GenGen workshop 15.02.2023

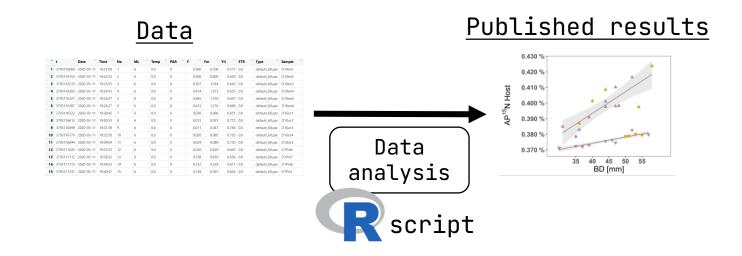


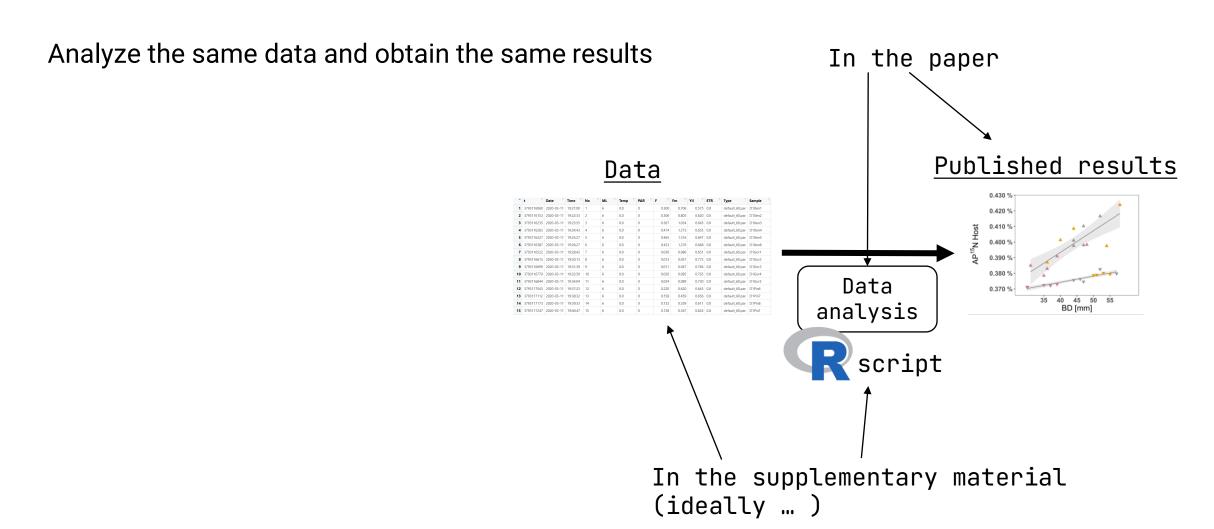
for Reproducible data wrangling

What happens before the stats:
the power of R Tidyverse for
wrangling, cleaning, and exploring your data

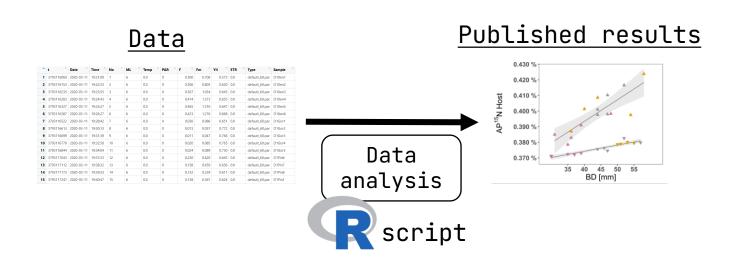
Giulia Puntin | > @sPuntinGi

Analyze the same data and obtain the same results

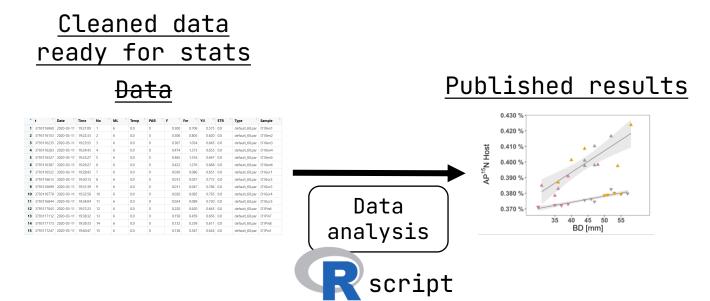




But there's also that other part ...



But there's also that other part ...



<u>Original data</u>



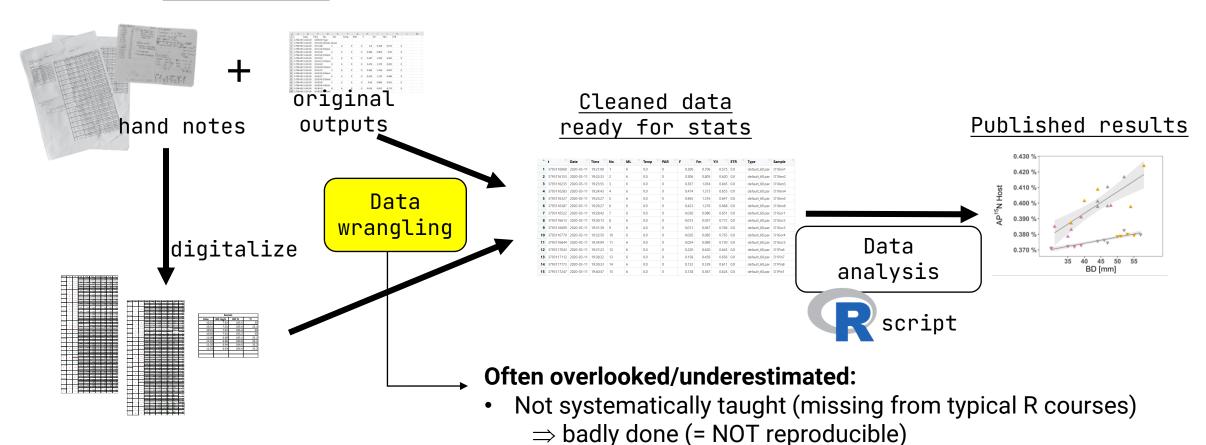
Unusable format ...

4	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										
6	3.79E+09	11.03.20	19:22:33	2	! 6	0		0	0.306	0.805	0.62	0		
7	3.79E+09	11.03.20	19:22:45	D1Xen2										
8	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										
10	3.79E+09	11.03.20	19:24:43	4	6	0		0	0.474	1.373	0.655	0		
11	3.79E+09	11.03.20	19:24:59	D1Xen4										
12	3.79E+09	11.03.20	19:25:27	5	6	0		0	0.465	1.316	0.647	0		
13	3.79E+09	11.03.20	19:25:52	D1Xen5										
14	3.79E+09	11.03.20	19:26:27	6	6	0		0	0.423	1.276	0.668	0		
15	3.79E+09	11.03.20	19:26:43	D1Xen6										
16	3.79E+09	11.03.20	19:28:42	7	' 6	0		0	0.03	0.086	0.651	0		
17	3.79E+09	11.03.20	19:28:59	D1Gor1										-
18	3.79E+09	11.03.20	19:30:13	8	6	0		0	0.013	0.057	0.772	0		
19	3.79E+09	11.03.20	19:30:29	D1Gor2										

... ready to be analyzed ©

^	t [‡]	Date [‡]	Time [‡]	No [‡]	ML [‡]	Temp [‡]	PAR [‡]	F [‡]	Fm ÷	YII ÷	ETR ÷	Type	Sample [‡]
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



- Time consuming (can take up as more time than stat testing)
- => **sensitive step** that can benefit a lot from improvement

<u>Original data</u>



Beware of spreadsheets

Problems derived from working with spreadsheets:

- Messy (many files) ...
- Error prone (e.g. genuine mistakes + autocorrection ...)
- Not scalable (it just doesn't work with large data sets)
- Not reproducible (hard to keep track of every action)



Pessimist: The glass is ½ empty. Excel: The glass is January 2nd.

 \bigcirc 70

1,241

9 40K

8

nature

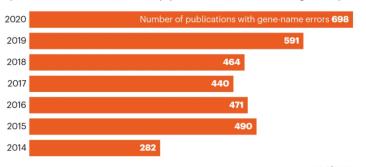
NEWS | 13 August 2021 | Correction 25 August 2021

Autocorrect errors in Excel still creating genomics headache

Despite geneticists being warned about spreadsheet problems, 30% of published papers contain mangled gene names in supplementary data.

GROWING PROBLEM

A 2016 analysis found that 20% of papers featuring gene names had errors created by spreadsheet autocorrect functions, but a bigger survey now finds the proportion is up to 30%. Since 2014, the number of papers with errors has increased significantly.



onature

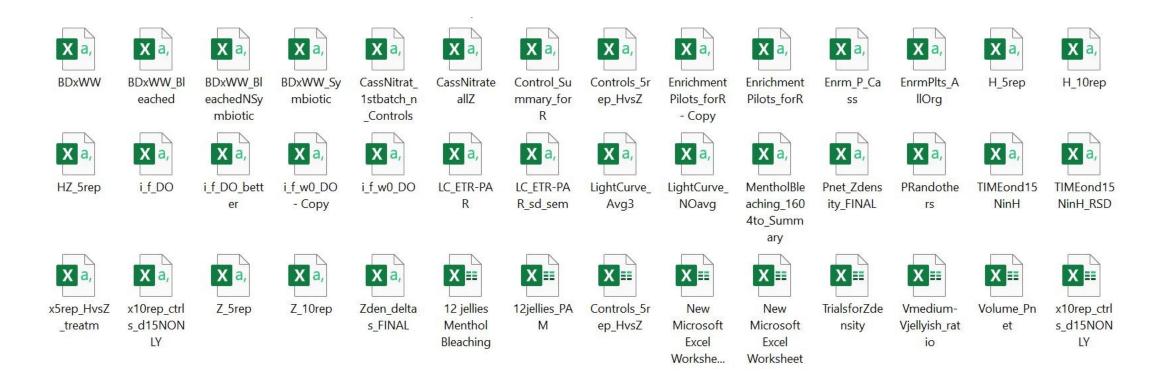
Beware of spreadsheets...

Problems derived from working with spreadsheets:

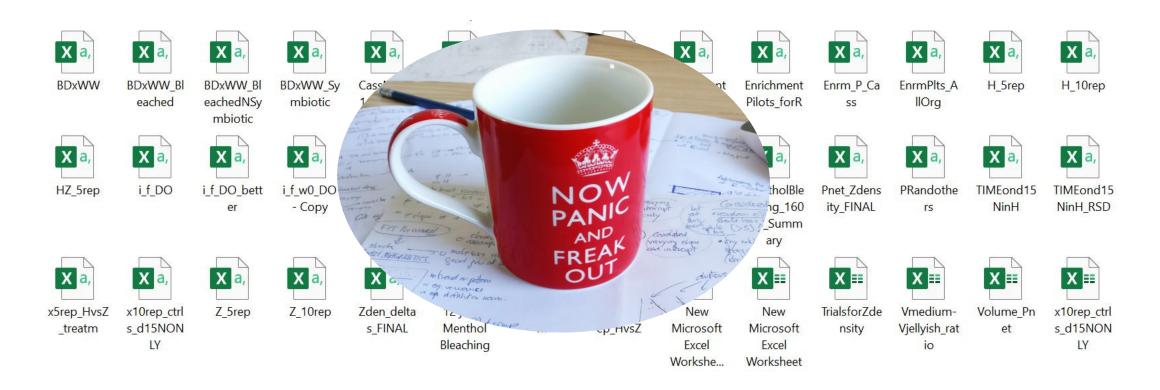
- Messy (many files) ...
- Error prone (e.g. genuine mistakes + autocorrection ...)
- Not scalable (it just doesn't work with large data sets)
- Not reproducible (hard to keep track of every action)

On the contrary, 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)

Old me before discovering Tidyverse ...



Old me before discovering Tidyverse ...



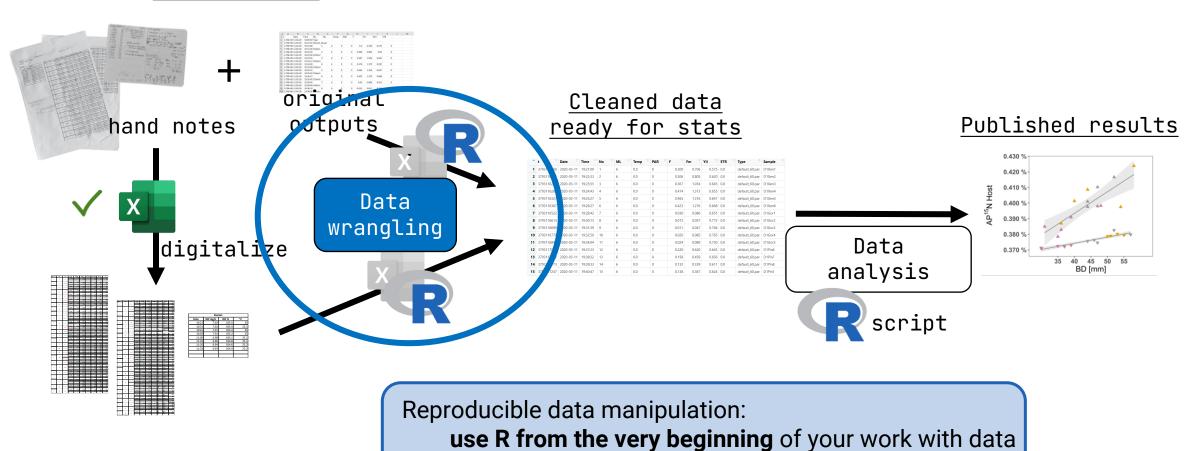
<u>Original data</u>



<u>Original data</u>



Original data



(not just for the stats and plots)!



Whatever gets the job done!

However, I recommend *also* implementing R in your analysis because:

- "Safer" approach: R doesn't modify data files directly, more wiggle room for trial and error (although disadvantages/additional steps)
- Analyses are scripted: you can always go back and check exactly what you did
- Convenience to have "all in one place": seamlessly proceed with data visualization (ggplot!)
 and statistical testing
- Deal with biologists: (unlike bioinformaticians) most biologists usually only know R …)

R vs Phyton:

- Phyton: more versatile (ML, web dev op, ...)
- R: best for stats and data viz
- Also, can just use both!

https://posit.co/blog/three-ways-to-program-in-python-with-rstudio/

Tidyverse

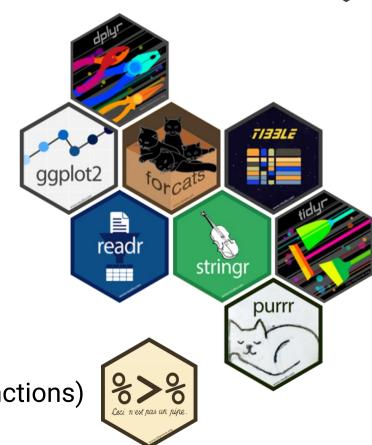


A **collection of R packages** designed **for data science**, that share an underlying design philosophy, grammar, and data structures.

"A gateway drug."
- my friend James

Noteworthy aspects:

- Concept of "Tidy data"
- 2. The pipe (%>%) (more human readable than nested functions)



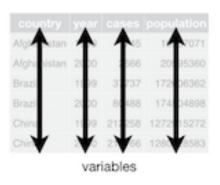
1. Tidy data

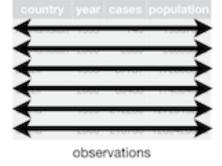
Happy families are all alike; every unhappy family is unhappy in its own way.

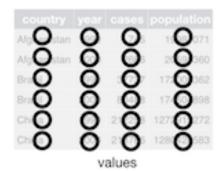
Leo Tolstoy

Simple rules:

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





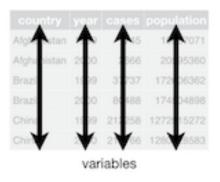


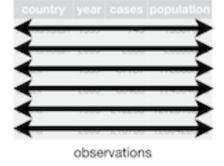
12 Tidy data | R for Data Science (had.co.nz)

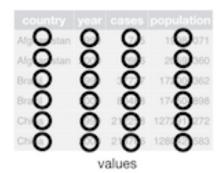
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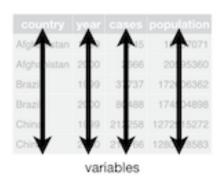
12 Tidy data | R for Data Science (had.co.nz)

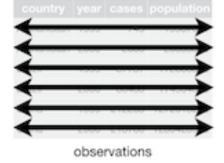
country	year	rate
Afghanistan	1999	745 / 19987071
Afghanistan	2000	2666 / 20595360
Brazil	1999	37737 / 172006362
Brazil	2000	80488 / 174504898
China	1999	212258 / 1272915272
China	2000	213766 / 1280428583

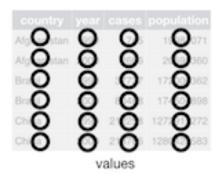
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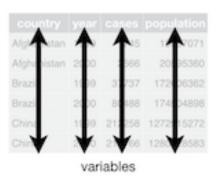
12 Tidy data | R for Data Science (had.co.nz)

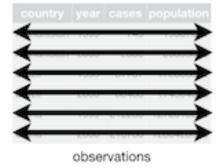


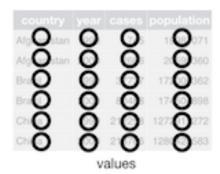
Leo Tolstoy

Simple rules:

- Every column is a variable.
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- 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

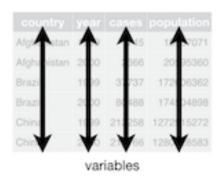
	John Smith	Jane Doe	Mary Johnson
treatmenta		16	3
treatmentb	2	11	1

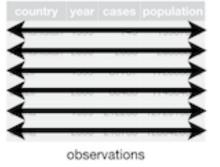
	1:
${ m treatment}$	result
a	
a	16
a	3
b	2
b	11
b	1
	a a b b

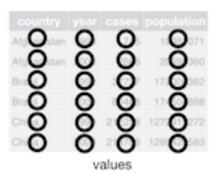
Leo Tolstoy

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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"

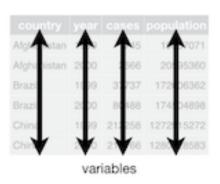
		1.
person	${ m treatment}$	result
John Smith	a	
Jane Doe	a	16
Mary Johnson	a	3
John Smith	b	2
Jane Doe	b	11
Mary Johnson	b	1

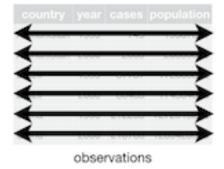
"long"

Leo Tolstoy

Simple rules:

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







values

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

Only column names <

Colum names

Row names



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

Not tidy

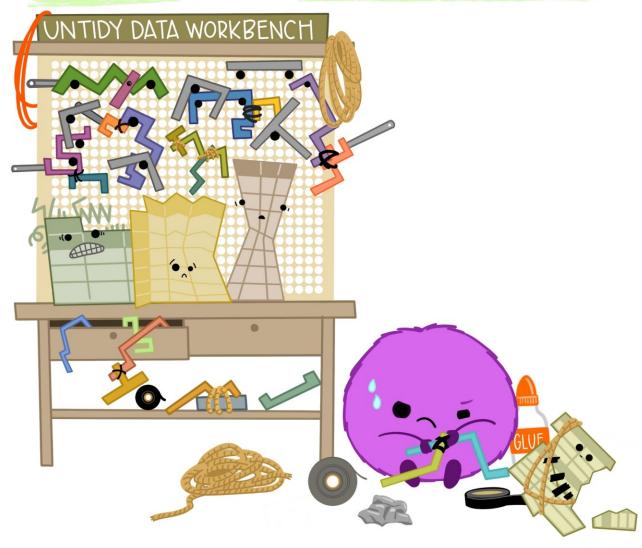
person	${\it treatment}$	result
John Smith	a	_
Jane Doe	\mathbf{a}	16
Mary Johnson	a	3
John Smith	b	2
Jane Doe	b	11
Mary Johnson	b	1

Tidy

When working with tidy data, we can use the same tools in similar ways for different datasets...

DATA WORKBENCH

...but working with untidy data often means reinventing the wheel with one-time approaches that are hard to iterate or reuse.



Credit: Allison Horst



2. Piping functions (vs nested)

```
Nested functions (base R)
3     2     1
length(unique(data$variable)))
```

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



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

2. Piping functions (vs nested)

A more complex example of piping (from this workshop script):

```
data %>%
  group_by(Species, Sex, Island) %>%
  summarise(across(where(is.numeric), ~ mean(.x, na.rm = TRUE))) %>%
  select(-Sample_Number) %>%
  arrange(desc(Sex)) %>%
  write_csv(., "./out/data_means.csv")
```

No need to create intermediate objects, just pipe the outcome of one function into the next (use "." as placeholder)

String manipulation stringr::str_*()



Work with character strings (text)

- Uses **regex** (regular expressions): a "codified" way to describe patterns in text strings, to do things with them (extract, select, replace, ...)
- Same rules as `grep` or `sed' in Unix and Bash

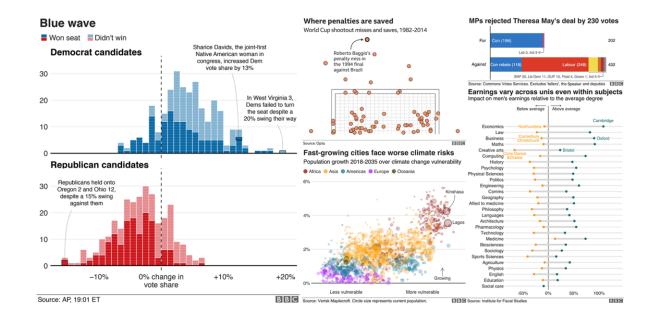
```
"d_Bacteria; p__Proteobacteria; c__Gammaproteobacteria; o__Pseudomonadales; f__Moraxellaceae; g__Acinetobacter"

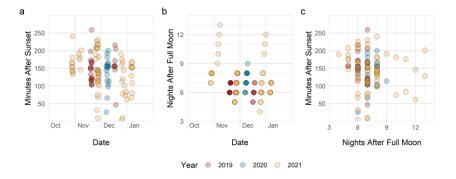
"d__Bacteria; p__Proteobacteria; /c__Gammaproteobacteria; /o__Pseudomonadales; /f__Moraxellaceae; g__Acinetobacter"

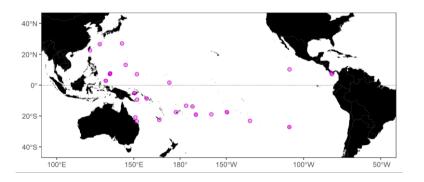
"d__Bacteria; p__Proteobacteria; c__Gammaproteobacteria; o__Pseudomonadales; f__Moraxellaceae; g__Acinetobacter"
```

Data Viz with ggplot

• Publication quality (also BBC, Economist ...)

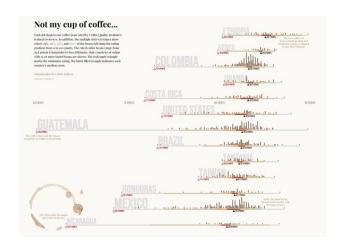


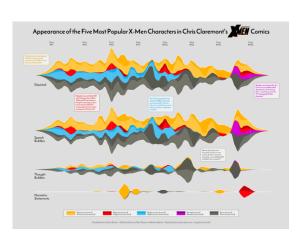


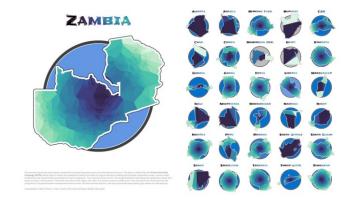


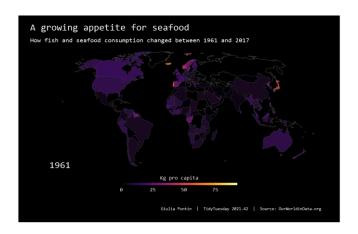
Data Viz with ggplot

- Publication quality (also BBC, Economist ...)
- Also just super beautiful:
 - Cedric Scherer tutorial blog
 - R graph gallery
 - #TidyTuesday









Practical part: R and Tidyverse in action!



The R script is based on **dummy data**(modified from open data set for didactic purposes by me)

Data on penguins' body dimensions, stable isotope measurements, and life stages by species, sex, location, etc

Chosen because of properties:

- numeric data
- character data and
- big enough that it would be annoying to do in Excel
- => good for showing my favorite Tidyverse functions
- Original data: palmerpenguins::penguins_raw
- For more info: ?penguins_raw



Data wrangling

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

But briefly:

- Create/modify variables
- Subset data
- Summarize
- Re-shape
- Merge
- Correct values
- Plot like a pro

Data wrangling

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

Use in combination with

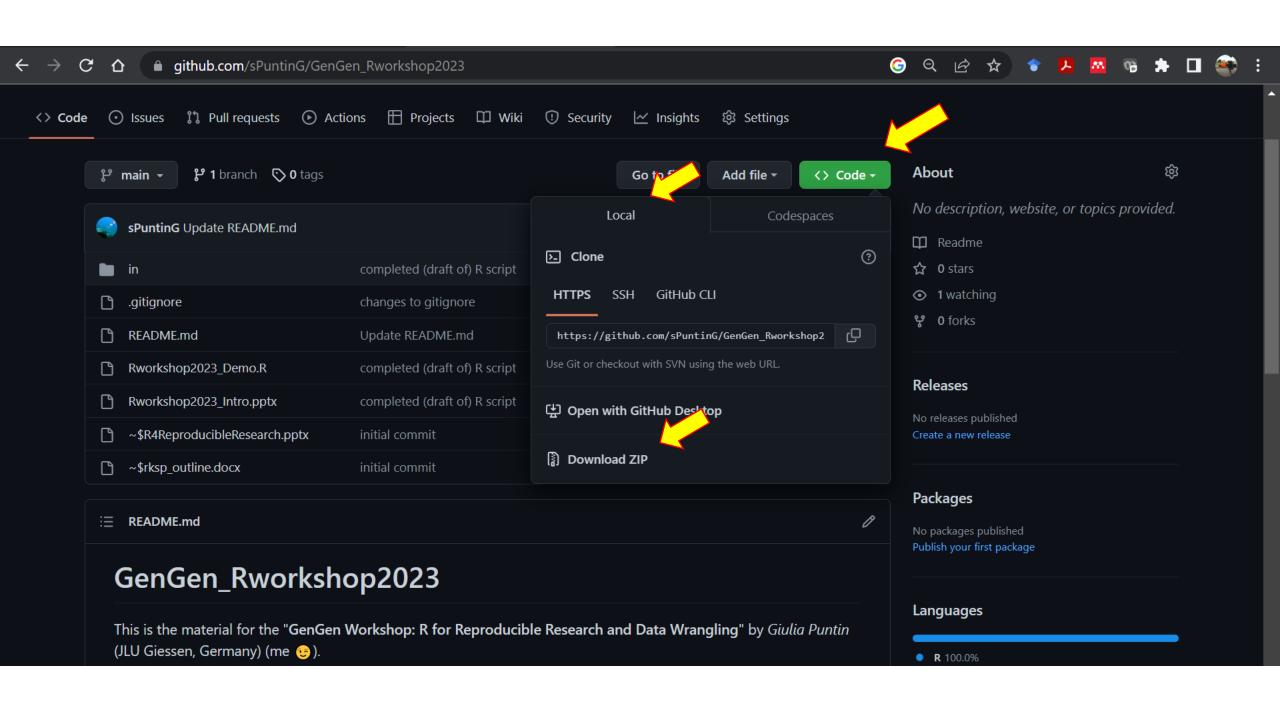
if_else(), case_when(), %in%

But briefly:

- Create/modify variables: mutate()
- Subset data: filter(), select()
- Summarize: summarise(), group_by()
- Re-shape: pivot_wider(), pivot_longer(), arrange()
- Merge: *_join() ... (e.g. left_join(), outer_join(), ...)
- Correct values: rename(), replace()
- Plot like a pro: ggplot()

All workshop material available at

https://github.com/sPuntinG/GenGen_Rworkshop2023



... and waaaay more!

This is **just a short demonstration** of what can be done (and how easily) in R Tidyverse,

BUT there's so much more out there!

Recommend:

- Today: ask me/us about specific tasks/operations that you'd like to learn to execute in R
- Any time: Check out the package cheat sheets for inspiration (I used them a lot!)
 https://posit.co/resources/cheatsheets/?type=posit-cheatsheets&_page=2/





