enter>
x; <enter>
```

“x = 3;” means store the number “3” at a variable named “x”

Variables and Data Types

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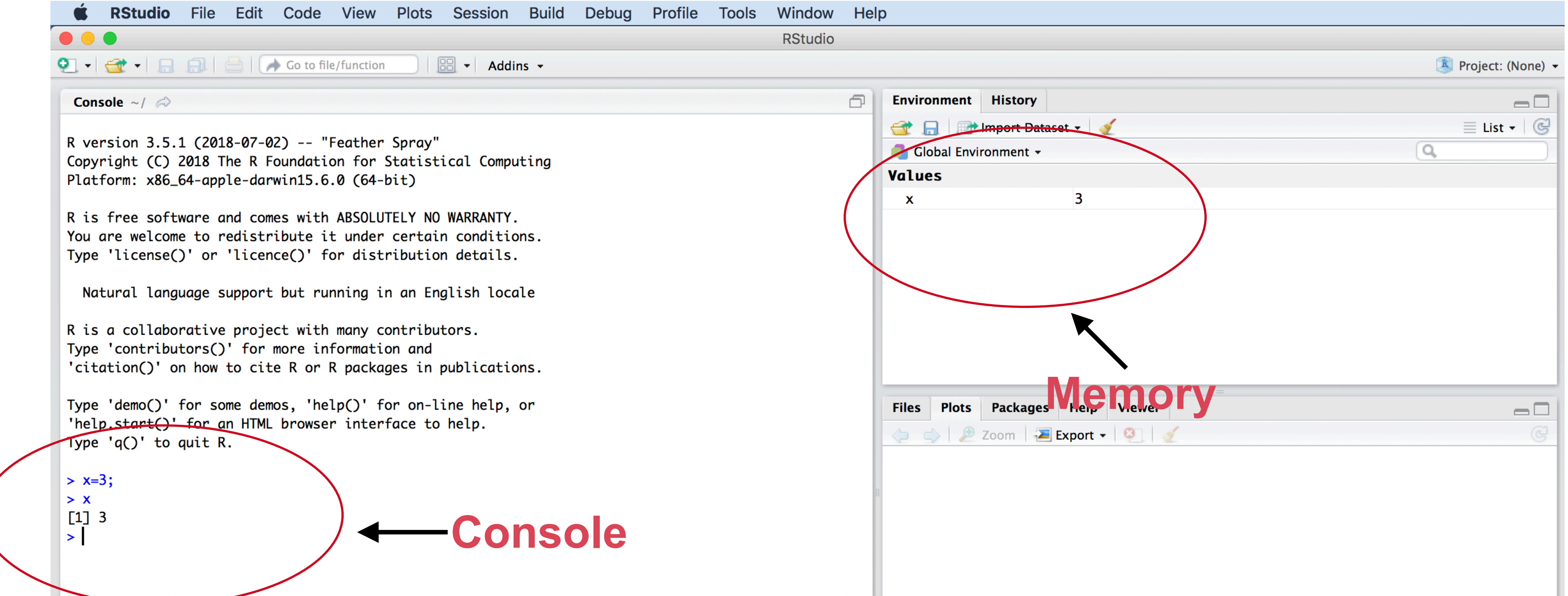
x = 3; <enter>
x; <enter>
```

“x = 3;” means store the number “3” at a variable named “x”



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Type 'q()' to quit R.

> x=3;
> x
[1] 3
> 
```

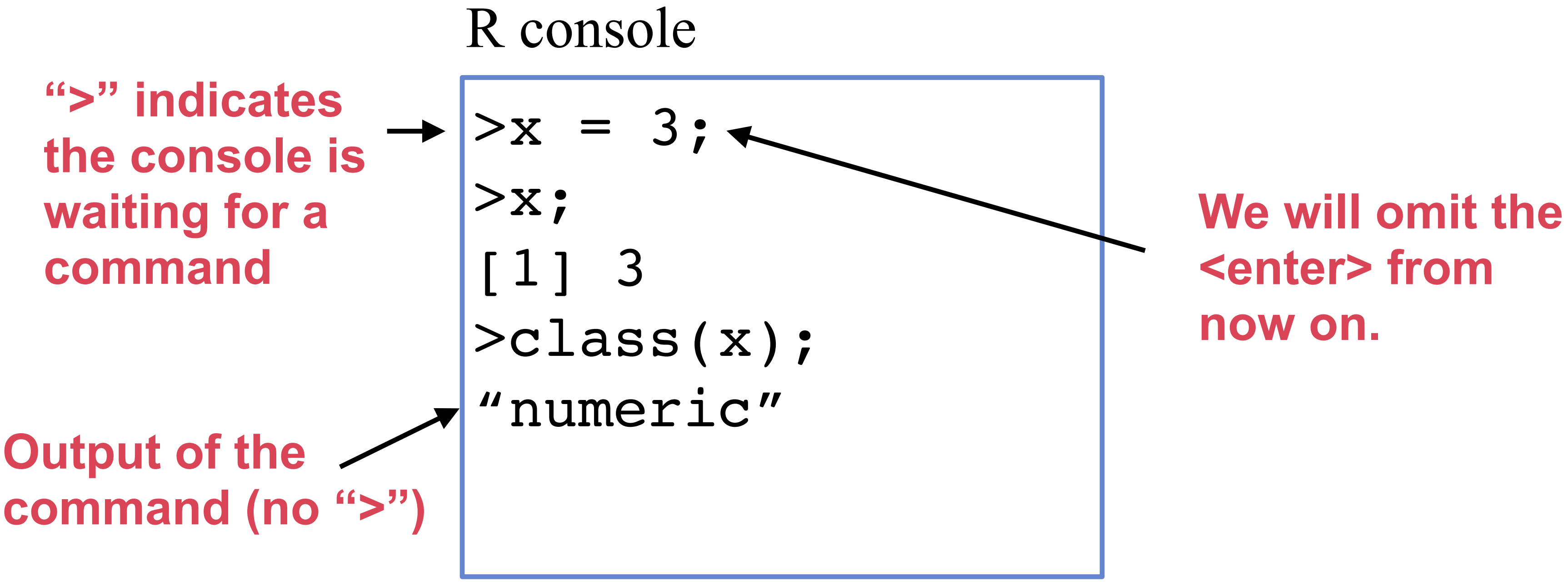
Values

x	3

Memory

Console

R Console



R console

```
>x = 3;
>x;
[1] 3
>class(x);
“numeric”
```

“>” indicates the console is waiting for a command

We will omit the <enter> from now on.

Output of the command (no “>”)

Variables and Data Types

Single data can be stored in variables

- Data Types: “numeric”, ”character”, “logical”, …

R console

```
> x = 3
> x
[1] 3
> class(x)
“numeric”
> y ="Bioinformatics"
> y
"Bioinformatics"
```

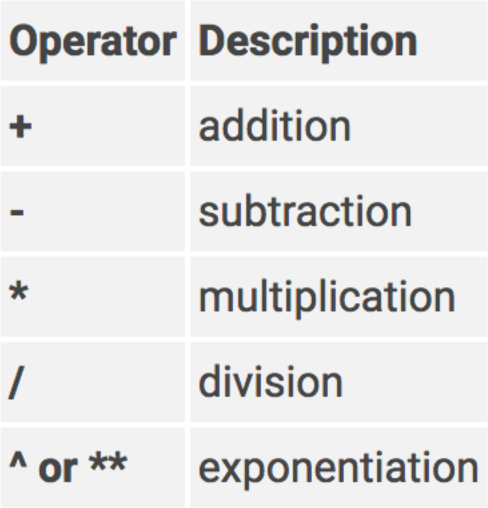
```
> class(y)
“character”
> z = TRUE
> z
TRUE
> class(z)
“logical”
```

Variables and Operations

We can apply arithmetic functions to variables

R console

```
> x = 3
> y = 4
> x + y
[1] 7
> x*y
[1] 12
> x/y
[1] 0.75
```



Operator	Description
+	addition
-	subtraction
*	multiplication
/	division
^ or **	exponentiation

Variables and Operations

We can apply arithmetic functions to variables

R console

```
> x = 3
> y = 4
> x + y
[1] 7
> x*y
[1] 12
> x/y
[1] 0.75
```

```
> z = x + y
> z
[1] 7
> z = z + 2
> z
[1] 9
```

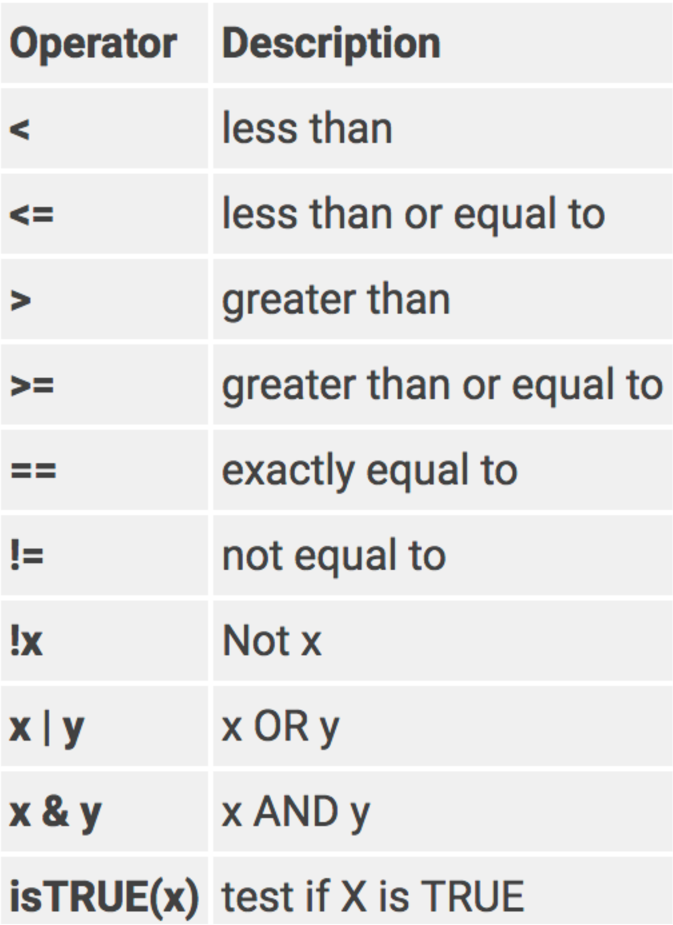
Variables and Operations

We can apply logical functions to variables

& (and) and | (or)

R console

```
> x = 3
> y = 4
> x > y
[1] FALSE
> z = TRUE
> z & (x > y)
[1] FALSE
> z | (x > y)
[1] TRUE
```



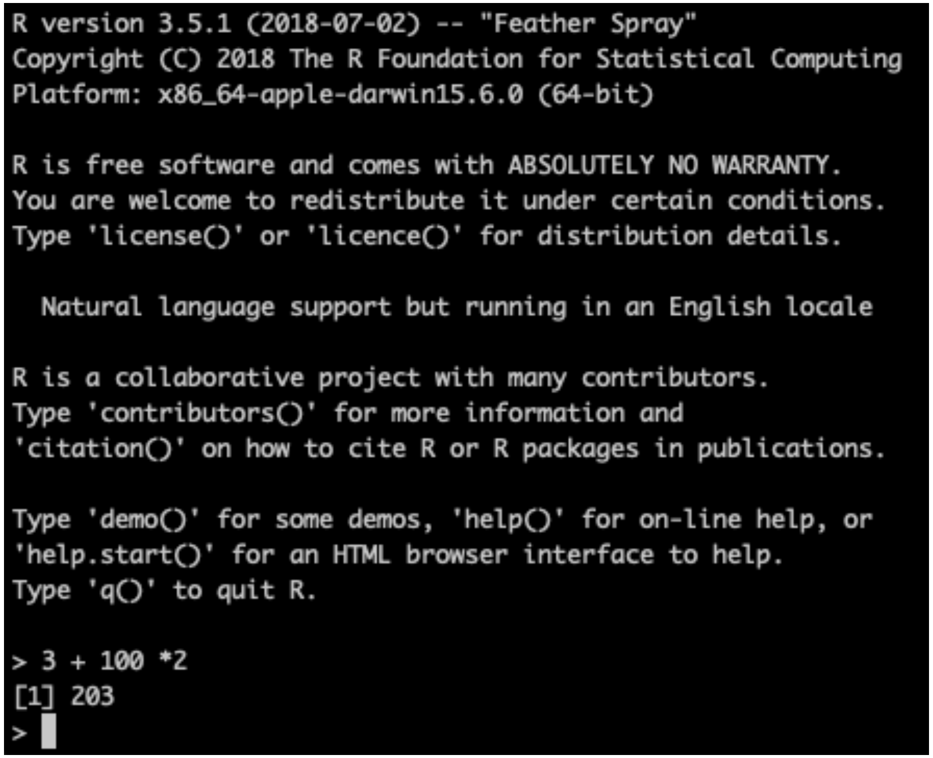
Operator	Description
<	less than
<=	less than or equal to
>	greater than
>=	greater than or equal to
==	exactly equal to
!=	not equal to
!x	Not x
x | y	x OR y
x & y	x AND y
isTRUE(x)	test if X is TRUE

Overview of RStudio

Intro to RStudio

- RStudio is not R itself, but an **i**ntegrated **d**evelopment **e**nvironment (IDE).

- It offers several panels for different purposes, such as console, help message, plots, history, scripts… etc.



```
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Type 'q()' to quit R.

> 3 + 100 *2
[1] 203
> 
```

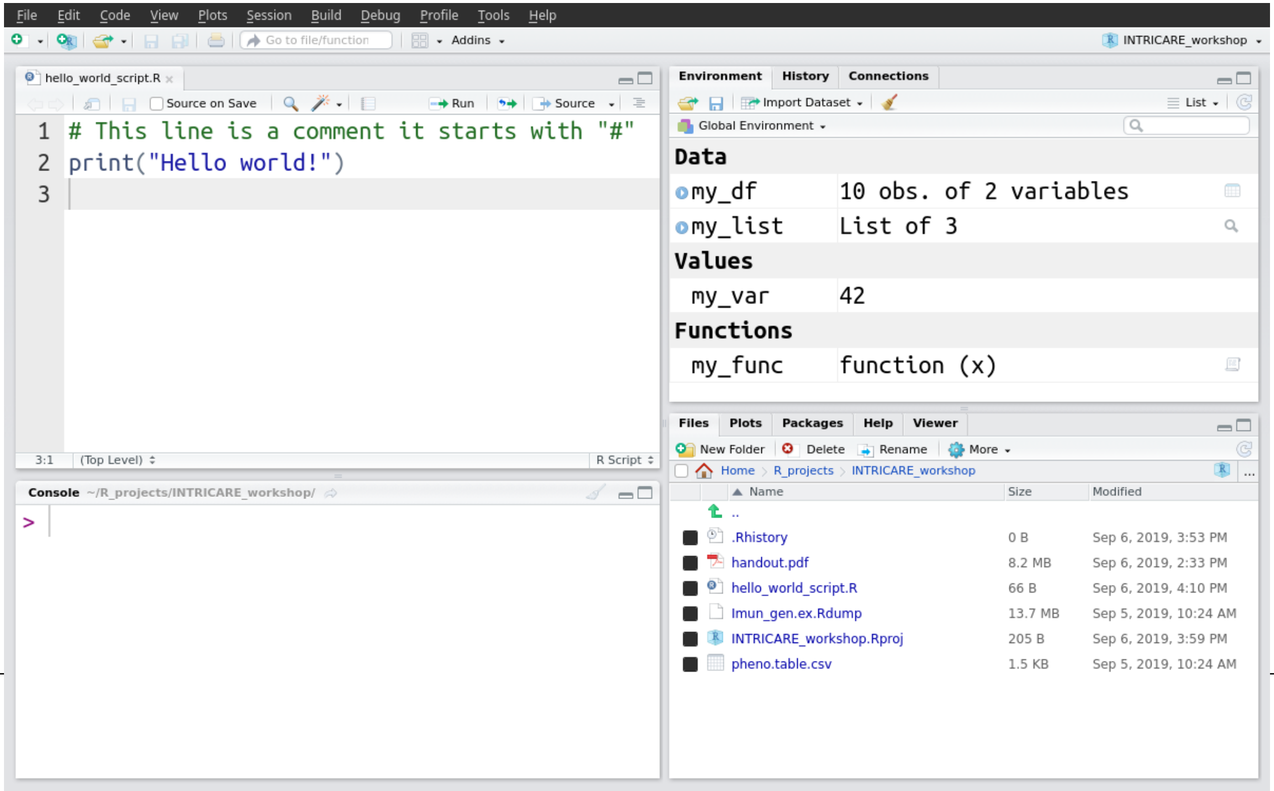
RStudio®

RStudio - Getting Started

- Install RStudio

  https://www.rstudio.com

- Run RStudio



```
# This line is a comment it starts with "#"
print("Hello world!")
```

```
>
```

Data

my_df	10 obs. of 2 variables
my_list	List of 3

Values

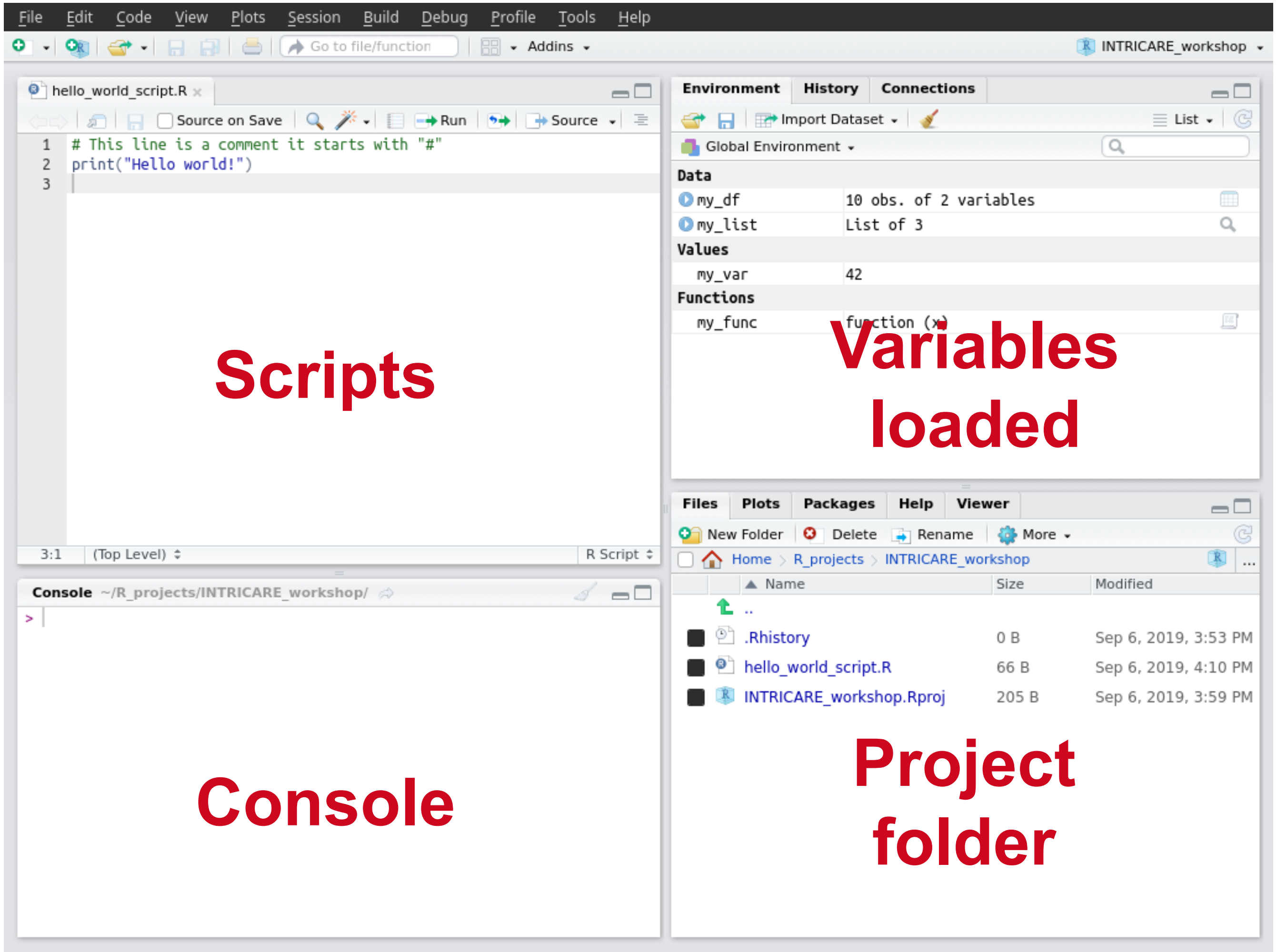
my_var	42

Functions

my_func	function (x)

Name	Size	Modified
..		
.Rhistory	0 B	Sep 6, 2019, 3:53 PM
handout.pdf	8.2 MB	Sep 6, 2019, 2:33 PM
hello_world_script.R	66 B	Sep 6, 2019, 4:10 PM
Imun_gen.ex.Rdump	13.7 MB	Sep 5, 2019, 10:24 AM
INTRICARE_workshop.Rproj	205 B	Sep 6, 2019, 3:59 PM
pheno.table.csv	1.5 KB	Sep 5, 2019, 10:24 AM

RStudio - Organisation



```r
# This line is a comment it starts with "#"
print("Hello world!")

```

Scripts

```
>
```

Console

Data	
my_df	10 obs. of 2 variables
my_list	List of 3
Values	
my_var	42
Functions	
my_func	function (x)

Variables loaded

Name	Size	Modified
..		
.Rhistory	0 B	Sep 6, 2019, 3:53 PM
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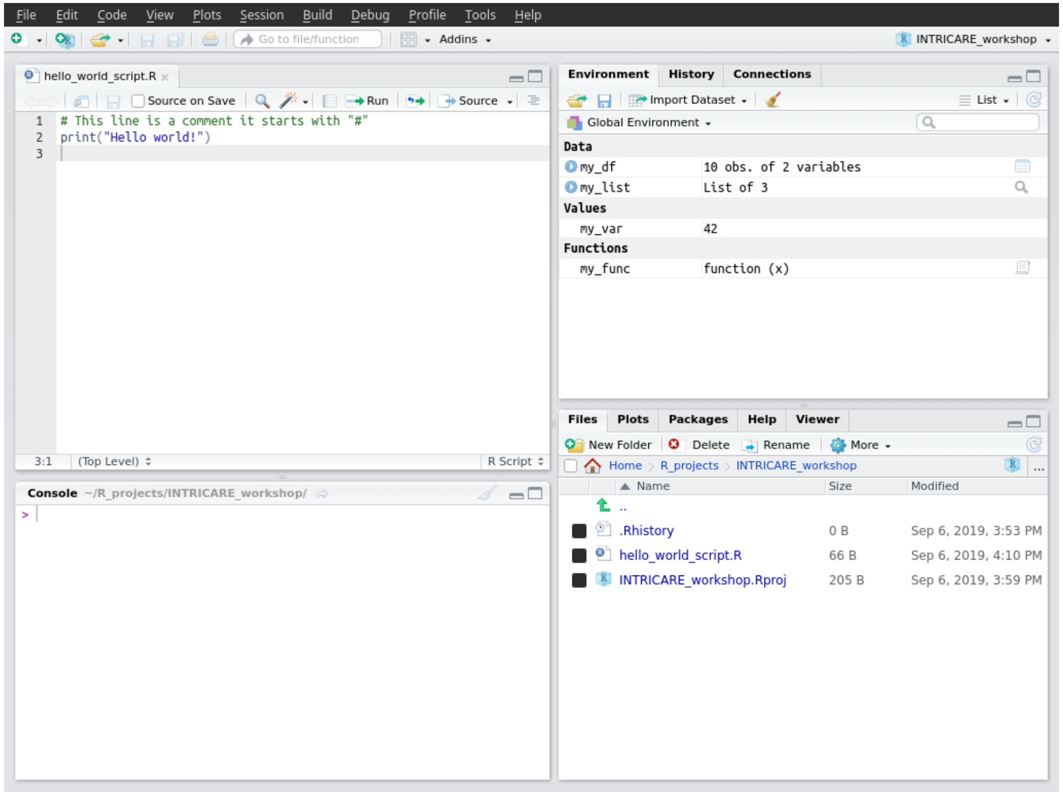
INTRICARE_workshop.Rproj	205 B	Sep 6, 2019, 3:59 PM

Project folder

RStudio - Configure Project Directory



```
# This line is a comment it starts with "#"
print("Hello world!")
```

Console ~/R_projects/INTRICARE_workshop/

```
>
```

Data	
my_df	10 obs. of 2 variables
my_list	List of 3
Values	
my_var	42
Functions	
my_func	function (x)

Home › R_projects › INTRICARE_workshop

Name	Size	Modified
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.Rhistory	0 B	Sep 6, 2019, 3:53 PM
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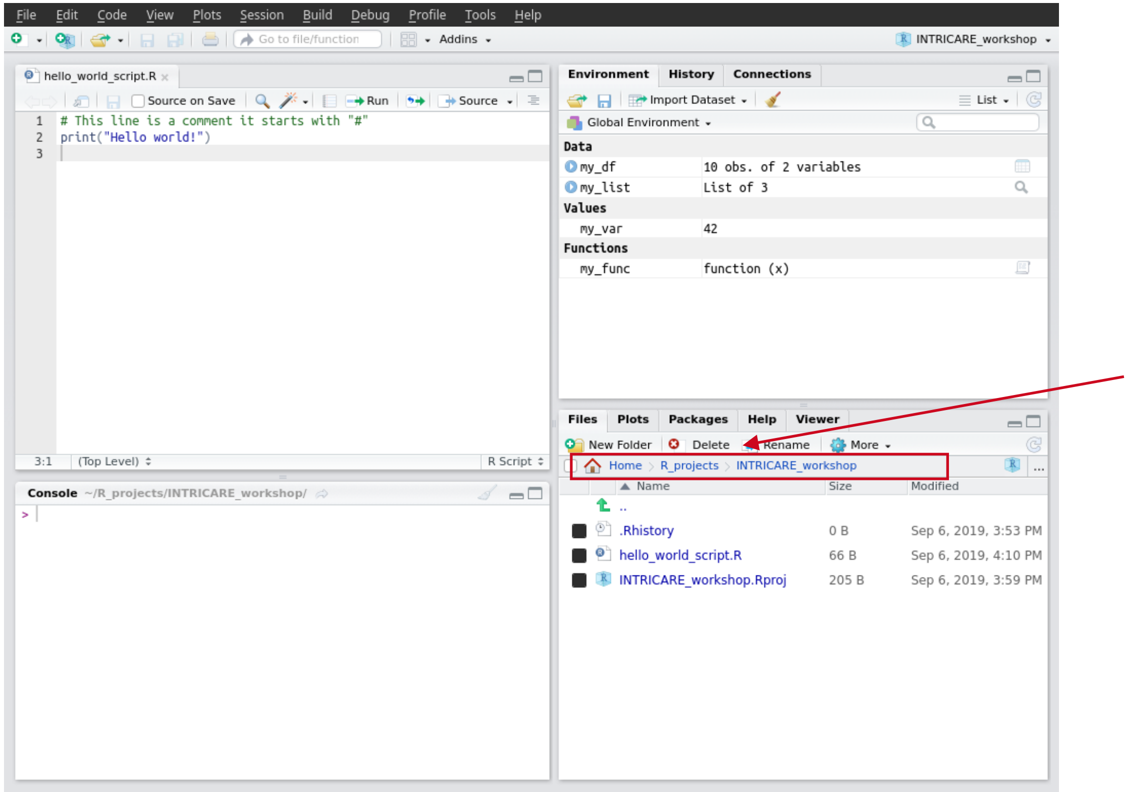
INTRICARE_workshop.Rproj	205 B	Sep 6, 2019, 3:59 PM

We need to configure the project directory:

RStudio - Configure Project Directory



```
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```

```
>
```

Data	
my_df	10 obs. of 2 variables
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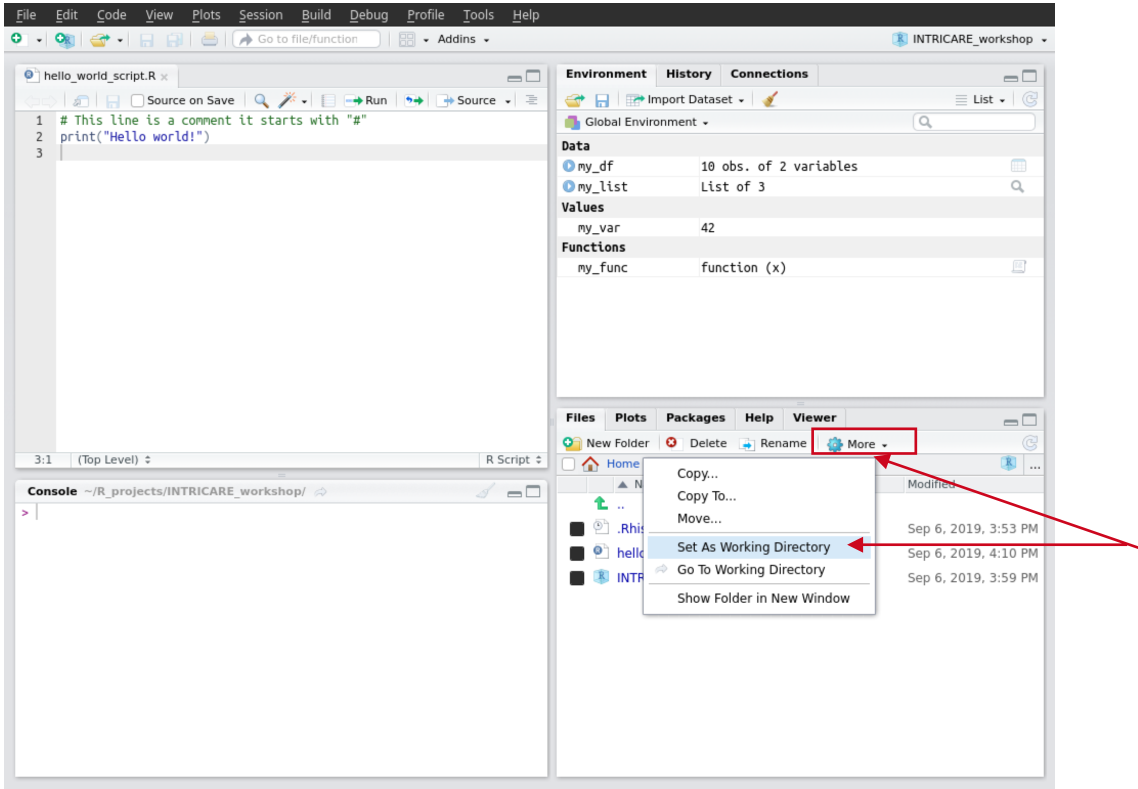
We need to configure the project directory:

1 - navigate until folder with course files

RStudio - Configure Project Directory



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my_func	function (x)

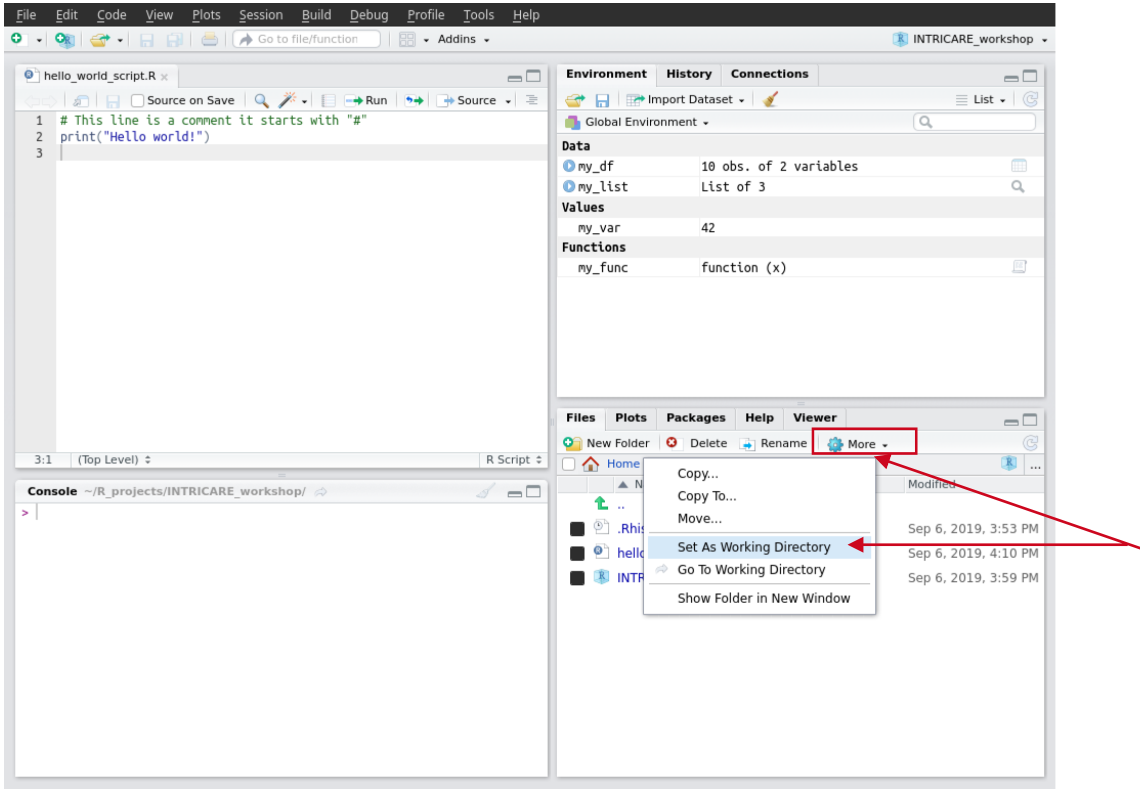
Name	Modified
..	
.Rhis	Sep 6, 2019, 3:53 PM
hell	Sep 6, 2019, 4:10 PM
INTR	Sep 6, 2019, 3:59 PM

We need to configure the project directory:

1 - navigate until folder with course files

2 - select the "More" option and "Set as Working Directory"

RStudio - Configure Project Directory



```
# This line is a comment it starts with "#"
print("Hello world!")
```

```
Data
my_df       10 obs. of 2 variables
my_list     List of 3
Values
my_var      42
Functions
my_func     function (x)
```

We need to configure the project directory:

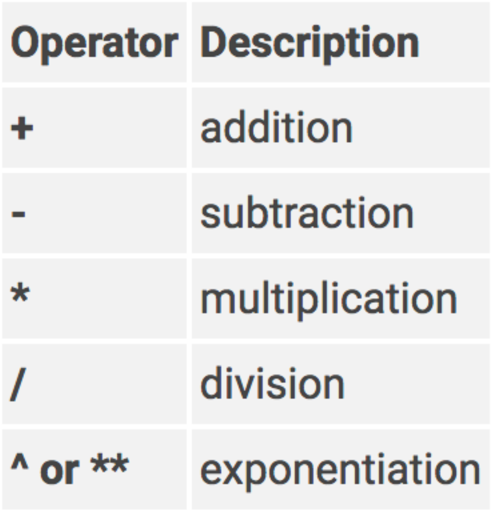
1 - navigate until folder with course files

2 - select the "More" option and "Set as Working Directory"

Now R Studio knows where to find files !

Exercise 1

- Use arithmetic operations to perform the following calculations
  - 1 plus 3
  - 3 minus 1
  - 2 multiplied by 2
  - 4 divided by 2
  - 3 to the power of 2



Operator	Description
+	addition
-	subtraction
*	multiplication
/	division
^ or **	exponentiation

- Repeat the exercise but this time "save" the results of the operations (using variables)

Exercise 2

- Use variables to store the amount of fruits in a shop. We have 5 green apples, 4 red apples, 10 bananas and 4 melons.
- Write a code using variables to answer the following questions:
  - How many fruits are there is total?
  - How many apples?
  - What is the average number of fruits per type?

Exercise 3

- An apple costs 0.5 cents, a banana 1.0 euro, a melon 3 euros (use variables to store these!).
  - How much does it cost to buy all the apples in the shop?
  - How much does it cost to buy all the fruits in the shop?
- There was an additional shipment of fruits with 20 additional bananas and 10 additional red apples.
  - Estimate the cost of buying all apples or fruits in the shop after the new shipment.

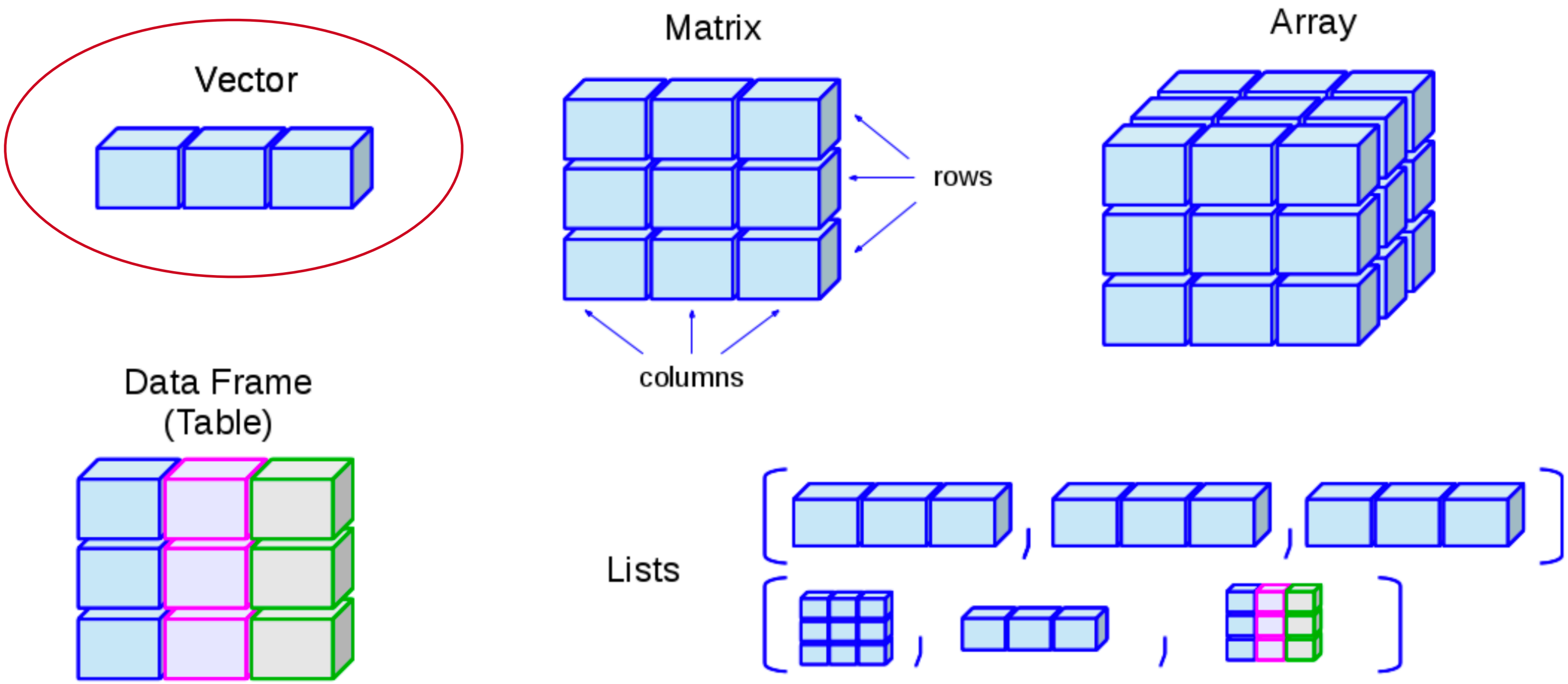
Exercise 4

- Use logical variables to answer the following questions.
  - Is buying all bananas cheaper than buying all apples?
  - You have 20 euros. Can you buy all apples?

Complex Data Structures

- Vector – variable containing a array of items of the same type
- Lists - a vector where items can have distinct types (tomorrow!)
- Matrix – two dimensional vector with items of the same type
- Data Frame – complex data structure for two dimensional data where columns can be of distinct type (as an excel sheet) (tomorrow!)

Complex Data Structures



Vector

- Creating, accessing and updating vector

```
> v = c(3.2, 4.1, 1.9)
> v
[1] 3.2 4.1 1.9
> v[2]          # access 2nd position of vector
[1] 4.1
> v[3] = 10.4   #update 3rd position of vector
> v
3.2  4.1 10.4

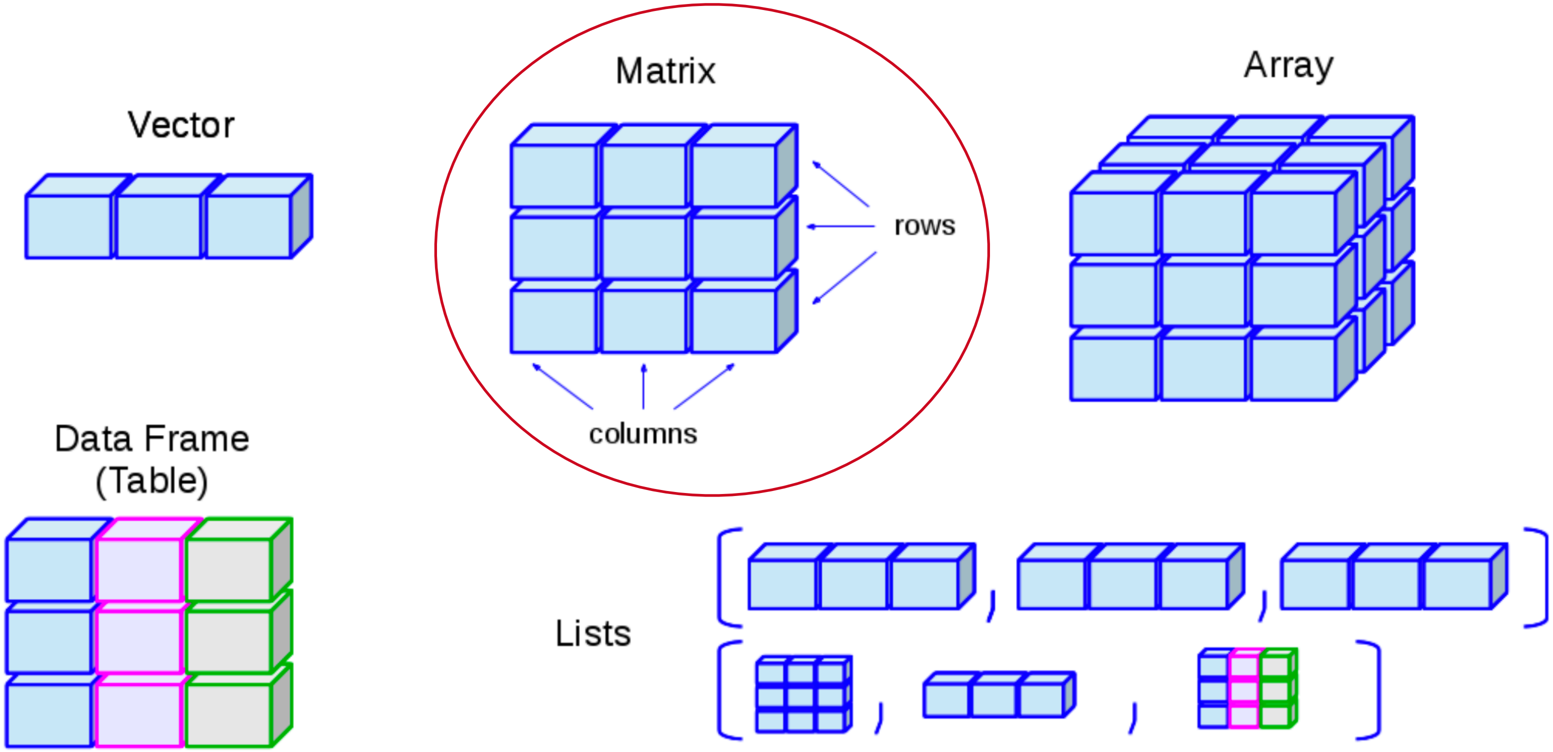
> u = c(1,2,3)
> z = u + v     #sum 2 vectors (if size is the same)
> z
[1]  4.2  6.1 13.4
```

Vector

- Operations, functions and access

```
> length(z)    # function indicating size of vector
[1] 3
> 1:2          # vector with 1 and 2.
[1] 1 2
> z[1:2]       #subsetting vector (1st and 2rd pos.)
[1] 4.2 6.1
> z > 6        #logical operator
[1] FALSE  TRUE  TRUE
> z[z > 6]     # return all values greater than 6
[1]  6.1 13.4
```

Complex Data Structures



Matrix

- Matrix – two dimensional vector / same type

```
> m = matrix(1:12, 4, 3)  # 4 by 3 matrix
> dim(m)                  # size of matrix
4  3
> m[1,]         # show first row of matrix
[1] 1  5  9
> m[3,1]        #show element at 3rd row / 1st column
[3]
> m
     [,1] [,2] [,3]
[1,]    1    5    9
[2,]    2    6   10
[3,]    3    7   11
[4,]    4    8   12
```

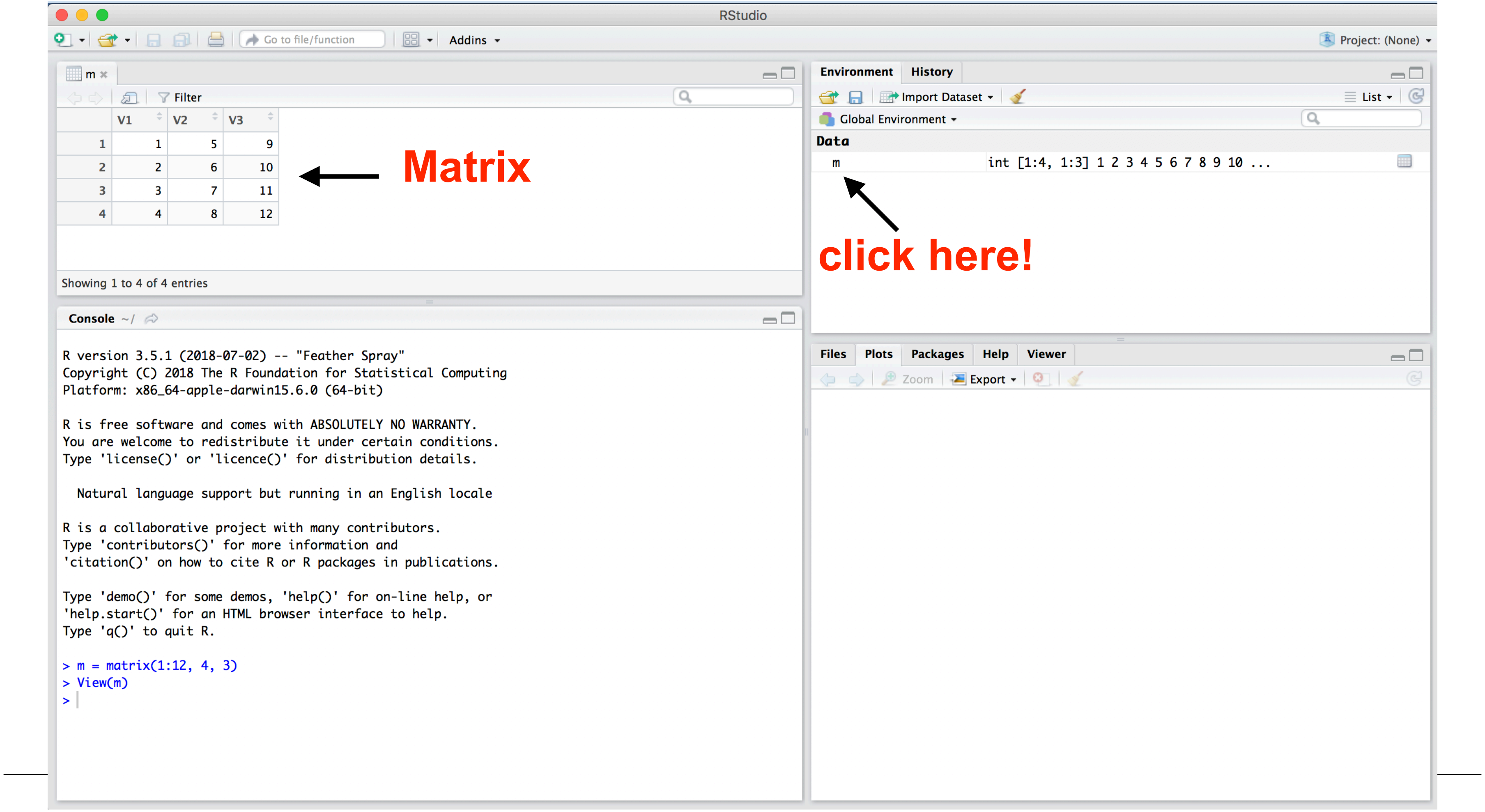
Matrix

- Matrix – two dimensional vector / same type

```
> v1 = c(10,4,10)  # a vector with 3 entries
> v2 = c(4,10,2)   # another 3 entry vector
> mat = rbind(v1,v2) # join two vectors as a matrix
> mat
   [,1] [,2] [,3]
v1   10    4   10
v2    4   10    2
```

Matrix

- RStudio also helps visualisation of a matrix



	V1	V2	V3
1	1	5	9
2	2	6	10
3	3	7	11
4	4	8	12

Showing 1 to 4 of 4 entries

Matrix

Data

```
m                    int [1:4, 1:3] 1 2 3 4 5 6 7 8 9 10 ...
```

click here!

```
R version 3.5.1 (2018-07-02) -- "Feather Spray"
Copyright (C) 2018 The R Foundation for Statistical Computing
Platform: x86_64-apple-darwin15.6.0 (64-bit)

R is free software and comes with ABSOLUTELY NO WARRANTY.
You are welcome to redistribute it under certain conditions.
Type 'license()' or 'licence()' for distribution details.

  Natural language support but running in an English locale

R is a collaborative project with many contributors.
Type 'contributors()' for more information and
'citation()' on how to cite R or R packages in publications.

Type 'demo()' for some demos, 'help()' for on-line help, or
'help.start()' for an HTML browser interface to help.
Type 'q()' to quit R.

> m = matrix(1:12, 4, 3)
> View(m)
> 
```

Matrix

- What happens if we have a large matrix? 450.000 lines by 1000 samples?

```
> m = matrix(1:12, 450000, 1000) # 4 by 3 matrix
> dim(m)      # size of matrix
[1] 450000   1000
> m[,1]       # show first column of matrix
[1] 1 2 3 4 5 6 …
```

Matrix

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[1] 1 2 3 4 5 6 …
```

- Large matrices use a lot of memory (1.7 GB)!

```
> remove(m) #  remove m from memory
```

Functions

Functions

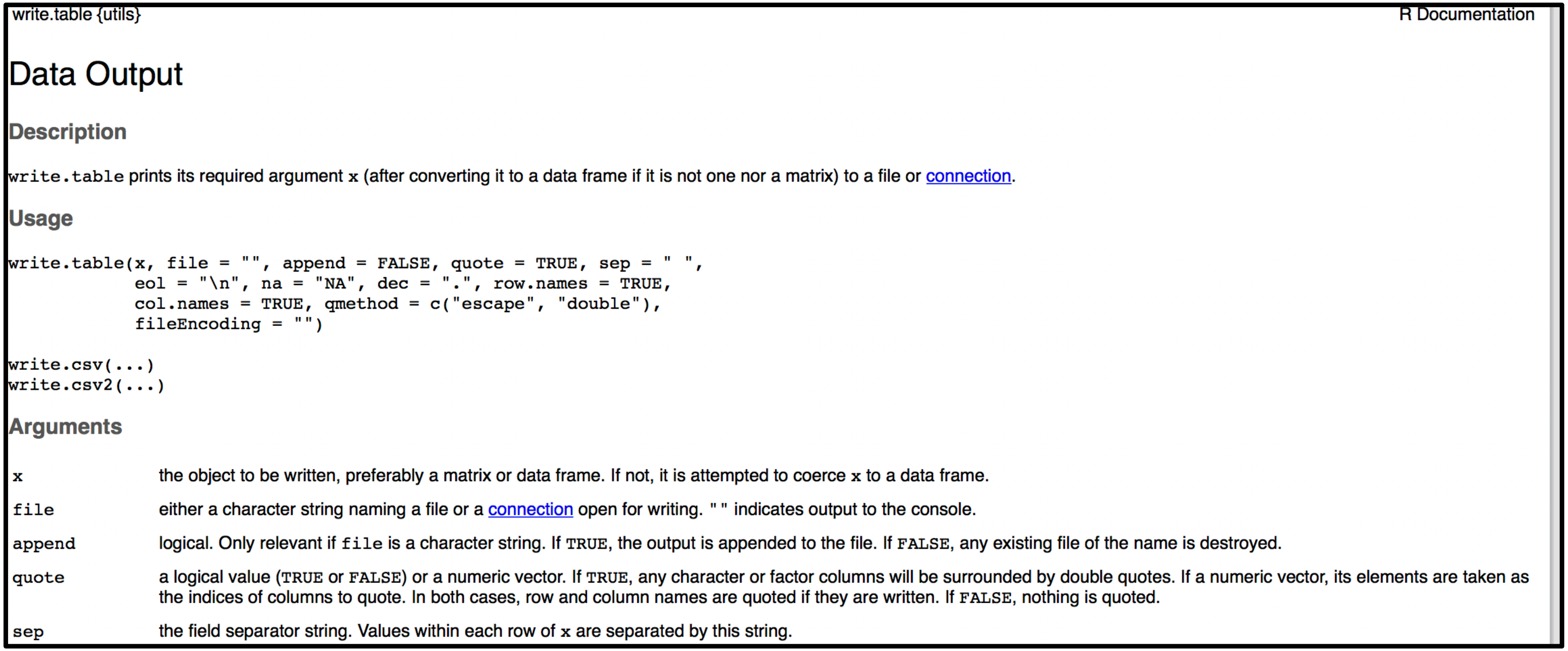
- A section of a program that perform a specific task
  - Takes values as input parameter and returns some new value (or performs an operation)
- R defines several types of functions
  - math: log, exp, abs, sqrt, min, max, …
  - array/matrix manipulation: length, dim, array, rep, …
  - Read/write files: read.table, write.table, …
- Can be created by user or defined in contributing packages (tomorrow!)

Example of Functions

```
> log2(4)
[1] 2
> m = matrix(1:12, 4, 3) # create a matrix
> dim(m)       # size of the data frame
[1] 4 3
> summary(m)   # statistics of the matrix columns
     V1             V2             V3
 Min.   :1.00   Min.   :5.00   Min.   : 9.00
 1st Qu.:1.75   1st Qu.:5.75   1st Qu.: 9.75
 Median :2.50   Median :6.50   Median :10.50
 Mean   :2.50   Mean   :6.50   Mean   :10.50
 3rd Qu.:3.25   3rd Qu.:7.25   3rd Qu.:11.25
 Max.   :4.00   Max.   :8.00   Max.   :12.00
> write.table(m,"mydata.txt")
# write matrix in a .txt file
> getwd()    # current working directory
```

Functions and help

```
> help.start() #opens a page with manual, tutorials and
help search
> help("write.table") #show options for write.table
```



write.table {utils}   R Documentation

Data Output

Description

`write.table` prints its required argument `x` (after converting it to a data frame if it is not one nor a matrix) to a file or connection.

Usage

```
write.table(x, file = "", append = FALSE, quote = TRUE, sep = " ",
            eol = "\n", na = "NA", dec = ".", row.names = TRUE,
            col.names = TRUE, qmethod = c("escape", "double"),
            fileEncoding = "")

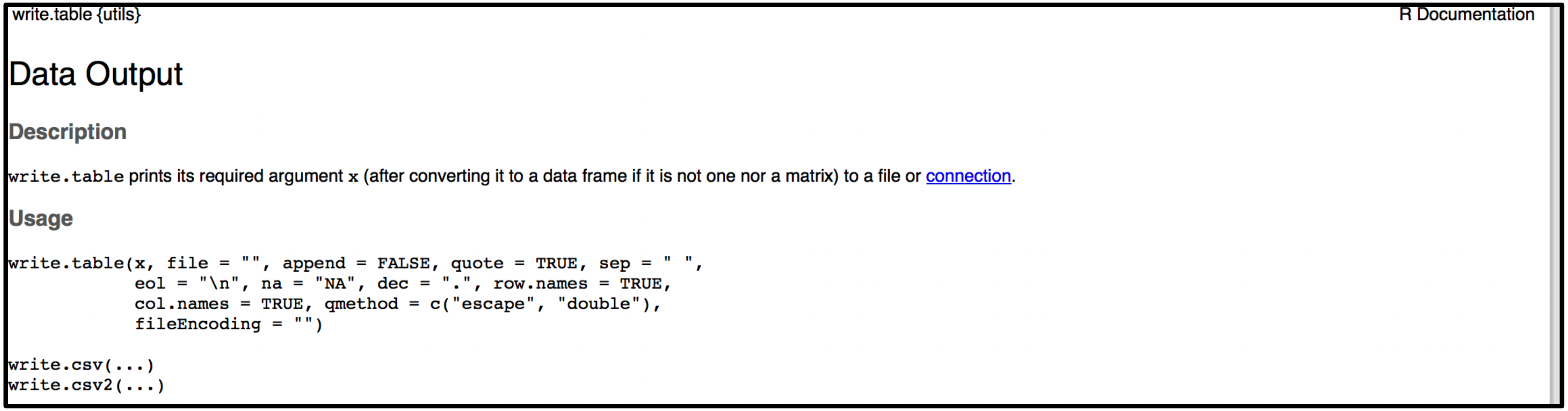
write.csv(...)
write.csv2(...)
```

Arguments

`x`	the object to be written, preferably a matrix or data frame. If not, it is attempted to coerce `x` to a data frame.
`file`	either a character string naming a file or a connection open for writing. `""` indicates output to the console.
`append`	logical. Only relevant if `file` is a character string. If `TRUE`, the output is appended to the file. If `FALSE`, any existing file of the name is destroyed.
`quote`	a logical value (`TRUE` or `FALSE`) or a numeric vector. If `TRUE`, any character or factor columns will be surrounded by double quotes. If a numeric vector, its elements are taken as the indices of columns to quote. In both cases, row and column names are quoted if they are written. If `FALSE`, nothing is quoted.
`sep`	the field separator string. Values within each row of `x` are separated by this string.

Functions / Multiple Parameters

```
>help.start()     #opens a page with manual, tutorials and
help search
>help("write.table") #show options for write.table
```



write.table {utils} R Documentation

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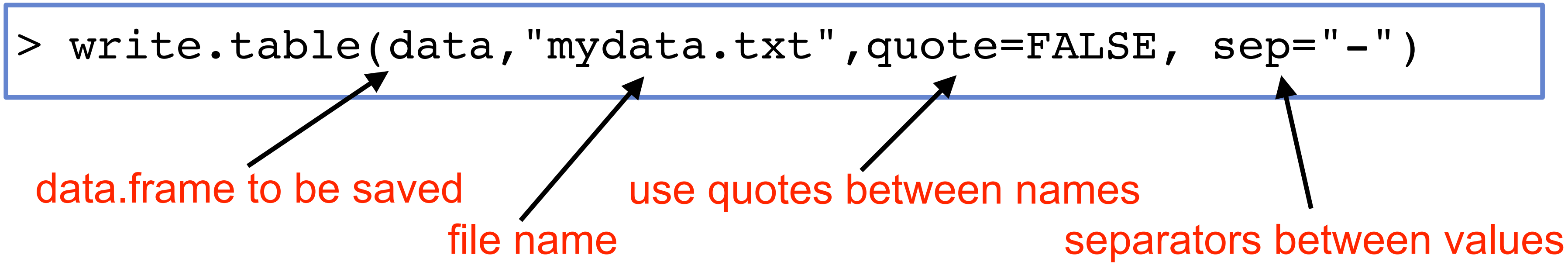

```
> write.table(data,"mydata.txt",quote=FALSE, sep="-")
```

data.frame to be saved

file name

use quotes between names

separators between values

Libraries

- In R the primary mechanism for distributing software (functions) is via packages
- CRAN is the major repository for packages.

```
> install.packages("packagename") # install a new package
```

- Bioinformatic packages are available at Bioconductor package.

```
> install.packages("BiocManager")
> BiocManager::install(c("packagename")
```

- Before using functions of a library they need to be opened.

```
> library("packagename")
```

Example of library / saving excel table

```
> install.packages("openxlsx") # installing package
> library("openxlsx") # loading package in memory
> help("openxlsx") # description of package
> m = matrix(1:12, 4, 3) # create a matrix
> write.xlsx(m,"mydata.xlsx")
# write matrix in a .xlsx file
> mydata = read.xlsx("mydata.xlsx") # read the file
and saves in another variable my data
> mydata
 V1 V2 V3
1  1  5  9
2  2  6 10
3  3  7 11
4  4  8 12
```

Try using openxlsx to load an excel table from yourself!

Exercise 1

- Define a vector to store the amount of fruits and another one to store their prices.
  - There are 5 green apples, 14 red apples, 30 bananas and 4 melons
  - An apple costs 0.5 cents, a banana 1.0 euro, a melon 3 euros
- Use vector operations/functions to calculate what is:
- The total amount of apples?
- The total amount of fruits?
- The total number of fruit types?
- The total price of all fruits?
- The maximum amount of any fruit?

Exercise 2

- Use logical operators to answer the following questions.
  - Which fruit types have more than 5 units?
  - Which fruit types you can buy all items with 10 euros?
  - Which fruit type has the least amount of units?
  - Which fruit types cost less than the average fruit cost?

Exercise 3

- The fruit shop became a chain. Use now a matrix to store the number of fruits in both shops. The first shop has 5 green apples, 14 red apples, 30 bananas and 4 melons. The second shop has 20 green apples, 10 red apples, 10 bananas and 6 melons.
  - What is the total number of fruits per shop?
  - How many apples are in both shops?
  - What is the total number of fruits?
  - How much does it cost to buy all fruits (prices are the same as before).
  - Save table as an excel sheet.

Exercise 4

Creating regular numeric sequences is a common task in statistical computing. You can use the seq function to create sequences.

1. Read the help page for seq by entering help(seq).
2. Generate a decreasing sequence from 50 to 1, then another sequence from 1 to 50.
3. Use seq to generate a sequence of the even integers between one and ten.

Exercise 5

- Create an integer vector i that can be used to subset v such that it will output the elements of v in decreasing order. For the general case, read the help pages for **order** and **sort**.

```
> v = c(1.1, 2, 100, 50, 60)
```

Afternoon Exercise

- Check exercise in https://www.costalab.org/bioinformatics-in-r-2020/

- See you at 1PM in discord!

Extra material

- More exercises at …

http://www.bioconductor.org/help/course-materials/2010/BioC2010/First_Steps_With_R_SOLUTIONS.pdf

(pages 1-17)

Inst. for Computational Genomics

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- Tiago Maie
- Johannes Schoeneich