Josep Carreras LEUKAEMIA Research Institute

# Introduction to 

Angelika Merkel (Head of Bioinformatics Unit IJC)
31/03/2025

IJC Bioinformatics

# The IJC Bioinformatics Unit

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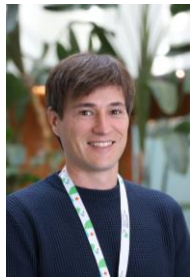
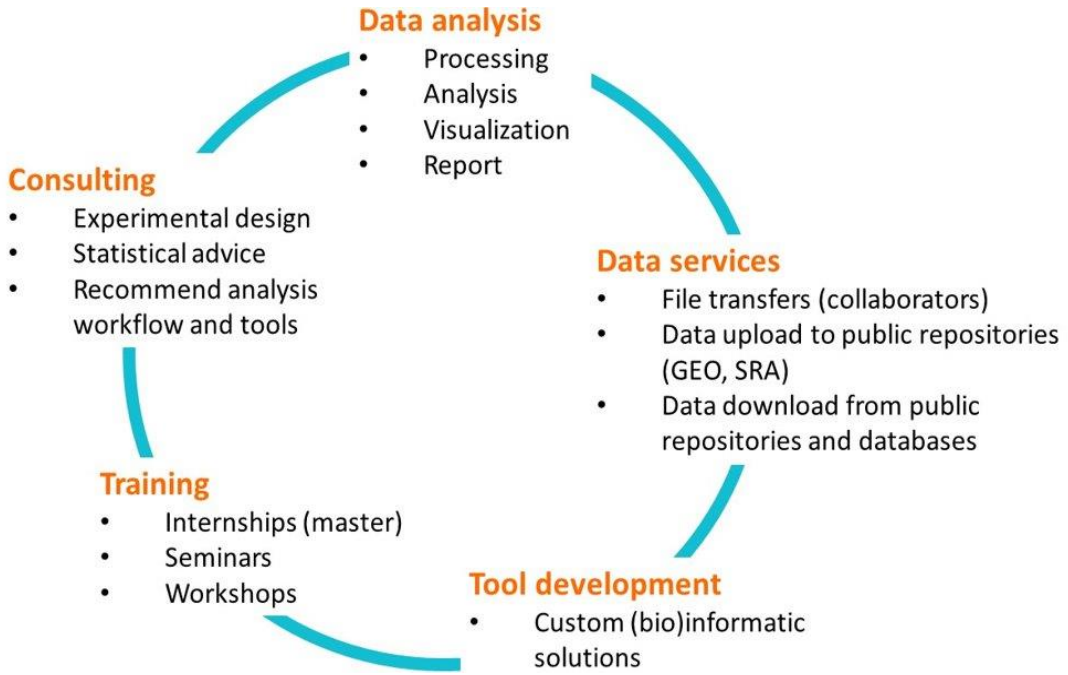
Unit Manager
Bioinformatician



Emilio Lario
Software Engineer

Marta Meroño
Bioinformatician

Paula Vela
Bioinformatician
(Student)




Office: 1st floor; phone: 4300
https://ijcbit.eu
https://www.carrerasresearch.org/en/bioinformatics-unit

# Workshop overview

Day 1:

- Why R, and what is R?
- Introduction to RStudio IDE (= 'POSIT' (July 2022))
- Practical session I: Get Started with R ( based on R Programming for Data Science (D. Peng, 2022))
  - basics, data classes and objects, control structure, functions
- My first R script, Running R scripts

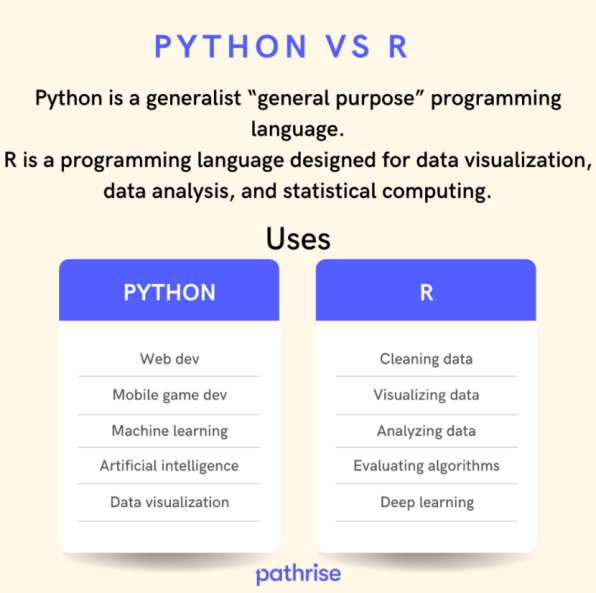
Day 2:

- Recap day 1
- R {base} and the Tidyverse
- Practical session II: Data analysis
  - Data import/export, wrangling and analysis in R
- Coding in style

All presentation and exercises are available here:

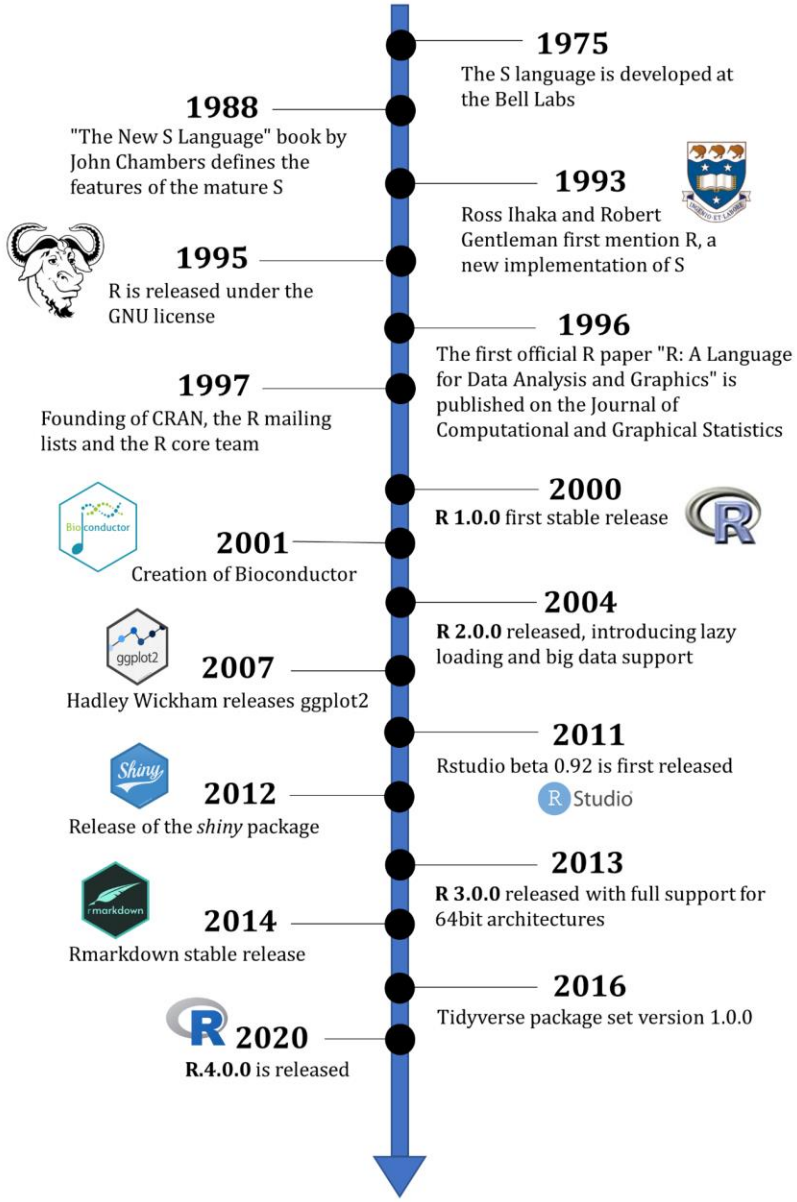
https://ijcbit.github.io/Workshops/

# Why learn R?

1. Statistical computing and graphics
2. Biological data analysis and data science
3. Free + open source, backed by a large interdisciplinary community
4. 


https://www.pathrise.com/guides/python-vs-r-data-science-languages-to-master/

# A little bit of R history...




Giorgi, F.M.; Ceraolo, C.; Mercatelli, D. The R Language: An Engine for Bioinformatics and Data Science. *Life* **2022**, *12*, 648. https://doi.org/10.3390/life12050648

# R - More than just data analysis

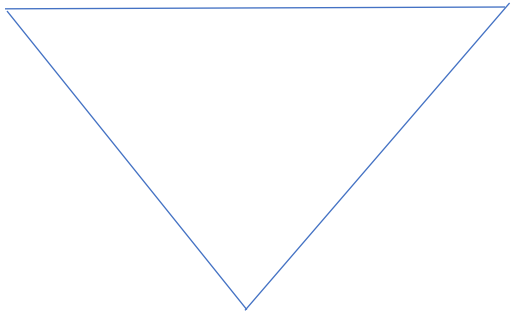
| | Extension | Output formats | Utilities |
|---|---|---|---|
| R script | .R | .csv, png, jpeg, .rds, .RData | Textfiles, images (plots), compressed R objects |
| R sweave * | .rnw | LaTeX ( PDF) | documents, presentations |
| R markdown * | .rmd | HTML, docx, LaTeX ( PDF) | Webpages, documents, notebooks, presentations |
| Quarto * | .qmd | HTML, docx, ppt, LaTeX ( PDF) | Webpages, documents, presentations |
| R Shiny | App.R, server.R | | Interactive web applications |

*literate programming = natural language with interspersed (embedded) pieces of code snippets

# R - More than just a programming language

Code repositories (packages) and collaborative development environments

Bioconductor
OPEN SOURCE SOFTWARE FOR BIOINFORMATICS



Integrated development environment (IDE)

RStudio

posit

Community

R-help -- Main R Mailing List: Primary help

stackoverflow >>R

R-bloggers

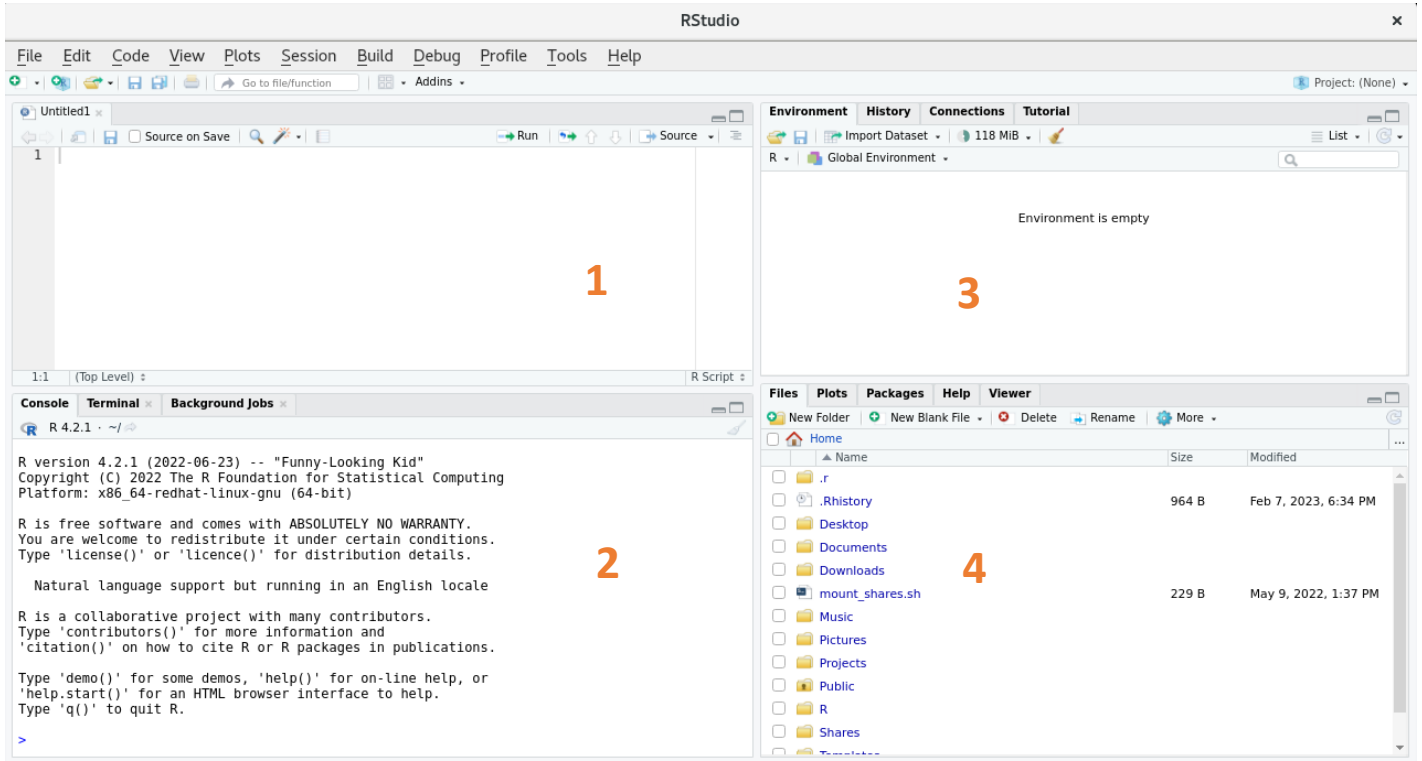
# RStudio: Integrated Development Environment (IDE)

Go to the RStudio course server

https://rstudio1.services.carrerasresearch.org/

RStudio spaces:

1. Source editor
2. Interactive console
3. Workspace (environment, command history)
4. 'Pane' area (Files, plots, package manager, integrated help)




Cheatsheet @ https://rstudio.github.io/cheatsheets/html/rstudio-ide.html

# R Studio

## 1) Source editor

= your working document (R script, R markdown, quarto document, text file) to write text or code

= data viewer

- tabs allow you have multiple documents/ data views open at the same time
- shows line numbers
- bracket high-lightning
- auto-completion of commands/object names with 'tab' key and integrated help
- Fold/extend code blocks (control structures)

# R Studio

## 2) Console

= R console to execute code

- each line starts with a prompt '>'
- auto-completion and integrated help as in the source editor
- use highlight + botton 'run to send code from the source editor to the R console (short cut: 'Ctrl' + 'Enter')

Terminal

= Unix like terminal

# R Studio

## 3) Work space

Environment

= object loaded within the environment

- Load previous/ save current workspace, import data sets, show current memory usage

History

= command history, show all previously executed commands in chronological order (can be send to the source editor or to the console)

=> other tabs:

- 'build' (e.g. render website from quarto document),
- 'git' (integration with git repository),
- 'tutorial' (R tutorials with the learnr package)

# R Studio

## 4) Viewing pane

Files

= file explorer (Home = current working directory)

- Create folders, rename, delete, view files, import dataset

Plots

= graphical display for plots

- Save, export plots

Packages

= package listing with description and version

- View, install, update, delete packages

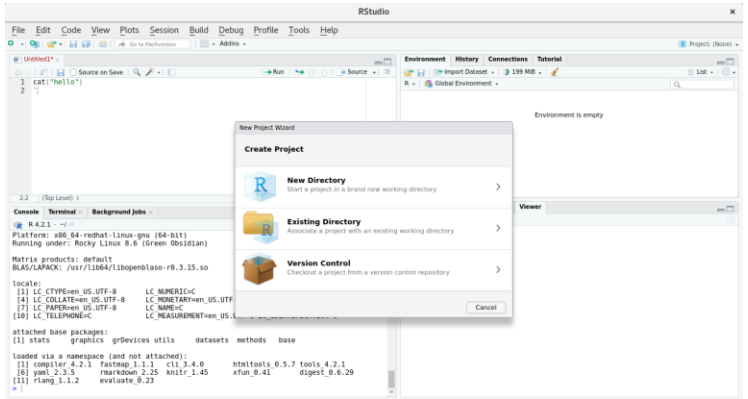
Help

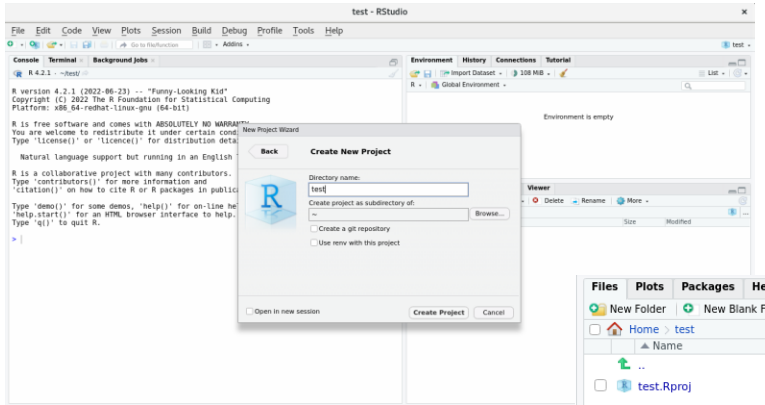
= integrated help

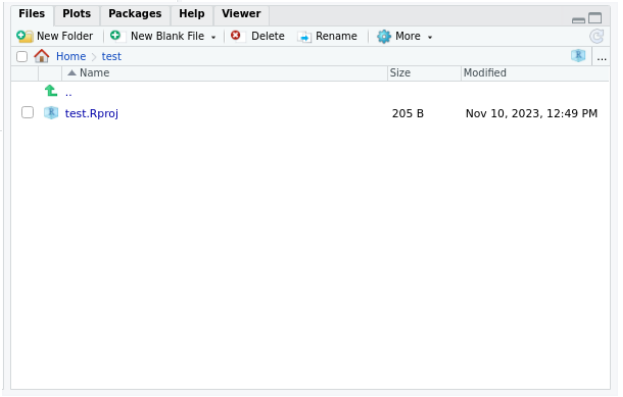
# R Studio: Working with projects

- Everything in one place
- Only relative paths

> File > New Project > New Directory



# Practical session I: R basics

## R Programming for Data Science (D. Peng, 2022)

- Chapter 4:
  - Nuts and bolts of R
  - Classes and types of objects
- Chapter 9:
  - Sub-setting (accessing) objects
- Chapter 13:
  - Control structures:
    if-else, for, while, repeat, next, break
- Chapter 14:
  - Functions

# Running R code from R scripts

From inside R:

```
> source(my_script.R)
```

From the terminal (outside) R using the `Rscript` utility

```
$ Rscript my_script.R [arguments]
```

Transfer arguments from terminal to R:

```
# function that captures all tokens ('words') after the script name on the terminal command line
# as elements of a vector
> args <- commandArgs( trailingOnly = TRUE )

# each argument can than retrieved from the vector and stored individually for further use inside the R
script
> argument_1 <- args[1]
> argument_2 <- args[2]
```

From the terminal (outside) R using the Rscript utility with arguments

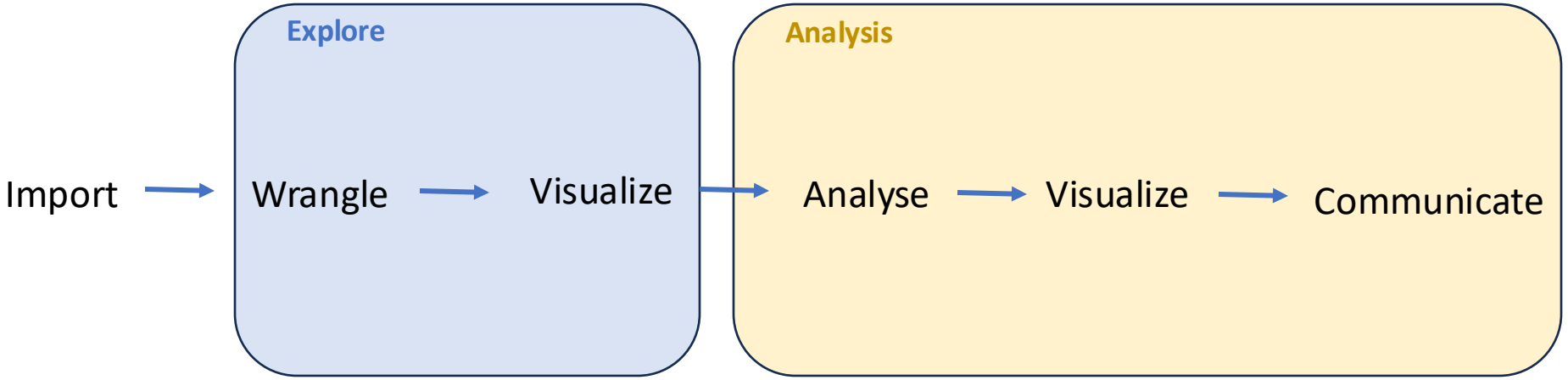
```
$ Rscript my_script.R argument1 argument2
```

# Day 2

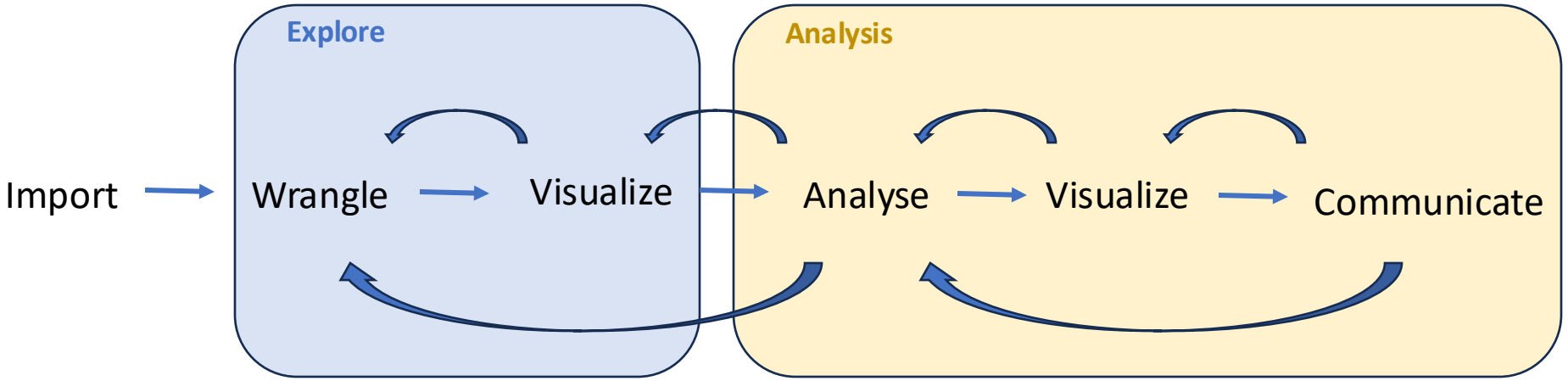
# Recap Day 1

- RStudio
- R basics
- R objects (vector, matrix, data frame, list) and classes (numeric, integer, complex, logical, character, factor)
- Accessing/Sub-setting R objects
- R control structure (if-else, while, for, next, repeat, break)
- R functions (definition, arguments)
- Running R scripts

# Data analysis



# Data analysis *in practice*



# Practical session: Data analysis in R

1. Import data

2. Data wrangling with {dplyr}: R programming for Data science (D. Peng 2022): Chapter 12
   - select(), filter(), mutate()
3. Exploratory analysis {base}{graphics}
   - summary(), histogram(), density(), plot(), boxplot(), pairs()
4. Analysis
   - smooth(), cor.test()

5. Export results

# Import data

Various functions across numerous packages:

{base}

- read.table(), read.csv() (tabular data)
- readLines (text)

{readr}

- read_table() (tabular data)
- read_csv() (comma separated)
- read_tsv() (tab separated)
- read_delim() (delimited)

{readxl}

- read_xls() (excel files)

{data.table}

- fread() (large tabular data)

R Studio integrates {readr} and {readxl} for data import using a graphical interface!

RStudio Server
https://rstudio1.services.carrerasresearch.org/

# The Tidyverse

Tidyverse = opinionated collection of R packages of approx. 25 packages for manipulation, visualization, transformation that share an underlying design philosophy, grammar, and data structures. (Hadley Wickham)

Tidy data (and data frames aka 'tibbles'):
= each value is placed in its own “cell”,
each variable in its own column,
and each observation in its own row.


tidy

```
table1
#> # A tibble: 6 × 4
#>   country      year  cases population
#>   <chr>       <dbl>  <dbl>      <dbl>
#> 1 Afghanistan  1999    745   19987071
#> 2 Afghanistan  2000   2666   20595360
#> 3 Brazil       1999  37737  172006362
#> 4 Brazil       2000  80488  174504898
#> 5 China        1999 212258 1272915272
#> 6 China        2000 213766 1280428583
```

Not so tidy

```
table2
#> # A tibble: 12 × 4
#>   country      year type           count
#>   <chr>       <dbl> <chr>          <dbl>
#> 1 Afghanistan  1999 cases            745
#> 2 Afghanistan  1999 population  19987071
#> 3 Afghanistan  2000 cases           2666
#> 4 Afghanistan  2000 population  20595360
#> 5 Brazil       1999 cases           37737
#> 6 Brazil       1999 population 172006362
#> # ℹ 6 more rows
```

Not so informative

```
table3
#> # A tibble: 6 × 3
#>   country      year rate
#>   <chr>       <dbl> <chr>
#> 1 Afghanistan  1999 745/19987071
#> 2 Afghanistan  2000 2666/20595360
#> 3 Brazil       1999 37737/172006362
#> 4 Brazil       2000 80488/174504898
#> 5 China        1999 212258/1272915272
#> 6 China        2000 213766/1280428583
```

# Base R versus the tidyverse

**{base}**

- better for software development
- better for running quick simulations
- generally faster performance
- more appealing to users with previous programming experience

Use if:

- Most of your work involves software or package development, advanced statistical procedures, or computationally expensive operations
- You're used to other languages that have more in common with Base-R
- Most of your collaborators and online network use it too

**{tidyverse}**

- ease of use, functions have the same structure and easier names, enables reading functions as instructions
- quick and easy data manipulation
- grouping datasets with many variable for summary statistics with dplyr
- over 25 packages in the tidyverse, each requiring its own updates to stay current
  -> adds overhead, difficult to reproduce, limits submission to code repros as R cran or bioconductor

Use if:

- Most of your work involves data cleaning, visualization, and common statistics
- You're newer to R and find it easier to read and understand than base-R
- Most of your collaborators and online network use it too

# Finally, a note on coding style...

*"Good coding style is like correct punctuation: you can manage without it, butitsuremakesthingseasiertoread."*

https://style.tidyverse.org/

# Scripts

- Script names should be meaningful and end in .R. Avoid using special characters in file names - stick with numbers, letters, -, and _.

```
# Good
fit_models.R
utility_functions.R

# Bad
fit models.R
foo.r
stuff.r
```

- If files should be run in a particular order, prefix them with numbers. If it seems likely you'll have more than 10 files, left pad with zero:

```
00_download.R
01_explore.R
...
09_model.R
10_visualize.R
```

# Organization

- Start your script with a descriptive header:

```
## AUTHOR:
## DATE:
## DESCRIPTION:
```

- If you use additional package, load them all at the beginning

- If you read files, read them at the beginning

```
library(dplyr)
library(scales)
```

- Use commented lines of - and = to break up your file into easily readable chunks.

```
# Load data ---------------------------

# Plot data ---------------------------
```

# Syntax

- Variable and function names should use only lowercase letters, numbers, and _. Use underscores (_) (so called snake case) to separate words within a name.

```
# Good
day_one
day_1

# Bad
DayOne
dayone
```

- Generally, variable names should be nouns and function names should be verbs. Strive for names that are concise and meaningful. Avoid re-using name of common functions and variables.

```
# Good
day_one

# Bad
first_day_of_the_month
djm1
```

# Syntax

- Always put a space after a comma, never before, just like in regular English.

```
# Good
x[, 1]

# Bad
x[,1]
x[ ,1]
x[ , 1]
```

- Do not put spaces inside or outside parentheses for regular function calls.

```
# Good
mean(x, na.rm = TRUE)

# Bad
mean (x, na.rm = TRUE)
mean( x, na.rm = TRUE )
```

# Syntax

- Place a space before and after () when used with if, for, or while.

```
# Good
if (debug) {
  show(x)
}

# Bad
if(debug){
  show(x)
}
```

- Place a space after () used for function arguments:

```
# Good
function(x) {}

# Bad
function (x) {}
function(x){}
```

# Syntax

- Most infix operators (==, +, -, <-, etc.) should always be surrounded by spaces:

```
# Good
height <- (feet * 12) + inches
mean(x, na.rm = TRUE)

# Bad
height<-feet*12+inches
mean(x, na.rm=TRUE)
```

- Adding extra spaces is ok if it improves alignment of = or <-.

```
# Good
list(
  total = a + b + c,
  mean  = (a + b + c) / n
)

# Also fine
list(
  total = a + b + c,
  mean = (a + b + c) / n
)
```

# Syntax

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# Also fine
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  mean = (a + b + c) / n
)
```

# Code blocks

- Curly braces, {}, define the most important hierarchy of R code. To make this hierarchy easy to see:
- { should be the last character on the line. Related code (e.g., an if clause, a function declaration, a trailing comma, ...) must be on the same line as the opening brace.
- The contents should be indented by two spaces.
- } should be the first character on the line.

```
# Good
if (y < 0 && debug) {
  message("y is negative")
}

if (y == 0) {
  if (x > 0) {
    log(x)
  } else {
    message("x is negative or zero")
  }
} else {
  y^x
}
```

# Comments

- In code, use comments to explain the “why” not the “what” or “how”. Each line of a comment should begin with the comment symbol and a single space: #.

```
# Good

# Objects like data frames are treated as leaves
x <- map_if(x, is_bare_list, recurse)


# Bad

# Recurse only with bare lists
x <- map_if(x, is_bare_list, recurse)
```

- If you discover that you have more comments than code, consider switching R markdown.

# Further resources

Books:

- R Programming for Data Science (D. Peng, 2022)
- R for data science 2ed (H.Wickham, M. Certinkaya-Rundel & G.Grolemund, 2023)

Tutorials:

- Datanovia

Musings:

- Medium: Towards data science

# Thank you!

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