

#### **ICRS Student Chapter**



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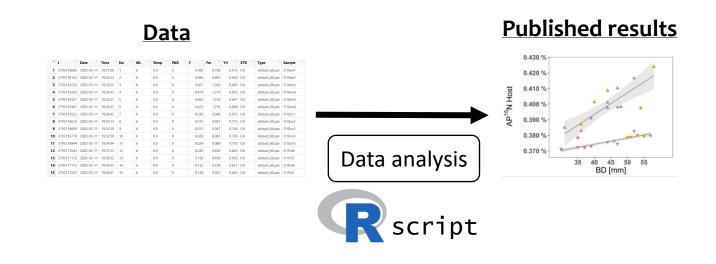
## An intro to **(** for reproducible research

What should happen between data collection and data analysis (that a lot of people do wrong)



02.12.2021

Analyze the same data and obtain the same results



Connected, but not the same as **replicability**: by repeating the same experiment reach the same conclusions

Analyze the same data and obtain the same results In the paper **Published results Data** 0.420 % 0.410 % 0.400 % 0.390 % 0.380 % 0.370 % Data analysis 40 45 50 55 Rscript In the supplementary material (ideally ...)

But there's also that other part ...

Cleaned data ready for stats

#### 

#### **Original data**



#### Unusable format ...

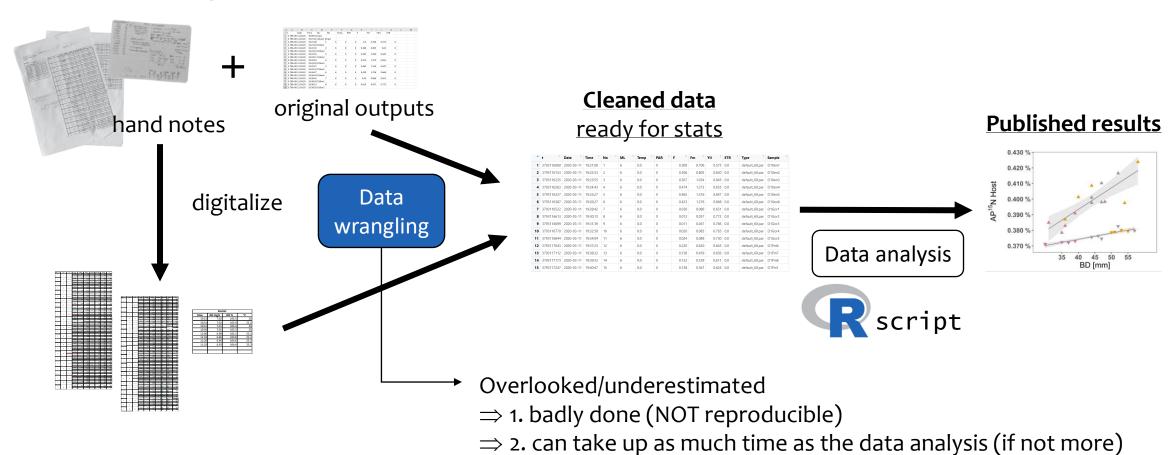
1	Α	В	С	D	E	F	G	Н	1	J	K	L	M
1	t	Date	Time	No.	ML	Temp.	PAR	F	Fm'	Y(II)	ETR		
2	3.79E+09	11.03.20	19:09:54	Type:									
3	3.79E+09	11.03.20	19:21:01	default_6	0.par								
4	3.79E+09	11.03.20	19:21:00	1	. 6	0	0	0.3	0.706	0.575	0		
5	3.79E+09	11.03.20	19:21:43	D1Xen1									
5	3.79E+09	11.03.20	19:22:33	2	2 6	0	0	0.306	0.805	0.62	0		
7	3.79E+09	11.03.20	19:22:45	D1Xen2									
3	3.79E+09	11.03.20	19:23:55	3	6	0	0	0.367	1.034	0.645	0		
9	3.79E+09	11.03.20	19:24:11	D1Xen3									
0	3.79E+09	11.03.20	19:24:43	4	6	0	0	0.474	1.373	0.655	0		
1	3.79E+09	11.03.20	19:24:59	D1Xen4									
2	3.79E+09	11.03.20	19:25:27	5	6	0	0	0.465	1.316	0.647	0		
3	3.79E+09	11.03.20	19:25:52	D1Xen5									
4	3.79E+09	11.03.20	19:26:27	6	6	0	0	0.423	1.276	0.668	0		
5	3.79E+09	11.03.20	19:26:43	D1Xen6									
6	3.79E+09	11.03.20	19:28:42	7	6	0	0	0.03	0.086	0.651	0		
7	3.79E+09	11.03.20	19:28:59	D1Gor1									-
8	3.79E+09	11.03.20	19:30:13	8	6	0	0	0.013	0.057	0.772	0		
9	3.79E+09	11.03.20	19:30:29	D1Gor2									



#### ... ready to be analyzed ©

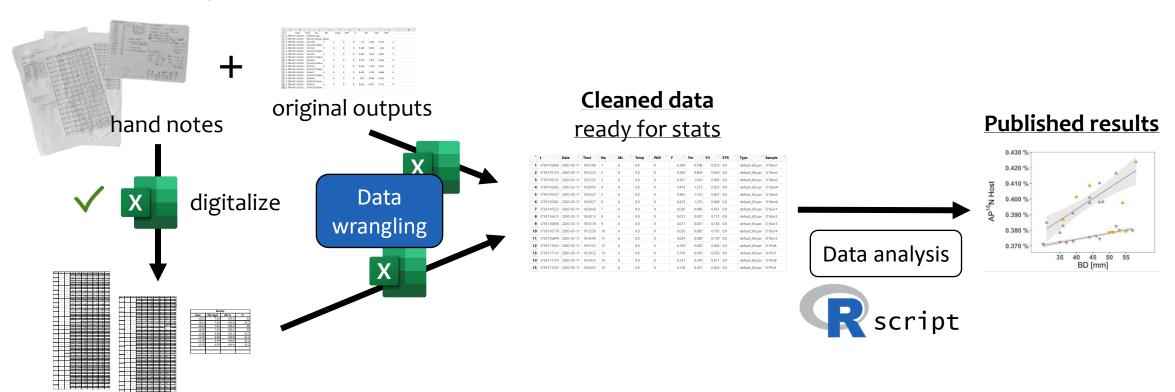
^	t <sup>‡</sup>	Date <sup>‡</sup>	Time <sup>‡</sup>	No <sup>‡</sup>	ML <sup>‡</sup>	Temp <sup>‡</sup>	PAR <sup>‡</sup>	F <sup>‡</sup>	Fm ÷	YII ÷	ETR ÷	Type	Sample <sup>‡</sup>
1	3793116060	2020-03-11	19:21:00	1	6	0.0	0	0.300	0.706	0.575	0.0	default_60.par	D1Xen1
2	3793116153	2020-03-11	19:22:33	2	6	0.0	0	0.306	0.805	0.620	0.0	default_60.par	D1Xen2
3	3793116235	2020-03-11	19:23:55	3	6	0.0	0	0.367	1.034	0.645	0.0	default_60.par	D1Xen3
4	3793116283	2020-03-11	19:24:43	4	6	0.0	0	0.474	1.373	0.655	0.0	default_60.par	D1Xen4
5	3793116327	2020-03-11	19:25:27	5	6	0.0	0	0.465	1.316	0.647	0.0	default_60.par	D1Xen5
6	3793116387	2020-03-11	19:26:27	6	6	0.0	0	0.423	1.276	0.668	0.0	default_60.par	D1Xen6
7	3793116522	2020-03-11	19:28:42	7	6	0.0	0	0.030	0.086	0.651	0.0	default_60.par	D1Gor1
8	3793116613	2020-03-11	19:30:13	8	6	0.0	0	0.013	0.057	0.772	0.0	default_60.par	D1Gor2
9	3793116699	2020-03-11	19:31:39	9	6	0.0	0	0.011	0.047	0.766	0.0	default_60.par	D1Gor3
10	3793116770	2020-03-11	19:32:50	10	6	0.0	0	0.020	0.085	0.765	0.0	default_60.par	D1Gor4
11	3793116844	2020-03-11	19:34:04	11	6	0.0	0	0.024	0.089	0.730	0.0	default_60.par	D1Gor5
12	3793117043	2020-03-11	19:37:23	12	6	0.0	0	0.220	0.620	0.645	0.0	default_60.par	D1Pin6
13	3793117112	2020-03-11	19:38:32	13	6	0.0	0	0.158	0.459	0.656	0.0	default_60.par	D1Pin7
14	3793117173	2020-03-11	19:39:33	14	6	0.0	0	0.132	0.339	0.611	0.0	default_60.par	D1Pin8
15	3793117247	2020-03-11	19:40:47	15	6	0.0	0	0.138	0.367	0.624	0.0	default_60.par	D1Pin1

#### **Original data**

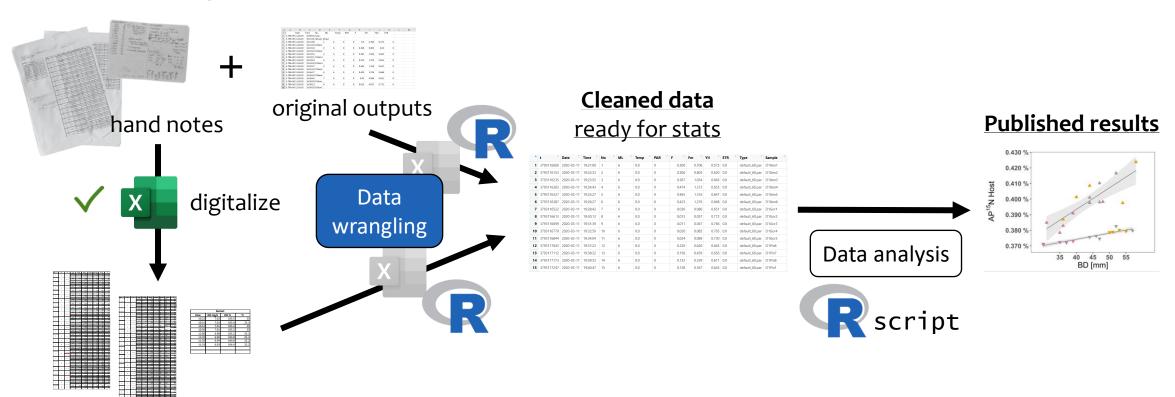


= sensitive step that can benefit a lot form improvement

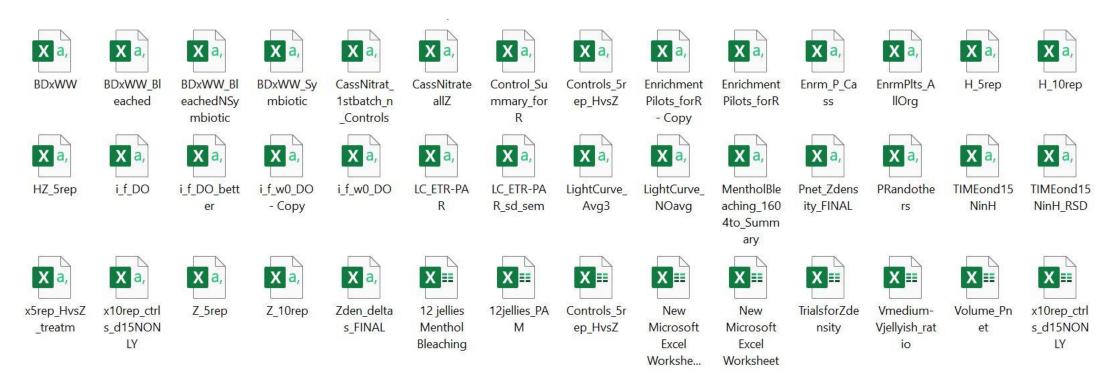
#### **Original data**



#### **Original data**



#### Does this look familiar?



Typical scenario of what happens when working in data in Excel: a new file is created for each version ... Naming can help only so far ...

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Typical scenario of what happens when working in data in Excel: a new file is created for each version ... Naming can help only so far ...

## Drop that spreadsheet already

Problems derived from working with spreadsheets:

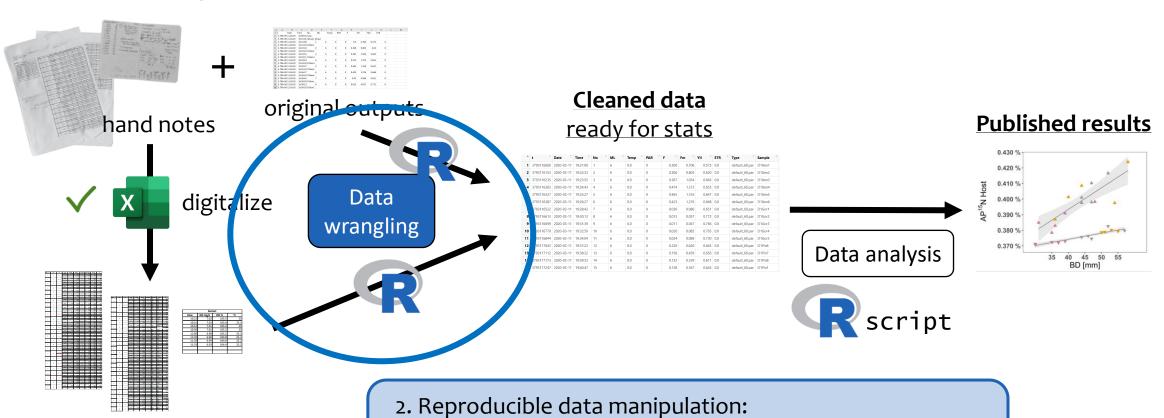
- Messy ...
- Error prone (e.g. manually copy-pasting the wrong thing in the wrong place)
- Not scalable (it just doesn't work with large data sets)
- Not reproducible (good luck trying to figure out what happened there ...!)

On the contrary, by working in **R**, you can do everything without ever altering the original data! (which also means that you can change your mind and easily un-do and re-do any operation)

#### **Original data**

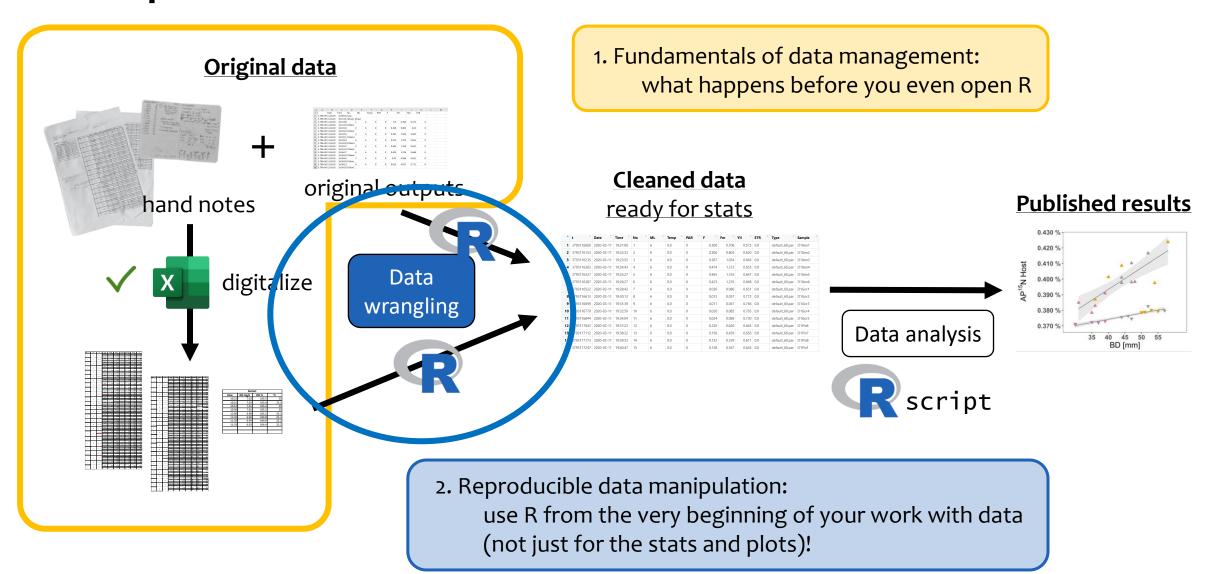


#### **Original data**



(not just for the stats and plots)!

use R from the very beginning of your work with data



# 1. Fundamentals of data management

Get your data in order **before** you start working on it ...



## Why this matters

• Ever looked at an **old project** and panicked because you could not make sense of what was what?

• Ever struggled to make sense of **data** that you **received from a collaborator**?



Panic, Frustration, and **bad science** ...

## Good data management = good data analysis

#### Projects generate a lot of:

- data (= stuff that you measured) and
- metadata (= additional information necessary to make sense of your data).

#### These come in

- different shapes and formats
- from different points in time,
- from different sources
- and likely get modified in multiple occasions.
- → things can get real messy ...

Messiness can hinder your ability to fully utilize your data, vanishing the efforts you made to generate that data!

Therefore, you need to set and follow rules ...

### Practically speaking: How to organize your project folder

- All data belonging to a project must be stored in one folder (there you can have as many subfolders as it is needed)
- Have a written description of how the data was generated and by who in a text file. It must be as clear and detailed as possible. Let's call it an "ultra-honest version of a papers' materials and methods"
- For each data set or table: provide a clear explanation of the meaning of each
  variable (column name) as well as of each observation (row). It must be clear what each name
  or measurement or attribute stands for (especially if it is an abbreviation) and in what units it
  is expressed
  - e.g. if a column named "DO", write somewhere that it means "Dissolved Oxygen [mg/L]" ...
  - This can be for example in another sheet within the same .xlsx file, or in a separate .txt or .csv file named in a way that can be unambiguously linked to the data it refers to (e.g. "rawdata shrimp 20201109.csv" and "rawdata shrimp 20201109 description.txt")

### Practically speaking: How to organize your project folder

Keep the raw / original data safe!

#### Meaning:

- name it clearly and unambiguously
- never modify it
- make a backup copy (or two or three ... ) saved somewhere else.



## Some definitions to clarify ....

**Original data** = the very original data that was collected: your hand notes if you have manual measurements (take pictures or make a scan copy of it) or what is outputted by a machine if you have automated or digital measurements. **AS IT IS**.

Raw data = basically, the same as original data, but for data analysis it should be in a digital format (what you manually enter in a spreadsheet).

**Manipulations** = include "cleaning" of the data to remove wrong or incomplete information, correction of typos, calculation of statistics (mean, sd or so) or reshaping of the data for preliminary plots.

If you manipulate it, you cannot call it "raw" or "original" anymore, therefore rename it!

## How to name your files in a meaningful way

#### Choose a naming system and stick to it.

Useful information to include in the filename are:

- The date of creation in the filename: "cmr\_intro\_20210104.R"
   (using the format YYYY-MM-DD is particularly handy because the files will automatically be sorted chronologically)
- The **version** number: "thesis\_intro\_v1.R", "thesis\_intro\_v2.R", "thesis\_intro\_v2.R" (but in this way it can be tricky to keep track of the actual version when you create a new one I prefer using the date)
- Your **initials** when you modify a file shared among collaborators: "thesis\_intro\_20210104\_GP.R", "cmr\_intro\_20210104\_GP\_ABC.R"

In this way, even if you have a million files at the end of the project you can always **track the changes chronologically** and arrive to the source ...

(but if you work on data, you should only modify it through scripts – not in Excel!)

## How to tell if your data is well kept: a simple rule ...

Ask yourself if **another person**, by looking at your data or project folder, without any additional input, **would be able to figure out**:

- Where does this data come from: how was it generated? What did you measure and how? Who generated it?
- Why, what is the rationale and what are the reason for specifically choosing that approach
- In each data table: what is the meaning of each variable (= column name): clearly define them as explicitly as possible (even if -you think- the naming is self-explanatory!)
- The **structure** of the data set is clear: how many treatments, how many levels, number of replicates ...



## Additional tips to simplify your (and everyone's) life

Characters choice – for filenames and for their content (aka your data)

Avoid anything that can have multiple interpretations.

- Avoid punctuation (.,:;?!)
- avoid special symbols (e.g. instead of "%", write "perc")
- avoid operational symbols ( + / \* ^ < >)
- never start with a number ("15thattemp.csv" is not good, rather: "attempt15.csv")
- Also good practice to leave no space in the filename
   (can be problem if in other OS, e.g. Linux, plus, in all coding languages I can think of, words separated by space are interpreted as separated objects)
  - Mario Rossi Data coral expm#3.xlsx
    1st version? 02.12.2019.csv

## Additional tips to simplify your (and everyone's) life

- Try as much as possible to generate the data directly in ENGLISH
- Try as much as possible to use the **English numerical system** (decimals as "." not as ",")
- Save your original data as .csv (or .tsv or even plain .txt), NOT as Excel spreadsheet
  - because .csv are universally read in the same way, while Excel spreadsheet read differently depending on the version and system locale





## To sum up ...

- Keep a complete and detailed written explanation of your data set together with your data (e.g. in the same folder)
- Never touch the raw/original data and keep at least one backup copy of it
- Be smart and just avoid anything that might create ambiguity (naming etc.)
- Make sure your work is ALWAYS REPRODUCIBLE = **modify** your **data only through scripts**! (yes, even corrections to obvious mistakes like typos)



# 2. Reproducible data manipulation: data wrangling in R (Tidyverse)

Work only through scripts  $\rightarrow$  R!

## Re-cap of what "data wrangling" means

Transform raw data into another format that is more suited for downstream applications (e.g., analytics).

#### Includes:

- Sorting/re-arranging of data (change order, transpose)
- Sub setting (separate a smaller part of a dataset from the rest -> e.g., to plot, remove outliers)
- Merging (put together data from different tables/sheets)
- Correcting errors (e.g., typos)

Typically takes more time than the actual analysis of the data!

## Tidyverse



A **collection of R packages** designed **for data science**, that share an underlying design philosophy, grammar, and data structures.

"A gateway drug ... "

#### Noteworthy aspects:

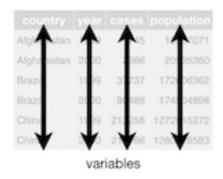
- Concept of "Tidy data"
- 2. The **pipe** (%>%) (move away from nested functions)

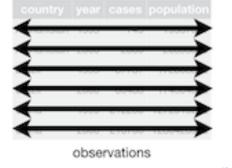


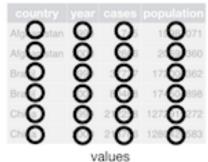
Leo Tolstoy

#### Simple rules:

- Every **column** is **variable**.
- Every **row** is an **observation**.
- Every **cell** is a **single value**.





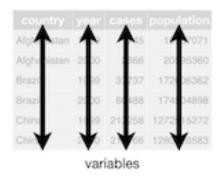


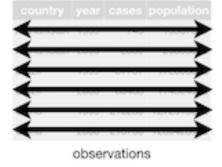
12 Tidy data | R for Data Science (had.co.nz)

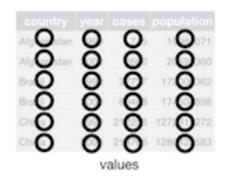
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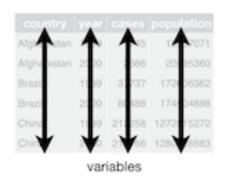
12 Tidy data | R for Data Science (had.co.nz)

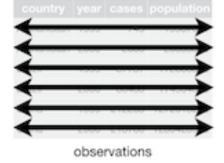
country	year	rate
Afghanistan	1999	<b>745</b> / 19987071
Afghanistan	2000	<b>2666</b> / 20595360
Brazil	1999	<b>37737</b> / 172006362
Brazil	2000	<b>80488</b> / 174504898
China	1999	<b>212258</b> / 1272915272
China	2000	<b>213766</b> / 1280428583

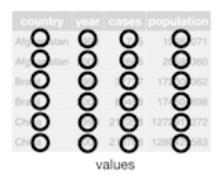
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12 Tidy data | R for Data Science (had.co.nz)

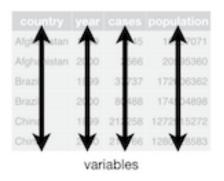


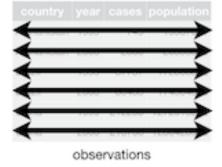
Leo Tolstoy

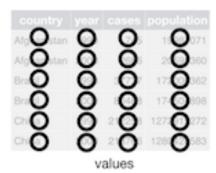
## 1. Tidy data

#### Simple rules:

- Every **column** is **variable**.
- Every **row** is an **observation**.
- Every **cell** is a single **value**.







12 Tidy data | R for Data Science (had.co.nz)

	treatmenta	treatmentb
John Smith	_	2
Jane Doe	16	11
Mary Johnson	3	1

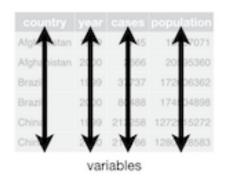
	John Smith	Jane Doe	Mary Johnson
treatmenta	_	16	3
treatmentb	2	11	1

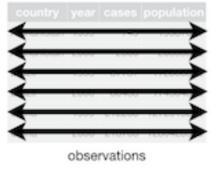
person	${f treatment}$	$\operatorname{result}$
John Smith	a	
Jane Doe	a	16
Mary Johnson	a	3
John Smith	b	$^2$
Jane Doe	b	11
Mary Johnson	b	1

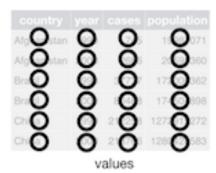
Leo Tolstoy

#### Simple rules:

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12 Tidy data | R for Data Science (had.co.nz)

	treatmenta	treatmentb
John Smith	_	2
Jane Doe	16	11
Mary Johnson	3	1



	John Smith	Jane Doe	Mary Johnson
treatmenta	_	16	3
treatmentb	2	11	1

"wide"

person	${\it treatment}$	$\operatorname{result}$
John Smith	a	
Jane Doe	a	16
Mary Johnson	a	3
John Smith	b	$^2$
Jane Doe	b	11
Mary Johnson	b	1

"long"

## 2. Piping functions (vs nested)

```
Nested functions (base R)
3     2     1

length(unique(data$column)))
```

Using the pipe makes the code easier to write and to read (Tidyverse)



```
data$column %>% unique() %>% length()
```

## A set of powerful and intuitive functions

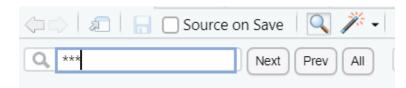
We'll see them in action in a minute ...!

#### But briefly:

- Create/modify variables: mutate()
- Subset data: filter(), select()
- Summarize: summarise(), group\_by()
- Restructure: pivot\_wider(), pivot\_longer()
- Merge: \*\_join() ... (e.g. left\_join() )
- Correct values: rename(), replace()
- Plot like a pro: ggplot()

These can take you a long way ...!

# \*\*\*
marked in the script
-> easy to find









all material available in GitHub to run at your own peace after the workshop

## Kidding, one last thing ....

We'll go through an example of exploratory data analysis (EDA\*)

- **Explore** structure of the data (understand it)
- Scout for mistakes (always present in real world data)
- Correct such mistakes exclusively through R
- Re-shape the data (tables) to our needs Prepare for stats (e.g. ANOVA)
- Make some plots (show the power of exploratory data viz! now because if earlier might be confusing)

<sup>\*</sup>use this terminology in your CV to sound more profesh;)

### Overview of the data set

The R script is based on dummy data (created for didactic purposes by me) that includes:

- PAM data, collected in 4 separate sessions + additional data regarding the experimental conditions → 5 files (.csv)
- "Metadata" with description of the dataset → text (.txt)
- Graphical representation of the experimental design → figure (.png)
   One picture figure is worth a thousand words ... even for scientists!

This is a **realistic example** of how to correctly store the raw/original data with the info necessary to understand it, and how to process/manipulate/wrangle it in R



Graphical representation of the experimental design for our dummy data ("PAM\_replication.png")

## Also keep in mind that ...

**Learning R coding is a hands-on effort**: you will never learn R just by watching (a lecture, a tutorial ... ) and memorizing. The only way is to try things for yourself: write (or copy paste) the code, read packages and functions descriptions, follow similar examples.

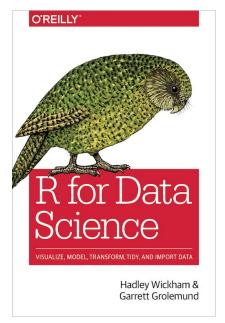
It's a lot of reading, and trial and error.

This can be discouraging at the beginning, but it is time well invested!

Therefore this script is **not** to be taken as **an explanation of how to do everything** – although it is heavily commented for ease of understanding – the idea is for **the script to be a starting point** (a **roadmap**) to show **examples of what R can do for you**. Then you will have to take the time to explore the functions by yourself (tip: use the "help" panel to check how the function works, what arguments it requires and in what shape ... ).

## (my favorite) Resources

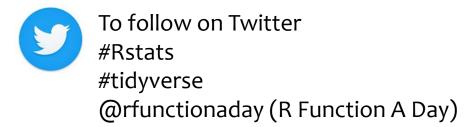
THE book, a must-read: "R4DS"

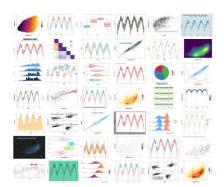


https://r4ds.had.co.nz/









Tutorials and inspiration for ggplot2

From data to Viz | Find the graphic you need (data-to-viz.com)

A ggplot2 Tutorial for Beautiful Plotting in R - Cédric Scherer (cedricscherer.com)

rfordatascience/tidytuesday: Official repo for the #tidytuesday project (github.com)