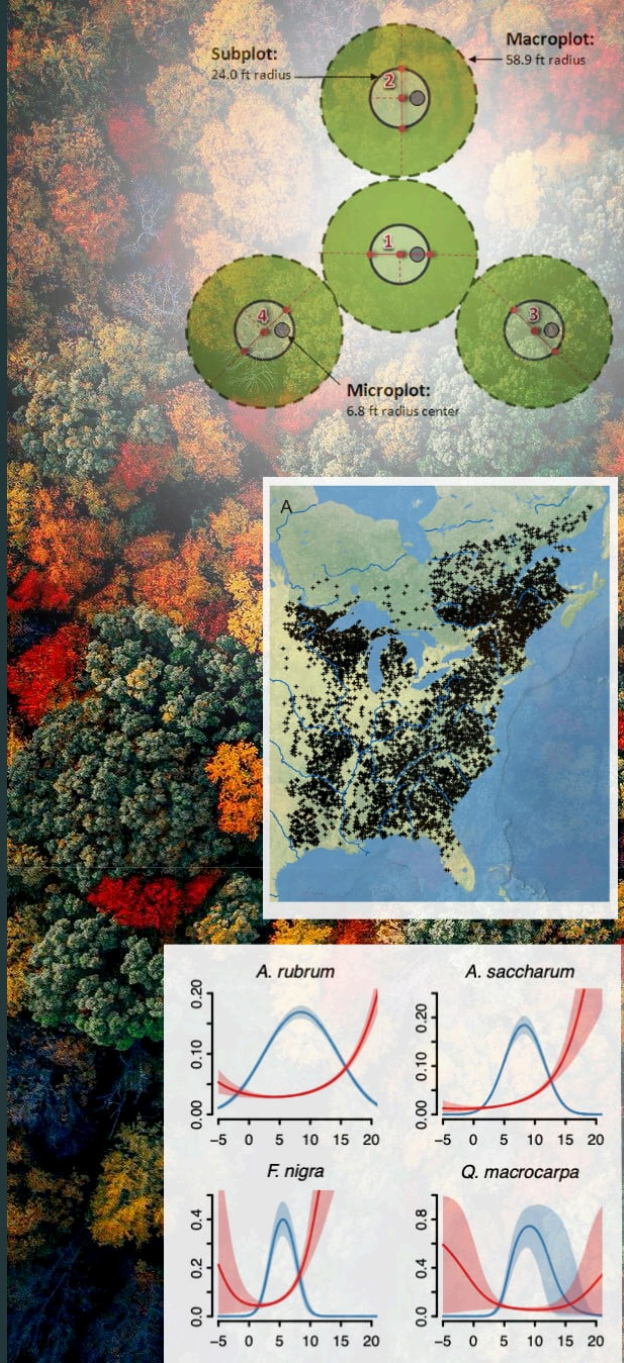
Lecture 1

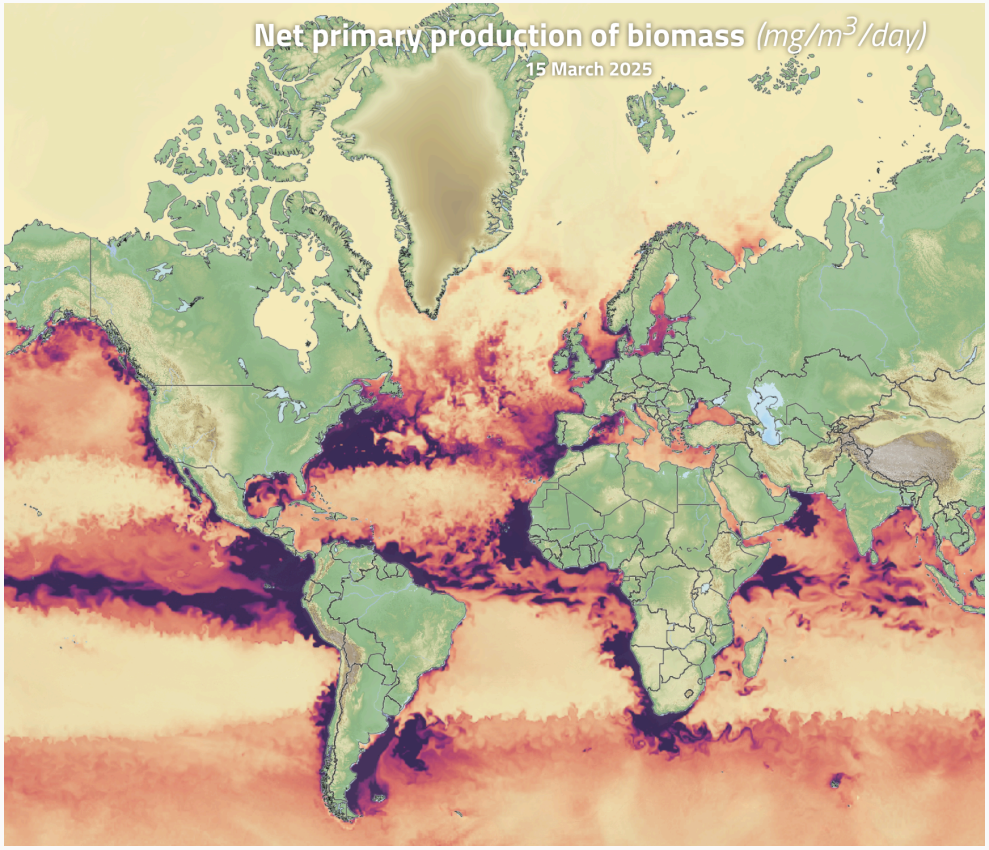
Introduction to scientific computing

Introduction to R for Biologists - Lauren Talluto



Why scientific computing?

- Growth in big data applications, remote sensing, monitoring, sequencing



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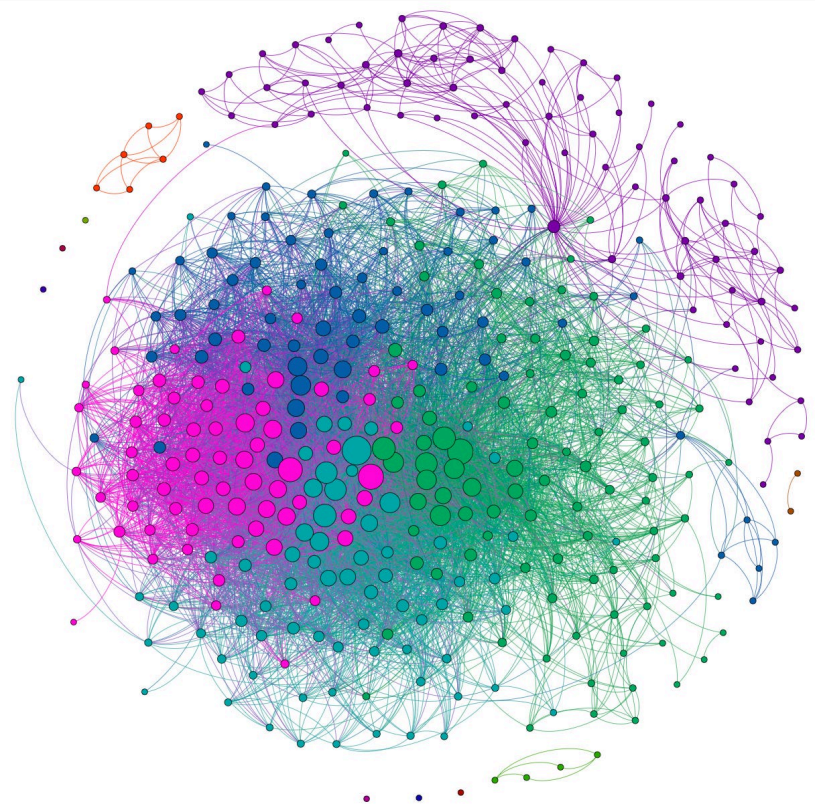
Why scientific computing?

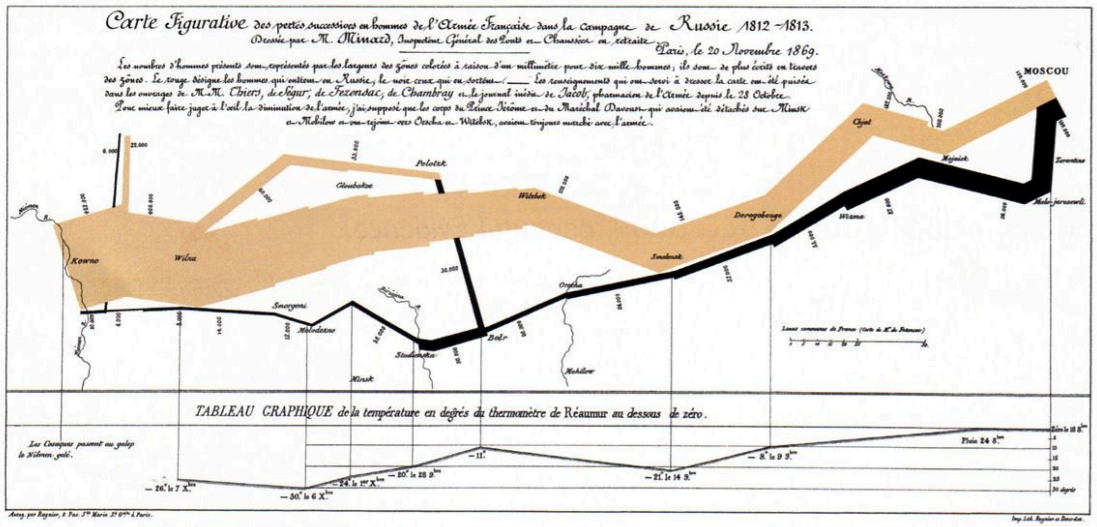
- Computation enables analyses that were previously impossible (permutation tests, Bayesian statistics, next-gen sequencing)



R package BNViewer

Why scientific computing?

- Enables the creation by non-artists of **highly effective visualisations**



This map drawn by Charles Joseph Minard portrays the losses suffered by Napoleon's army in the Russian campaign of 1812. Beginning at the left on the Polish-Russian border near the Niemen, the thick band shows the size of the army (422,000 men) as it invaded Russia. The width of the band indicates the size of the army at each position. In September, the army reached Moscow with 100,000 men. The path of Napoleon's retreat from Moscow in the bitterly cold winter is depicted by the dark lower band, which is tied to temperature and time scales. The remains of the Grande Armée struggled out of Russia with 10,000 men. Minard's graphic tells a rich, coherent story with its multivariate data, far more enlightening than just a single number bouncing along over time. Six variables are plotted: the size of the army, its location on a two-dimensional surface, direction of the army's movement, and temperature on various dates during the retreat from Moscow. It may well be the best statistical graphic ever drawn. Napoleon's March poster $14 postpaid; English/French version $18 postpaid.

Edward R Tufte. *The Visual Display of Quantitative Information*

Why/what is R?

- Open-source **domain-specific** language
- Scientific computing is built-in
- Large number of packages specifically oriented around statistics, data science, visualisation
- Standard language for statistics, and (to a lesser extent) bioinformatics
- Excellent tools for scientific communication
  - *Rmarkdown* for websites, reports, presentations
  - *Shiny* for webapps

Course objectives

- Learn fundamental concepts of R programming
  - RStudio IDE
  - Key programming concepts
  - Planning, structuring, debugging
  - Good scientific computiung practises
- Data visualisation
- Basic data science

This course is for beginners! No programming experience is needed

We will *not* cover statistical theory or advanced concepts in computer science

Course Format

- Brief lectures to introduce general concepts (< 1 hour per session)
- Structured exercises to get you coding in R

Grading

- Participation in class, working on exercises (40%)
- Submission of a (group) report on the exercises (60%)

Resources & Materials

- Course web page
- Getting help: stackoverflow.com, R help files, **avoid chatGPT**.

You will need

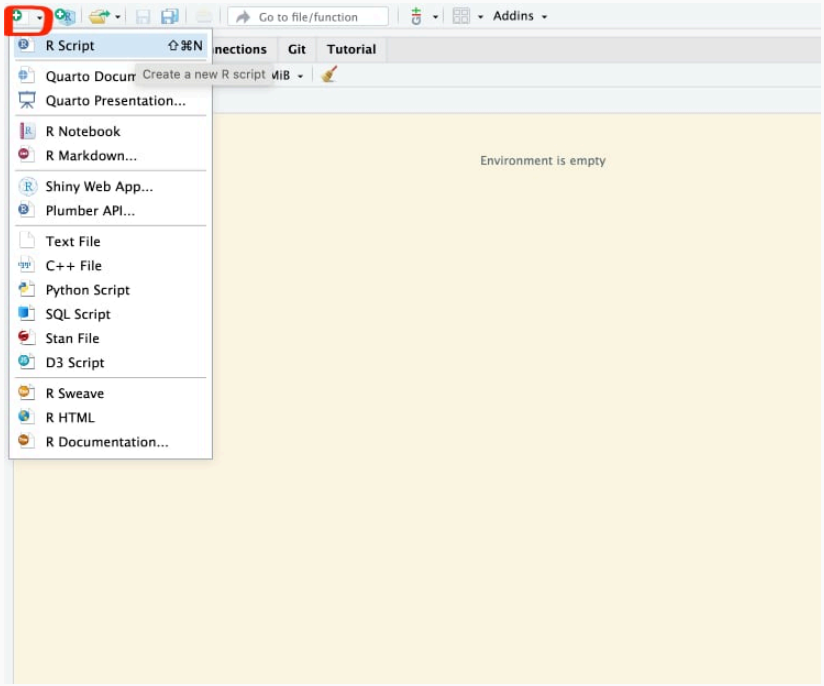
- (recommended): your own laptop (you can also use university computers)
- Extra time outside class to finish exercises (if needed)

The R environment

- `R` is two things:
  1. A statistical programming language
  2. A software package implementing the R language (available at https://cran.r-project.org/)
- `RStudio` is a comprehensive working environment for R (https://rstudio.com/products/rstudio/)
  - An editor, for writing R programs
  - Tools to help you write and analyse code
  - An R console and interpreter

Parts of RStudio

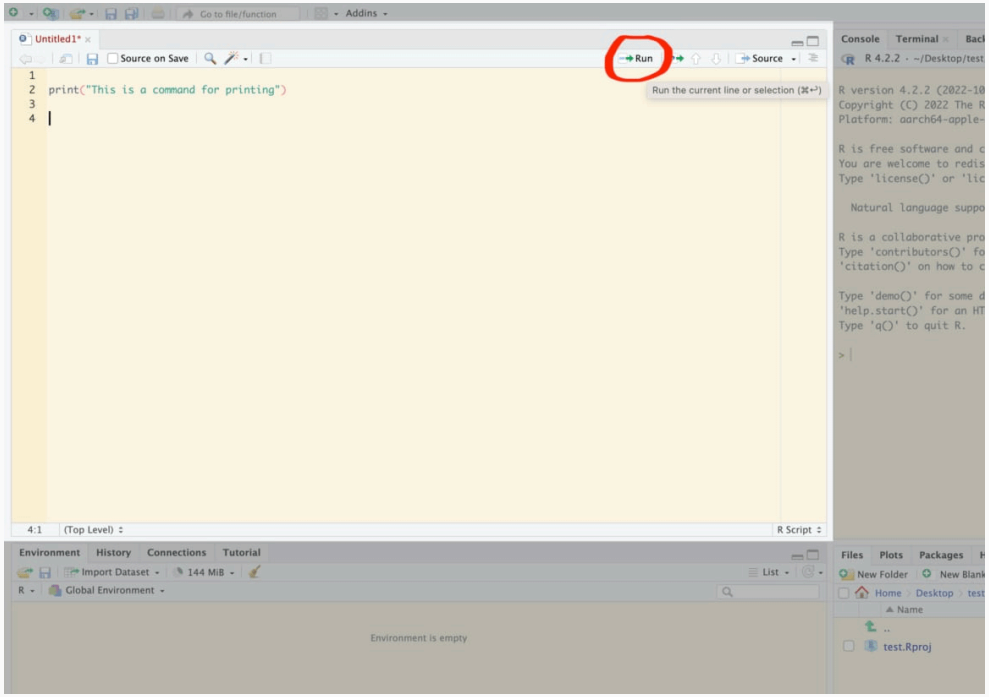
After launching Rstudio, create a new R **script** using the button in the upper left



Script: a text file where you will write an R-program. Commands in a script will be run in order, from the top to the bottom.

Parts of RStudio

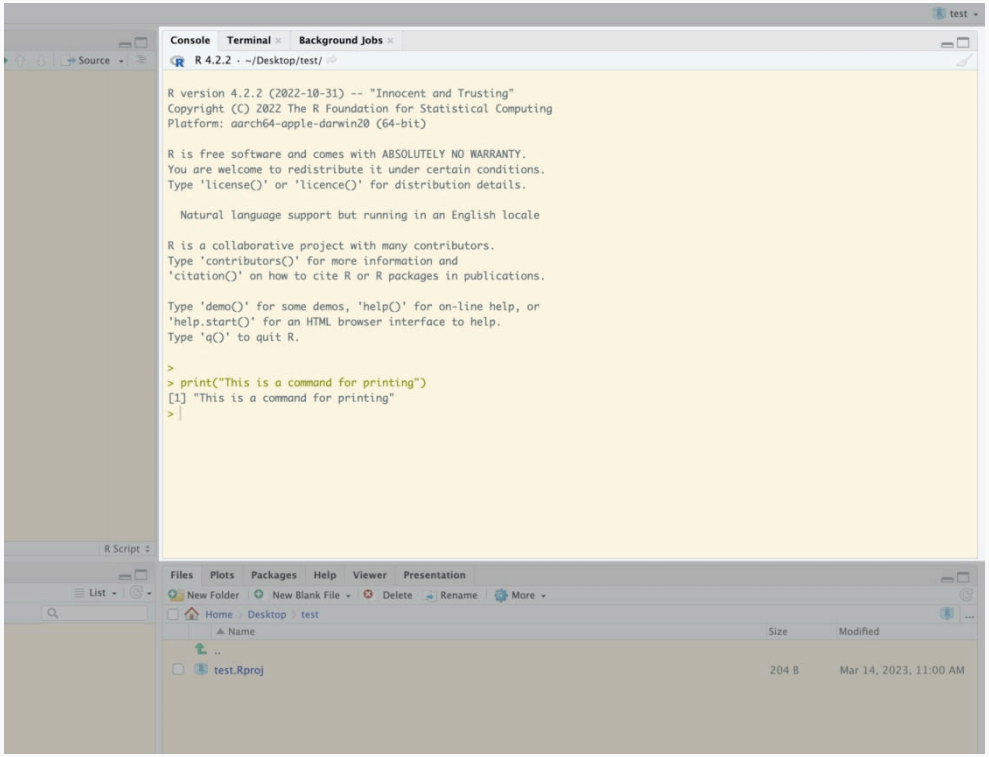
- The **editor** pane is where you will write your scripts.
- Execute commands by using **run** (control-return [1])



[1]Mac users: usually you can substitute the command (⌘) key for control, and option for alt

Parts of RStudio

- The **console** pane is where commands are executed.



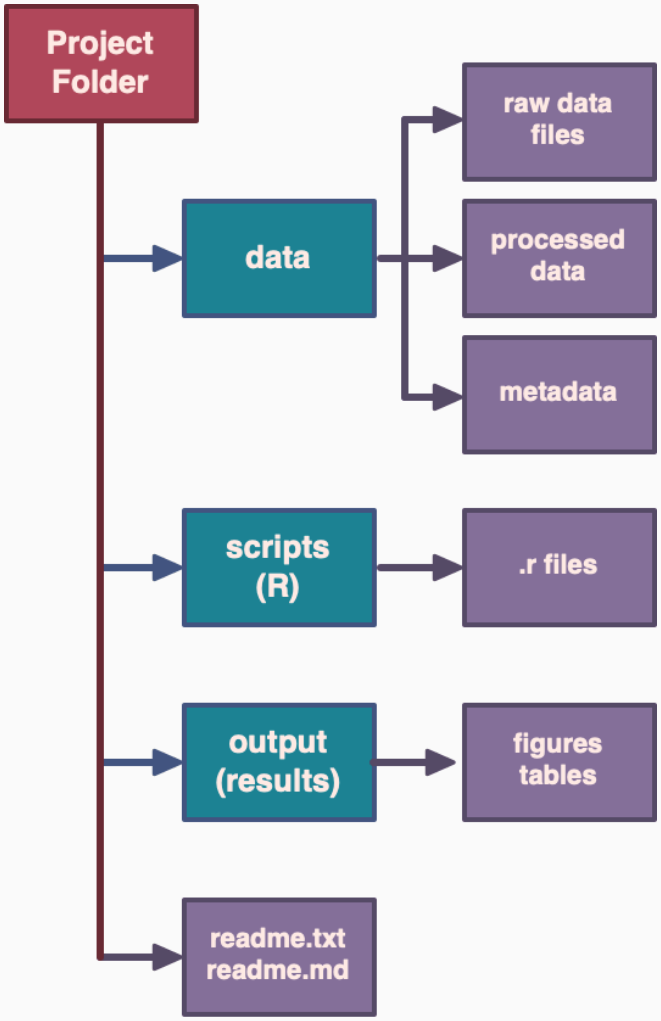
Helpful Vocabulary

- **console**: A window where you can type commands and view (text) results and output
- **interpreter**: Software that translates R commands into instructions for your computer in real time
- **script**: a text file containing a program, or series of commands
  - can be run **interactively** (sending commands one at a time to the console)
  - or in **batch mode** (all commands run, one after the other)
- **working directory**: location on your computer where R will search for files, data, etc.

Organising scientific projects

- Create a project in RStudio to organise your work (File => New Project)
- Store all files in the project folder (your project will be **self-contained**).
- Filenames: ASCII letters (No accents), numbers, underscores (_) ONLY

Project folder/file structure



Preparing your data

- Prepare data in excel
- The first row is a header with column names
- Column names should be **legal variable names**
- In a separate file, describe the dataset, how it was collected, and the meaning of each column (including units!)
- Arrange your data so that each row is a single observation, each column is a variable ("tidy" data)

The working directory

Your **working directory** is the folder where R will look for files, folders, data.

- It is displayed at the top of the **Console** window.
- You can also type `getwd()` in the console

The working directory

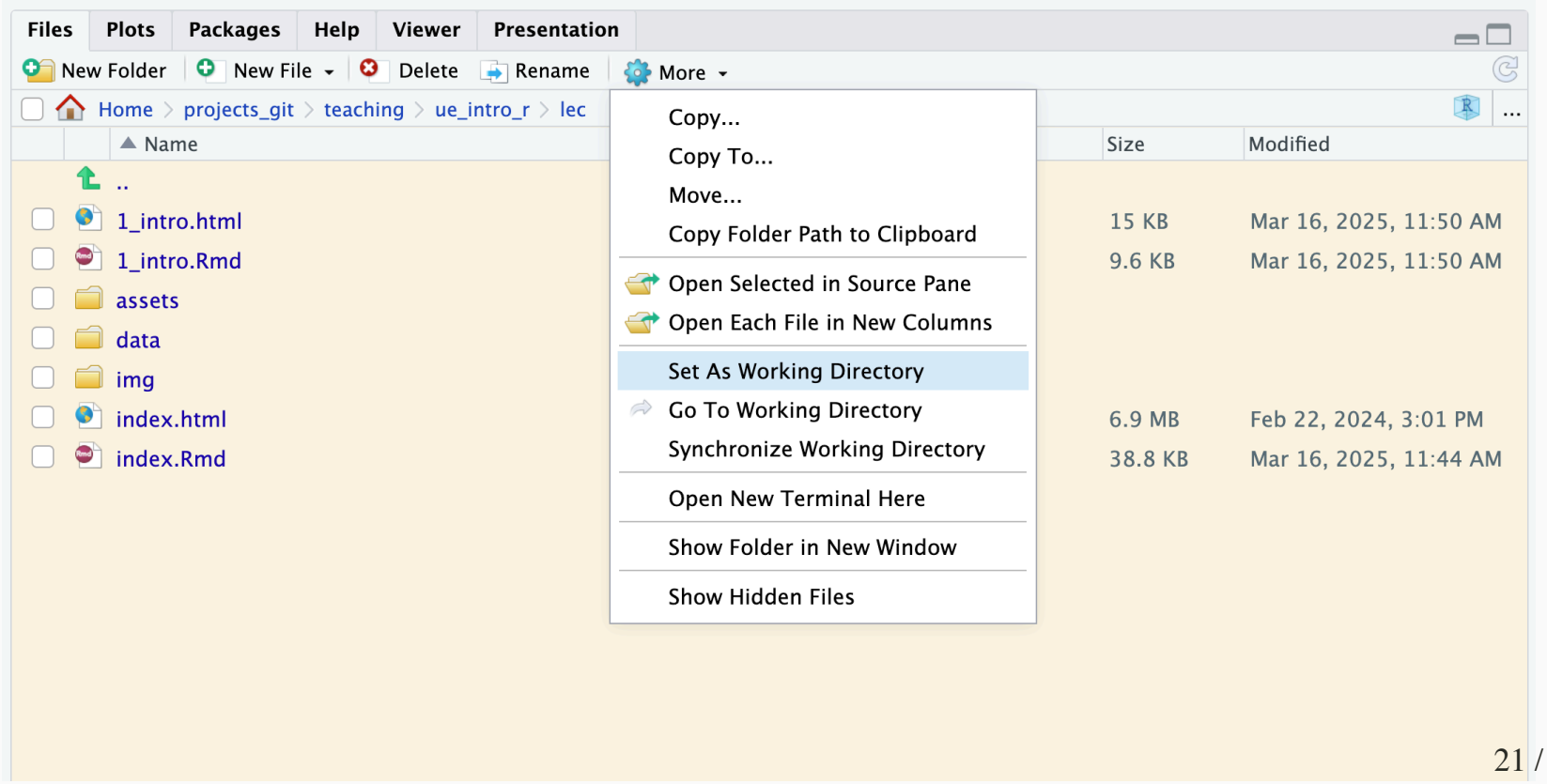
Your **working directory** is the folder where R will look for files, folders, data.

- Usually set this to the **project root directory**
- It is set automatically for you if you open R by double-clicking the `project_name.Rproj` file

The working directory

Your **working directory** is the folder where R will look for files, folders, data.

- Change it in the `Files` pane under `More`
- Or use `setwd("path/to/new/folder")` in the console.



Variables

- A **variable** is a name that points to some data.
- Variable names can contain lower- or upper-case letters, numbers, and the `_` symbol.
- Names must start with letters and (when possible) should be descriptive
- Variables are given values by **assignment** using either the `=` or `<-` symbol

```
# Comments in R start with the # symbol
# Legal variable names
x = 1
y0 = 5
time_of_day = "20:15"
dayOfWeek <- "Monday"
```

Variables

Recommendations

- Use descriptive variable names instead of comments.
- Avoid 1- and 2- letter names.
- Separate words with underscores.
- Use a consistent assignment operator (`=` or `<-`)

```
# bad!
# d is the diversity in our site, in species
d = 8

# better!
site_diversity = 8
```

Data types

`numeric` — `integer` — `logical` — `character` — `factor`

The **type** of a variable tells us what kind of information it contains.

- **numeric**: integers and floating-point (decimal) numbers
  - **integer**: a special case of numeric variable
- **logical**: yes/no, true/false data; in R represented by the special values `TRUE` and `FALSE`
- **character**: strings, text
- **factor**: special variable type for categorical (nominal & ordinal) data

Data types

`numeric` — `integer` — `logical` — `character` — `factor`

Useful functions for querying a data type are `class()` and `mode()`.

```
x = "a string"
mode(x)
## [1] "character"
```

```

y = 5.5
mode(y)
## [1] "numeric"
```

Data types

`numeric` — `integer` — `logical` — `character` — `factor`

Convert between data types using `as`

```
y = 5.5
as(y, "integer")
## [1] 5
```

Operators

Operators perform computations on variables and constants.

- The **assignment operators** give a value to a variable
  - `=`, `<-`
  - Both work mostly the same, use alt-dash (-) for `<-`

```
# assignment
x = 5
```

Operators

Operators perform computations on variables and constants.

- **Mathematical operators** allow us to do arithmetic
  - `+`, `-`, `*`, `/`, `^`

```
# math
x + 2
## [1] 7
```

```
(3 + x) * 2
## [1] 16
```

```
3^2
## [1] 9
```

Functions

Functions allow for more complex operations on data

- Functions take **arguments** inside the brackets `()`
  - arguments can be variables or constants

```
x = 16
sqrt(x)
## [1] 4
```

```
sqrt(25)
## [1] 5
```

Functions

Functions allow for more complex operations on data

- Separate multiple arguments with a comma
- Clarify your code by **naming** the arguments
  - see the help files (here: `?log`) to learn argument names!

```
x = 100
log(x)
## [1] 4.60517
```

```
log(x, base = 10)
## [1] 2
```

Vectors

Group multiple values of the same type together in a **vector**.

- create a vector with the concatenate function `c()`.

```
five_numbers = c(3, 2, 8.6, 4, 9.75)
print(five_numbers)
## [1] 3.00 2.00 8.60 4.00 9.75
```

Vectors

Group multiple values of the same type together in a **vector**.

- Create a sequence of integers with the `:` operator

```
one_to_ten = 1:10
print(one_to_ten)
##  [1]  1  2  3  4  5  6  7  8  9 10
```

```
class(one_to_ten)
## [1] "integer"
```

Vectors

Group multiple values of the same type together in a **vector**.

- Create arbitrary sequences using `seq()`
- Repeat a value using `rep()`

```
seq(1, 5, 0.5)
## [1] 1.0 1.5 2.0 2.5 3.0 3.5 4.0 4.5 5.0
```

```
rep(0, 5)
## [1] 0 0 0 0 0
```

Vectorized operations

- Many of R's basic operators and functions are **vectorized**: they apply one-at-a-time to the whole vector.

```
five_numbers = c(3, 2, 8.6, 4, 9.75)
# math on vectors is performed on each element
five_numbers + 1
## [1]  4.00  3.00  9.60  5.00 10.75
```

```
five_numbers^2
## [1]  9.0000  4.0000 73.9600 16.0000 95.0625
```

```
sin(five_numbers)
## [1]  0.1411200  0.9092974  0.7343971 -0.7568025 -0.3195192
```

Indexing

We can use **indexing** with the `[]` operator to get a part of a vector by its position

```
five_numbers = c(3, 7, 8.6, 4, 9.75)
five_numbers[3]
## [1] 8.6
```

Indexing

We can use **indexing** with the `[]` operator to get a part of a vector by its position

- The index itself can be a vector!

```
five_numbers = c(3, 7, 8.6, 4, 9.75)
five_numbers[2:3]
## [1] 7.0 8.6
```

```
five_numbers[c(2,5)]
## [1] 7.00 9.75
```

Indexing

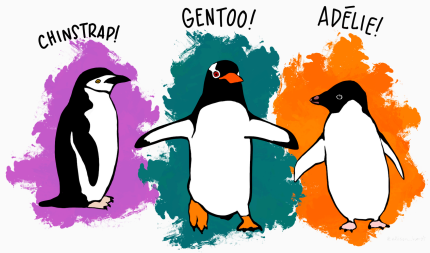
We can use **indexing** with the `[]` operator to get a part of a vector by its position

- Any legal **expression** that returns integers can be used inside `[]`!

```
i = 1
five_numbers = c(3, 7, 8.6, 4, 9.75)
five_numbers[i + 2]
## [1] 8.6
```

Reading data

- Use `read.csv()` to read in a csv file, or `read.table()` for tab- or space-delimited files.
- Here I read in the Palmer Penguins dataset




```
# read.csv will also accept a url!
# url = "https://raw.githubusercontent.com/allisonhorst/
# palmerpenguins/main/inst/extdata/penguins.csv"
# penguins = read.csv(url)
penguins = read.csv("data/penguins.csv")
```

Data frames

A **data frame** is a data structure for tabular data

- `head()` shows the first few rows of a data frame
- `View()` will open the data frame in a spreadsheet-like viewer

```
head(penguins)
##   species    island bill_length_mm bill_depth_mm flipper_length_mm body_mass_g
## 1  Adelie Torgersen           39.1          18.7                181        3750
## 2  Adelie Torgersen           39.5          17.4                186        3800
## 3  Adelie Torgersen           40.3          18.0                195        3250
## 4  Adelie Torgersen             NA            NA                 NA          NA
## 5  Adelie Torgersen           36.7          19.3                193        3450
## 6  Adelie Torgersen           39.3          20.6                190        3650
##      sex year
## 1   male 2007
## 2 female 2007
## 3 female 2007
## 4   <NA> 2007
## 5 female 2007
## 6   male 2007
```

Data frames

A **data frame** is a data structure for tabular data

- Each row in a data frame is a single **case**
- Each column is a single variable, stored as a **vector**

```
head(penguins)
##   species    island bill_length_mm bill_depth_mm flipper_length_mm body_mass_g
## 1  Adelie Torgersen           39.1          18.7                181        3750
## 2  Adelie Torgersen           39.5          17.4                186        3800
## 3  Adelie Torgersen           40.3          18.0                195        3250
## 4  Adelie Torgersen             NA            NA                 NA          NA
## 5  Adelie Torgersen           36.7          19.3                193        3450
## 6  Adelie Torgersen           39.3          20.6                190        3650
##      sex year
## 1   male 2007
## 2 female 2007
## 3 female 2007
## 4   <NA> 2007
## 5 female 2007
## 6   male 2007
```

Data frames

A **data frame** is a data structure for tabular data

- `str()` gives you a summary of the **str**ucture of the data

```
str(penguins)
## 'data.frame':    344 obs. of  8 variables:
##  $ species          : chr  "Adelie" "Adelie" "Adelie" "Adelie" ...
##  $ island           : chr  "Torgersen" "Torgersen" "Torgersen" "Torgersen" ...
##  $ bill_length_mm   : num  39.1 39.5 40.3 NA 36.7 39.3 38.9 39.2 34.1 42 ...
##  $ bill_depth_mm    : num  18.7 17.4 18 NA 19.3 20.6 17.8 19.6 18.1 20.2 ...
##  $ flipper_length_mm: int  181 186 195 NA 193 190 181 195 193 190 ...
##  $ body_mass_g      : int  3750 3800 3250 NA 3450 3650 3625 4675 3475 4250 ...
##  $ sex              : chr  "male" "female" "female" NA ...
##  $ year             : int  2007 2007 2007 2007 2007 2007 2007 2007 2007 2007 ...
```

Data frames

A **data frame** is a data structure for tabular data

- `nrow()`, `ncol()` and `dim()` give you data frame dimensions

```
nrow(penguins)
## [1] 344
```

```
ncol(penguins)
## [1] 8
```

```
dim(penguins)
## [1] 344   8
```

Data frames

A **data frame** is a data structure for tabular data

Data frame variables are normally **hidden**

```
str(penguins)
## 'data.frame':    344 obs. of  8 variables:
##  $ species          : chr  "Adelie" "Adelie" "Adelie" "Adelie" ...
##  $ island           : chr  "Torgersen" "Torgersen" "Torgersen" "Torgersen" ...
##  $ bill_length_mm   : num  39.1 39.5 40.3 NA 36.7 39.3 38.9 39.2 34.1 42 ...
##  $ bill_depth_mm    : num  18.7 17.4 18 NA 19.3 20.6 17.8 19.6 18.1 20.2 ...
##  $ flipper_length_mm: int  181 186 195 NA 193 190 181 195 193 190 ...
##  $ body_mass_g      : int  3750 3800 3250 NA 3450 3650 3625 4675 3475 4250 ...
##  $ sex              : chr  "male" "female" "female" NA ...
##  $ year             : int  2007 2007 2007 2007 2007 2007 2007 2007 2007 2007 ...
```

```
print(bill_length_mm[1:5])
## Error in eval(expr, envir, enclos): object 'bill_length_mm' not found
```

Indexing with $

You can use the `$` operator to access a single variable *within* a data frame

```
print(bill_length_mm[1:5])
## Error in eval(expr, envir, enclos): object 'bill_length_mm' not found
```

```
print(penguins$bill_length_mm[1:5])
## [1] 39.1 39.5 40.3   NA 36.7
```

The with function

The `with()` function is a special function that makes data frame variables visible insde the `{}` operator

```
with(penguins, {
    bill_length_mm[1:5] + bill_depth_mm[1:5]
})
## [1] 57.8 56.9 58.3   NA 56.0
```

Data frame subsets

- You can use the `subset` function to extract part of a data frame that meet certain **conditions**
- The `==` operator *tests* if two things are equal

```
penguins_gentoo_only = subset(penguins, species == "Gentoo")
head(penguins_gentoo_only)
##     species island bill_length_mm bill_depth_mm flipper_length_mm body_mass_g
## 153  Gentoo Biscoe           46.1          13.2               211        4500
## 154  Gentoo Biscoe           50.0          16.3               230        5700
## 155  Gentoo Biscoe           48.7          14.1               210        4450
## 156  Gentoo Biscoe           50.0          15.2               218        5700
## 157  Gentoo Biscoe           47.6          14.5               215        5400
## 158  Gentoo Biscoe           46.5          13.5               210        4550
##        sex year
## 153 female 2007
## 154   male 2007
## 155 female 2007
## 156   male 2007
## 157   male 2007
## 158 female 2007
```

Data frame subsets

- You can use the `subset` function to extract part of a data frame that meet certain **conditions**
- The `>` and `<` operators test greater-than and less-than

```
penguins_big = subset(penguins, body_mass_g > 6000)
head(penguins_big)
##     species island bill_length_mm bill_depth_mm flipper_length_mm body_mass_g
## 170  Gentoo Biscoe           49.2          15.2               221        6300
## 186  Gentoo Biscoe           59.6          17.0               230        6050
##      sex year
## 170 male 2007
## 186 male 2007
```