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GOBIERNO DE LA CIUDAD DE MÉXICO
SECRETARÍA DE EDUCACIÓN, CIENCIA, TECNOLOGÍA E INNOVACIÓN

ASPP LatAm

Best practices in data visualization

Guillermo Aguilar & Carlos Cernuda

With material from Aina Frau-Pascual & Nicolas P. Rougier

Mexico City, ASPP LATAM 2023

Plan

17:00	Principles of data visualization
	Hands-on Exercise 1: **mastering matplotlib**
	Types of visualizations - Use of color - Common pitfalls
	Hands-on Exercise 2: which visualization should I use?
	Review of your solutions as PR
19:30	**END**

Visualization is a method of computing. It transforms the symbolic into geometric, **enabling researchers to observe** their simulations and computations. Visualization offers **a method for seeing the unseen.** It **enriches** the process of scientific discovery and fosters profound and unexpected insights.

Visualization in Scientific Computing, NSF report, 1987

Classical example: Anscombe's quartet

I		II		III		IV	
x	y	x	y	x	y	x	y
10.0	8.04	10.0	9.14	10.0	7.46	8.0	6.58
8.0	6.95	8.0	8.14	8.0	6.77	8.0	5.76
13.0	7.58	13.0	8.74	13.0	12.74	8.0	7.71
9.0	8.81	9.0	8.77	9.0	7.11	8.0	8.84
11.0	8.33	11.0	9.26	11.0	7.81	8.0	8.47
14.0	9.96	14.0	8.10	14.0	8.84	8.0	7.04
6.0	7.24	6.0	6.13	6.0	6.08	8.0	5.25
4.0	4.26	4.0	3.10	4.0	5.39	19.0	12.50
12.0	10.84	12.0	9.13	12.0	8.15	8.0	5.56
7.0	4.82	7.0	7.26	7.0	6.42	8.0	7.91
5.0	5.68	5.0	4.74	5.0	5.73	8.0	6.89

statistic	value
mean of x	9
sample variance of x	11
mean of y	7.50
sample variance of y	4.125
correlation coefficient	0.816
linear regression line	y = 3.00 + 0.500x
coefficient of determination	0.67

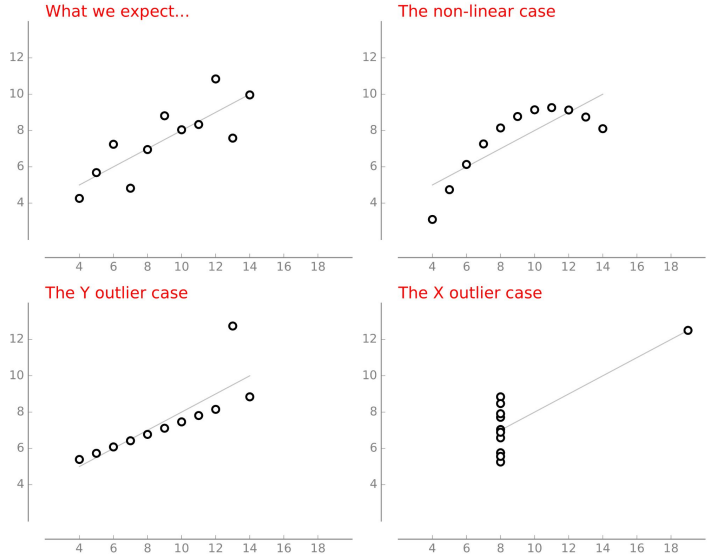
Anscombe (1973)

Classical example of why visualization is important

Anscombe, an statistician, created these four datasets, pairs of x and y points. They all share the 'summary statistics': mean and variance of each variable, and the correlation coefficient between x and y.

Are they identical? For a computer or an algorithm that only looks at these numbers, these four datasets would be identical.

Classical example: Anscombe's quartet



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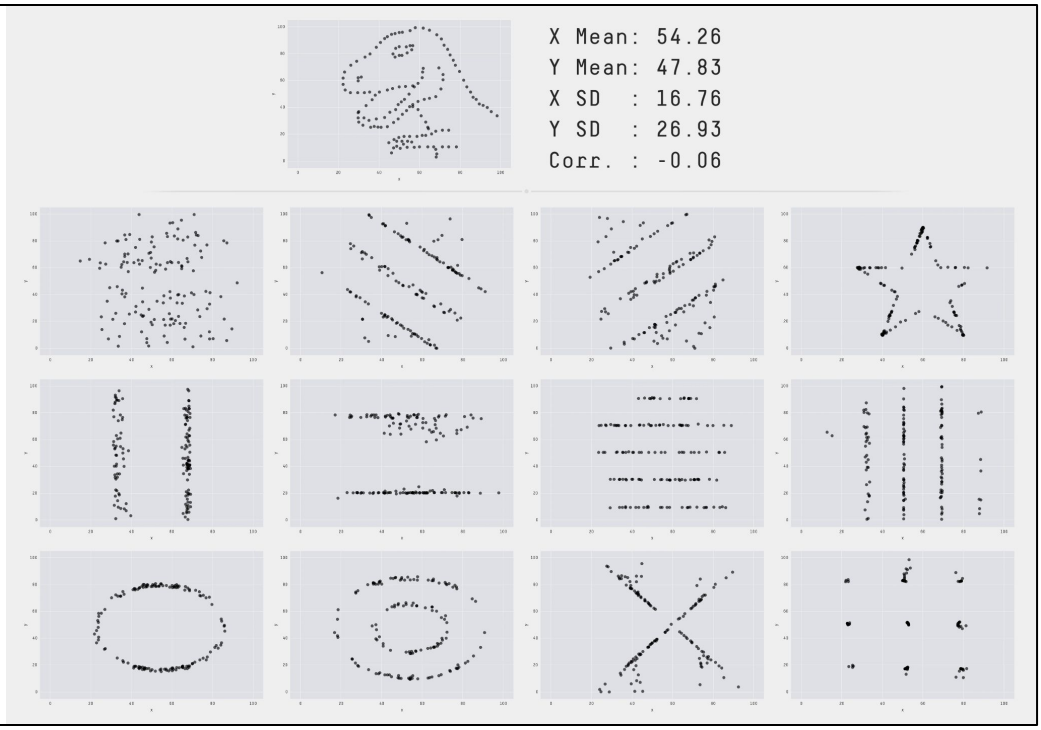
However when we visualize them, we see that actually these datasets are completely different!

We need of vision and our cognitive interpretation to comprehend these differences.

Datasaurus



In the extreme, from a given set of points - here a cute dinosaur - we can create arbitrarily many different datasets with the same statistics - same mean, standard deviation etc, but looking completely different.
The R package Datasaurus implements this idea.

Datasaurus
https://cran.r-project.org/web/packages/datasauRus/vignettes/Datasaurus.html,
https://www.autodesk.com/research/publications/same-stats-different-graphs

So although you might think that number are just numbers and you just need statistics, that's not the whole story.

Because we are humans that see, and we communicate our findings (of science) to other humans, we do need to consider these 'human factors'...
and one of the most important ones in scientific communication is how we visualize things.

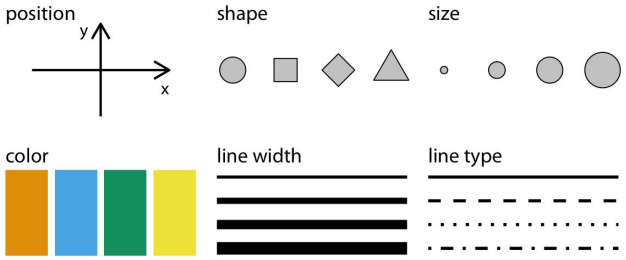
We put his example as a demo of how we do not read always from top to bottom, instead we prioritize size.

Thus we need to know a little bit of how we see in order to better present our results and communicate.

Main challenge: **mapping from data info to visual info**

Data → **Graphical elements**

Type of variable	Examples	Appropriate scale
quantitative/numerical continuous	1.3, 5.7, 83, $1.5x10^{-2}$	continuous
quantitative/numerical discrete	1, 2, 3, 4	discrete
qualitative/categorical unordered	dog, cat, fish	discrete
qualitative/categorical ordered	good, fair, poor	discrete
date or time	Jan. 5 2018, 8:03am	continuous or discrete



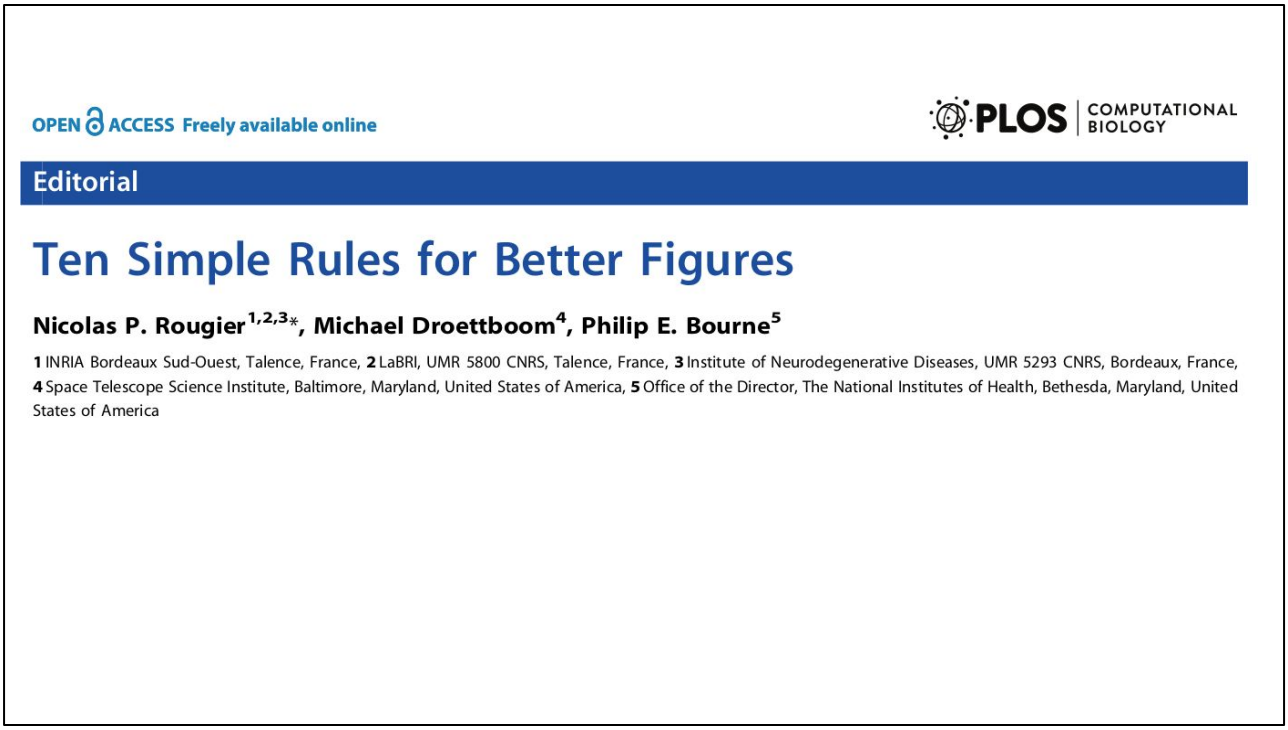
Claus O. Wilke (2019)

Thus the main challenge in data visualization is the **mapping between pure numbers and variables**, which a table or dataset in a computer stores, **to graphical elements, visual features which a human understands**.

We have **different kinds of data**, you probably know this classification: **quantitative** or numerical variables, either continuous or discrete, for example like things that are measured with real numbers.
And then **qualitative** or categorical variables (ordinal or not), for example things without an order, dog, cat, fish… or with an order: good, fair, poor.

Some variables can be assigned to some graphical elements and not others. A **continuous variable** can be assigned to **x and y axis**.
But for example a categorical not ordinal variable (dog, cat, fish) cannot be assigned to e.g. the line width or the size of a dot. That doesn't make sense. As it is categorical **it should be mapped to something categorical, like line type, or a categorical color palette**.

Rules for this mapping are numerous and we will not go into the details here, as also different **fields have different internal 'conventions' or 'standards'** on how they do this mapping. **BUT in the 2nd exercise you will see and practice this mapping and the decisions that you need to take**.



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PLOS | COMPUTATIONAL BIOLOGY

Editorial

Ten Simple Rules for Better Figures

Nicolas P. Rougier[1,2,3]*, Michael Droettboom[4], Philip E. Bourne[5]

1 INRIA Bordeaux Sud-Ouest, Talence, France, **2** LaBRI, UMR 5800 CNRS, Talence, France, **3** Institute of Neurodegenerative Diseases, UMR 5293 CNRS, Bordeaux, France, **4** Space Telescope Science Institute, Baltimore, Maryland, United States of America, **5** Office of the Director, The National Institutes of Health, Bethesda, Maryland, United States of America

So **instead of doing a full lecture on how to do plotting**, we go through **some simple rules** that you can follow.
If you follow these, your visualizations could be very much improved.

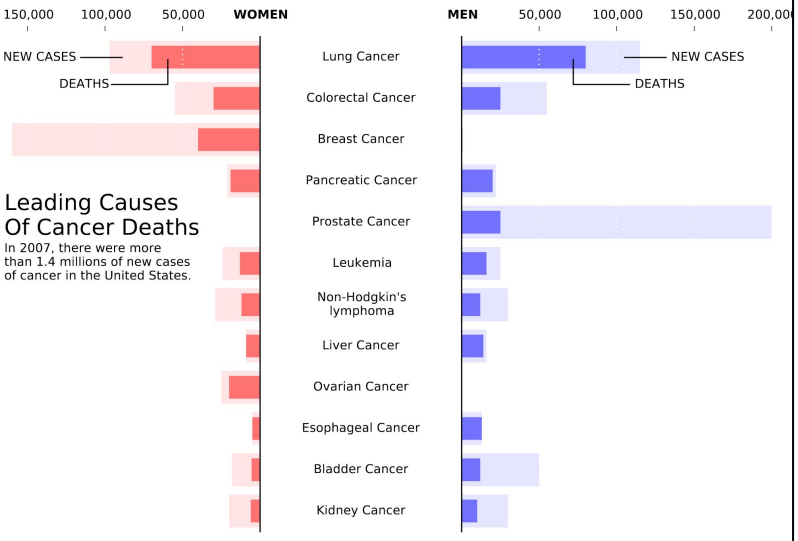
1) Know your audience

My colleagues

Scientific community

Student audience

General public



Audience: general public

Main message: cancer

Separated in sex groups: Women / Men

The graphical design of the visual should be **informed by the audience and the message** the visual is to convey.

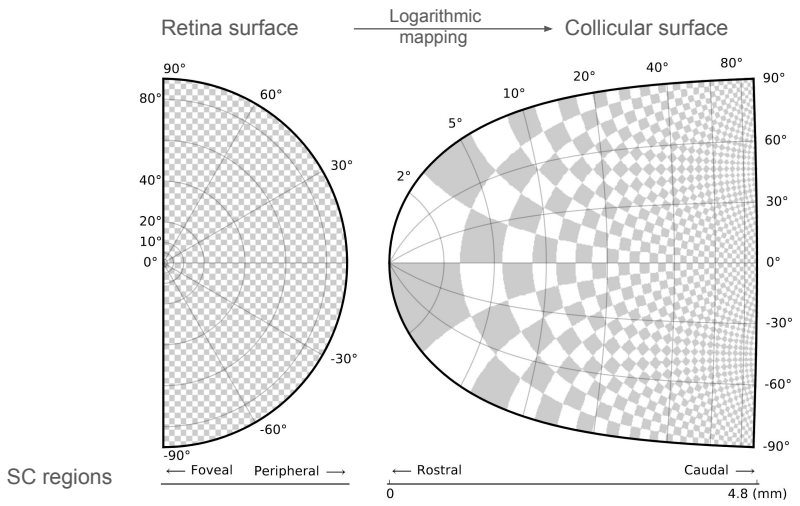
Focus of this figure:

- Audience: general public
- Qualitative (you can't tell the exact numbers)
- Main message in the center: cancer
- As NEW CASES are always higher than DEATHS and DEATHS are part of the cases, so **we can visually have them together**

2) Identify your message

Audience:

neuroscience scientific community



Main message: Artificial checkerboard pattern demonstrates the magnification of the foveal region in the superior colliculus (brainstem structure). This has to do with the induction of saccadic eye movement that the SC plays a role in.

Depending on the audience the complexity of your message has to be different.

Once you **identify** which is the **right level of complexity** for your message, **then** you **visualize** your message.

For the audience the **main message should be easily graspable at a first sight, with minimal reading of captions and text**.
That means that **the more general the audience is, the simplest the visualization has to be**.

One message -> one figure

On this example:
Audience → neuroscientific community.
Main message: artificial checkerboard pattern log mapping from a brainstem substructure to another

3) Adapt the figure to support the medium

Figure for a Paper

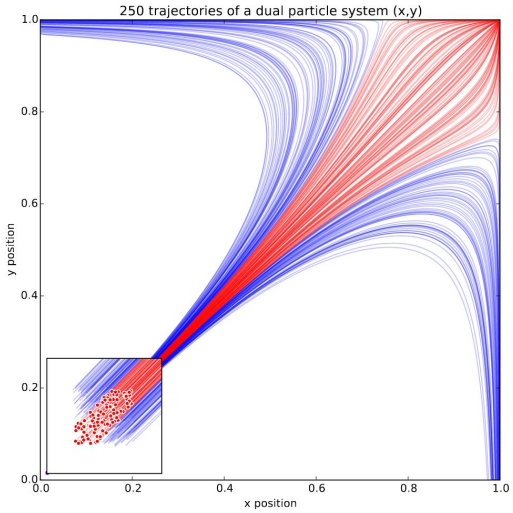
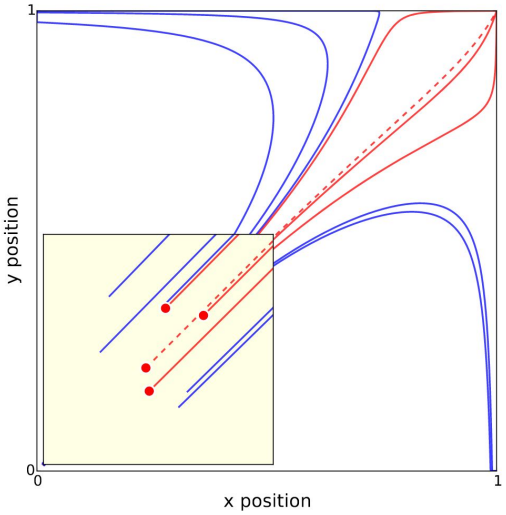


Figure for a Talk



Each medium is different. For instance, seeing a **figure in a printed poster on a conference** is **different than having it digitally in a computer**, and **different that a figure projected in an oral presentation**. All these media have **different physical sizes, but more importantly**, each of them also implies **different ways of viewing and interacting with the figure**.

On the **left**:

- Image for a **journal article** where **the reader is free to look at every detail**. **Red lines**: initial conditions & **Line transparency**: show density of lines

On the **right**:

- Image for an **oral presentation**. **Time-limited display. Many details have been removed**. Some **parts modified** so that it is **easier to reference**.

4) Captions are not optional. Neither x and y-labels

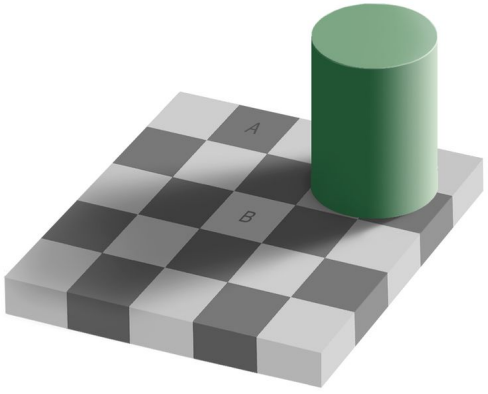
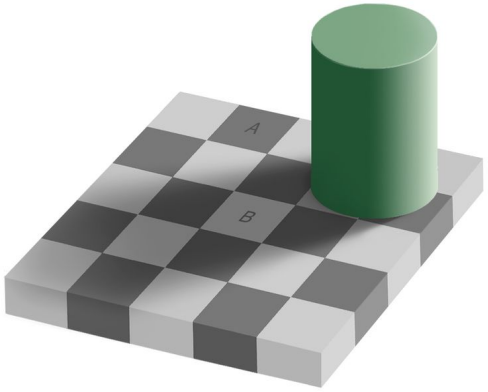


Figure 1. Optical illusion

The **caption explains how to read the figure** and **provides additional precision for what cannot be graphically represented**.

Be **concrete and explicit in the caption**. **Describe all what is going on**, if there are different panels, colors, line types, you should mention what they all mean.

4) Captions are not optional. Neither x and y-labels



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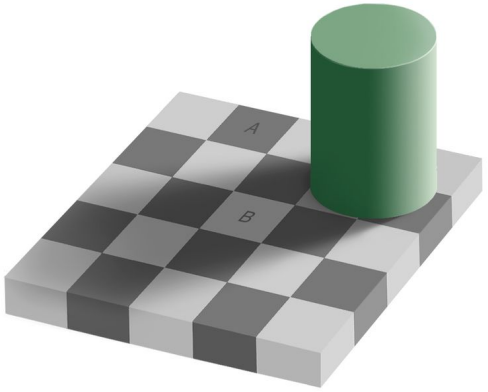

Figure 1. A and B patches are actually the same color even though we perceive them at being different color

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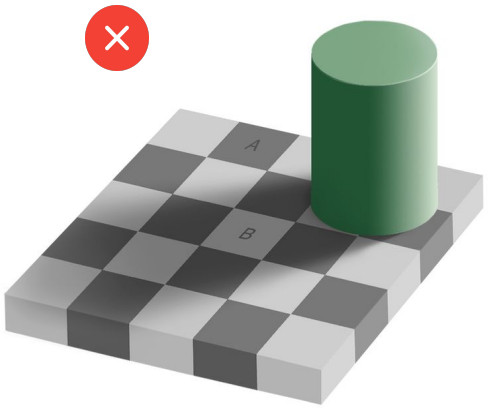
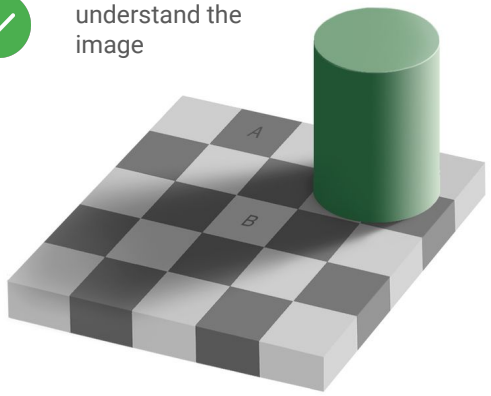


Figure 1. Optical illusion

Caption helps you understand the image



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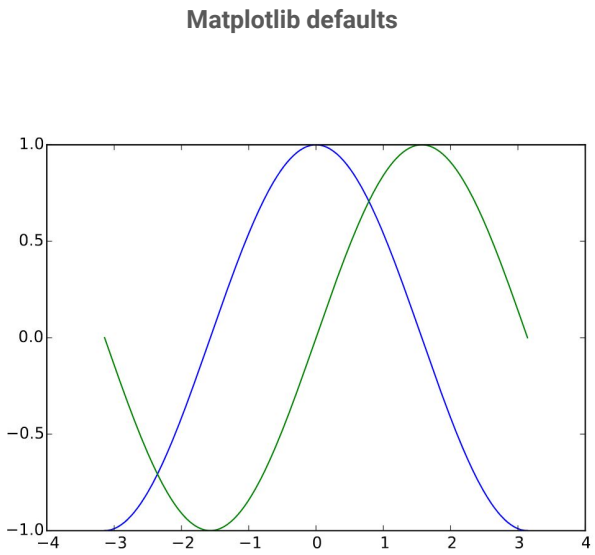
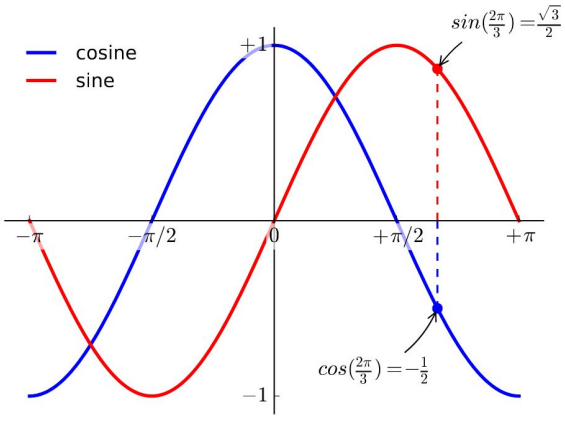
5) Do not trust the defaults



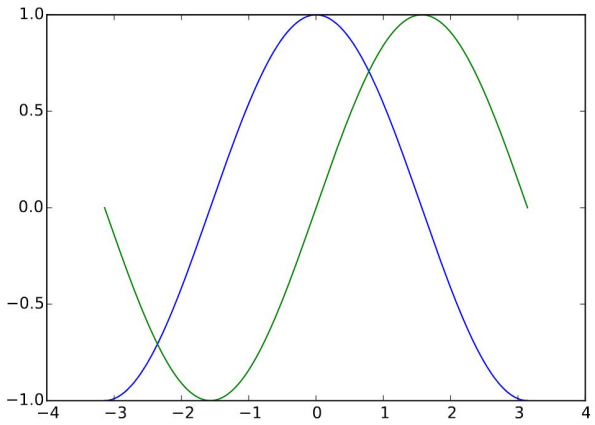


Defaults are good enough for any plot but best for none. Fine-tuning the plot will allow you to better express the message.

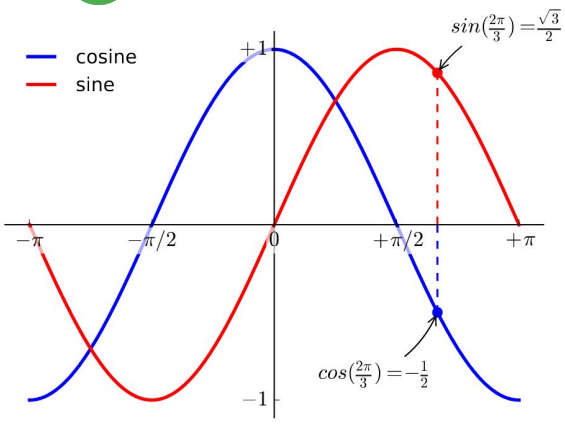
All plots require at least some manual tuning of the different settings to better express the message, be it for making a precise plot more salient to a broad audience, or to choose the best colormap for the nature of the data.

5) Do not trust the defaults

Matplotlib defaults



With a bit of work....
(Exercise 1 today)



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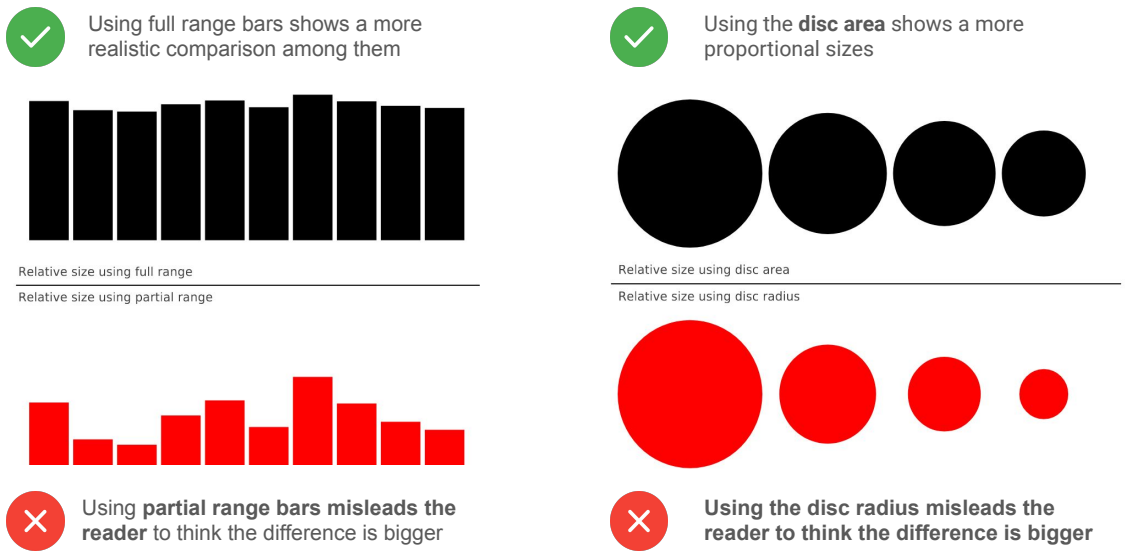
6) Use color effectively → more on this later

7) Do not mislead the reader



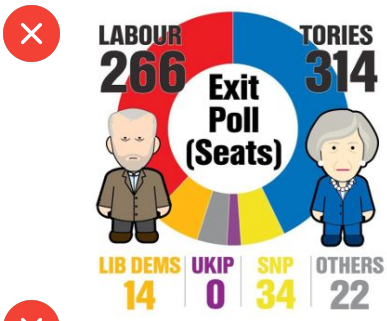
What distinguishes a scientific figure from other graphical artwork is the presence of **data** that **needs to be shown as objectively as possible**.

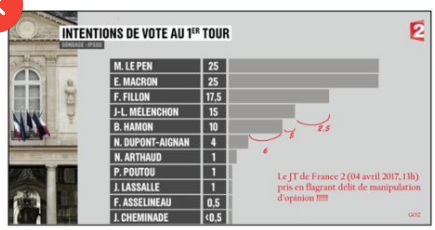
A **scientific figure** is, by definition, **tied to the data** (be it an experimental setup, a model, or some results) and if you loosen this tie, you may unintentionally project a different message than intended. However, **representing results objectively is not always straightforward**.

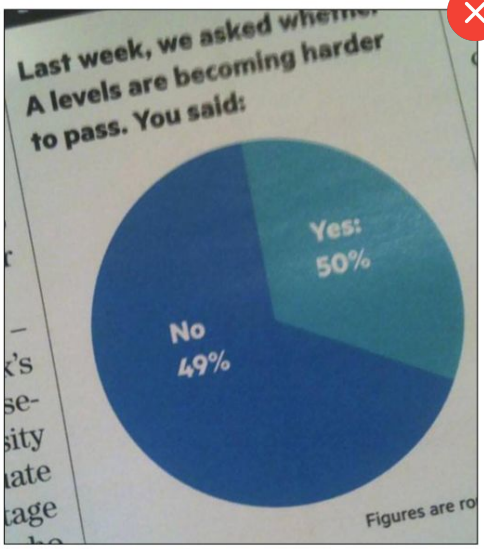
As a **rule of thumb**, make sure to always **use the simplest type of plots that can convey your message** and **make sure to use labels, ticks, title, and the full range of values when relevant**.

Lastly, do not hesitate to ask colleagues about their interpretation of your figures.

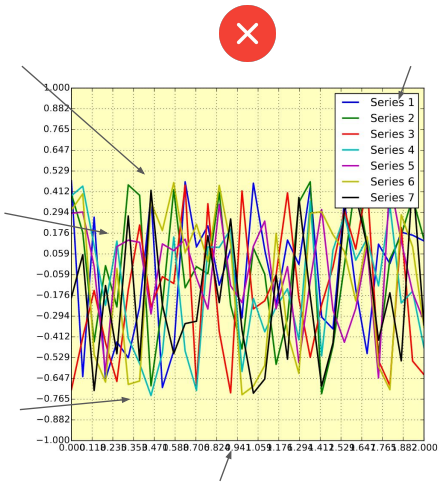
7) Do not mislead the reader. Really.

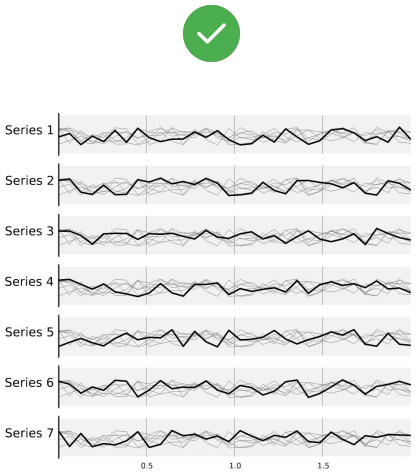






8) Avoid **chartjunk**





Chartjunk refers to all the **unnecessary or confusing visual elements** found in a figure. They **do not improve the message (in the best case) or add confusion (in the worst case)**.

For example, chartjunk may include the **use of too many colors, too many labels, gratuitously colored backgrounds, useless grid lines, etc**.

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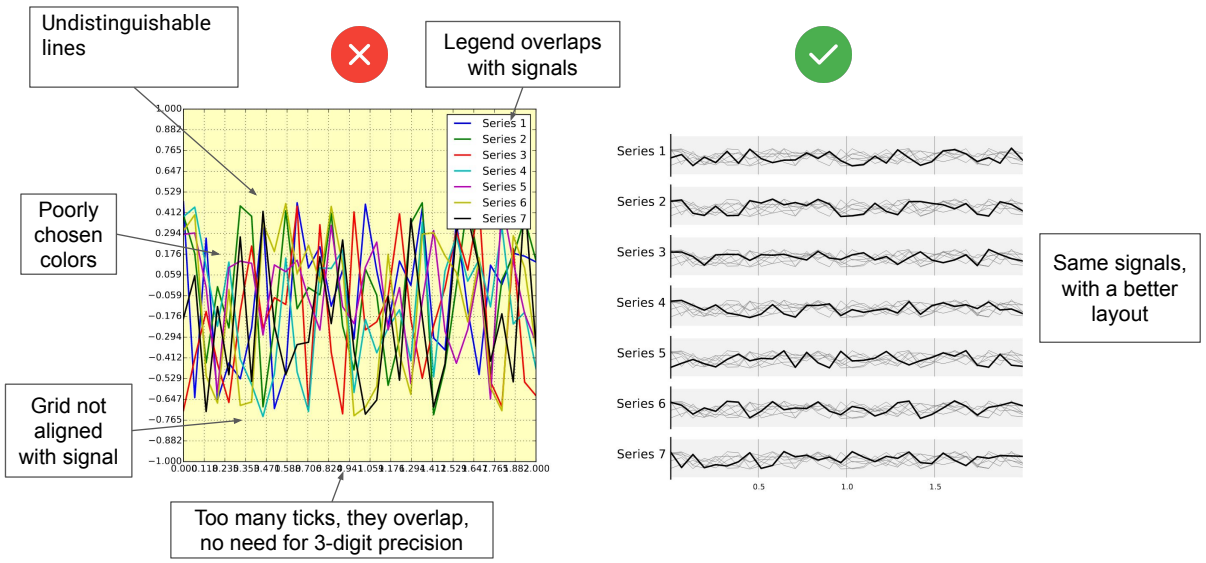

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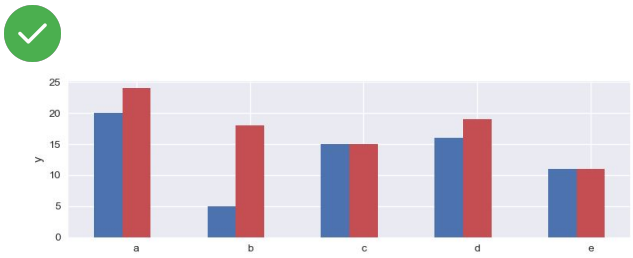
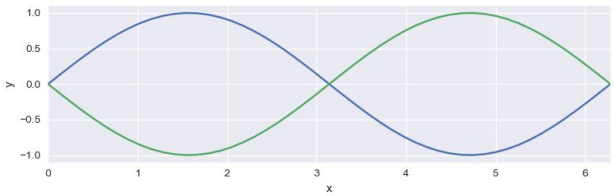
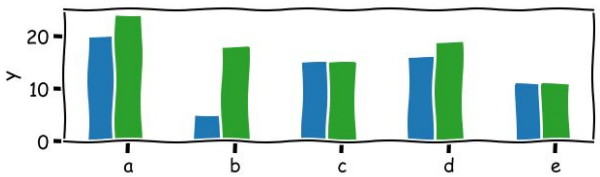
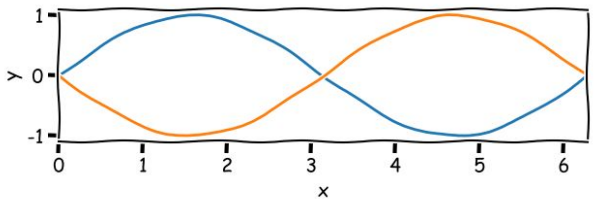
9) Message trumps beauty:

To convey an idea, sometimes an sketch suffices









To deliver an idea or sometimes you don't have to be super precise and accurate. You can give a rough idea, with a sketch. This is OK!

10) Get the right tool

PDFCrop to remove white borders

GraphViz for creating easy graphs

ImageMagick for scripted image processing

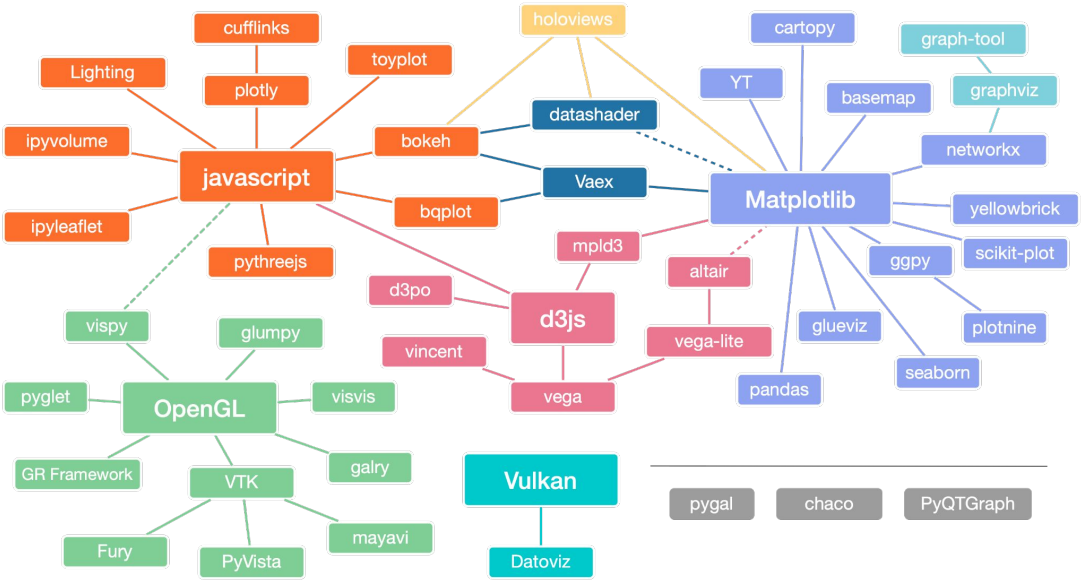
Gimp for bitmap image manipulation

Inkscape for vector image manipulation

Tikz for scripted vector art

And many, many, many others…

Overview of visualization libraries



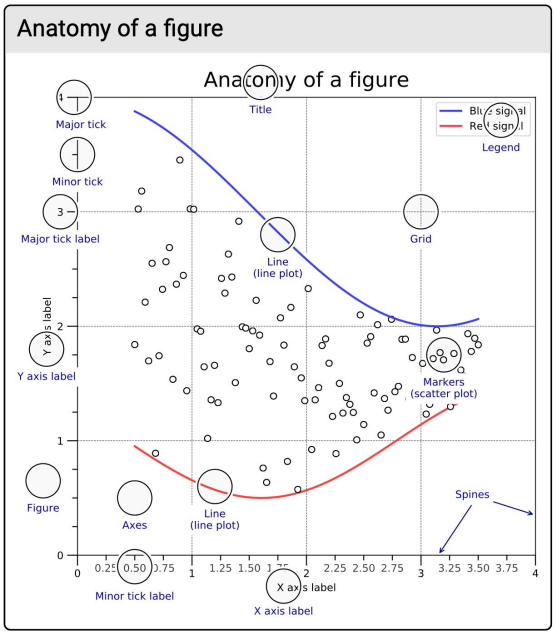
A jungle of visualization libraries. Here we will focus on the most used one: **matplotlib.**
After today's session feel free to expand your knowledge of other libraries, seaborn, plotnine, etc. Check out the Repo's README for links to further resources.

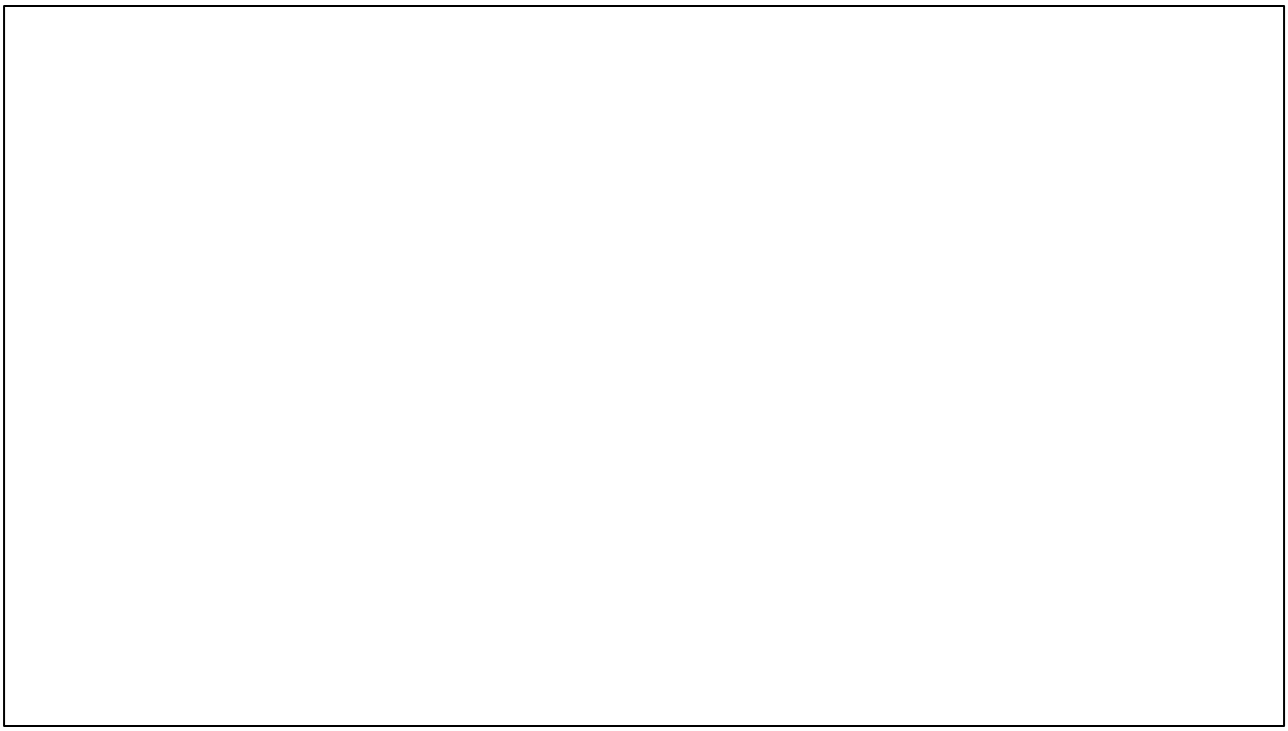
Time for hands-on exercises!

Exercise 1: Mastering matplotlib

Have your cheatsheet at hand!:

https://matplotlib.org/cheatsheets/





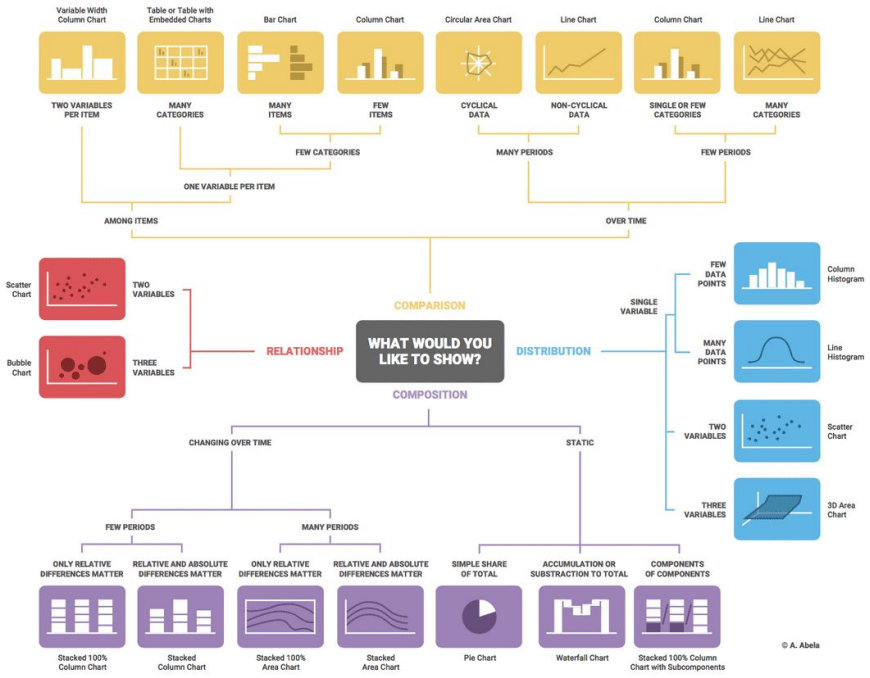
An useful tool:

datavizcatalogue.com

https://datavizcatalogue.com/search.html
https://datavizcatalogue.com/blog/chart-selection-guide/

Another,
older tool

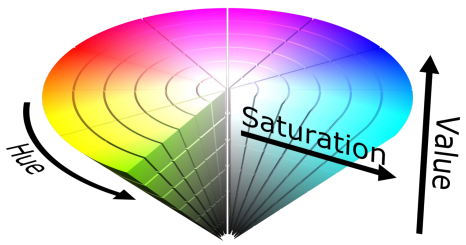
Chart
suggestions
by Abela



If you're completely overwhelmed or lost in the amount of options out there… you can use this workflow to decide which visualization to use first. You will get already something very reasonable!

6) Use color effectively

Three dimensions of color: Hue, saturation and brightness

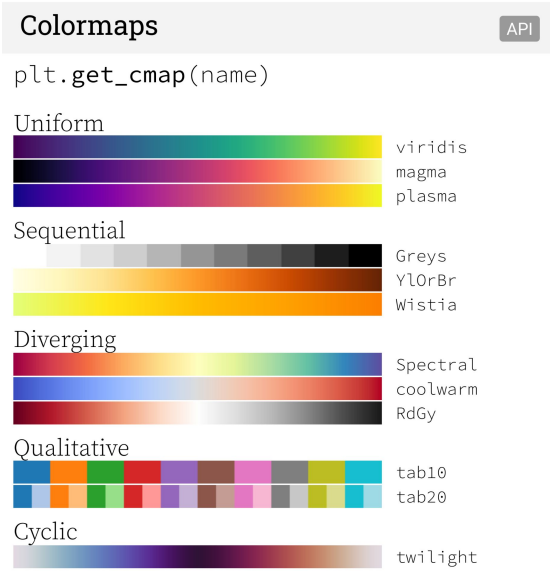


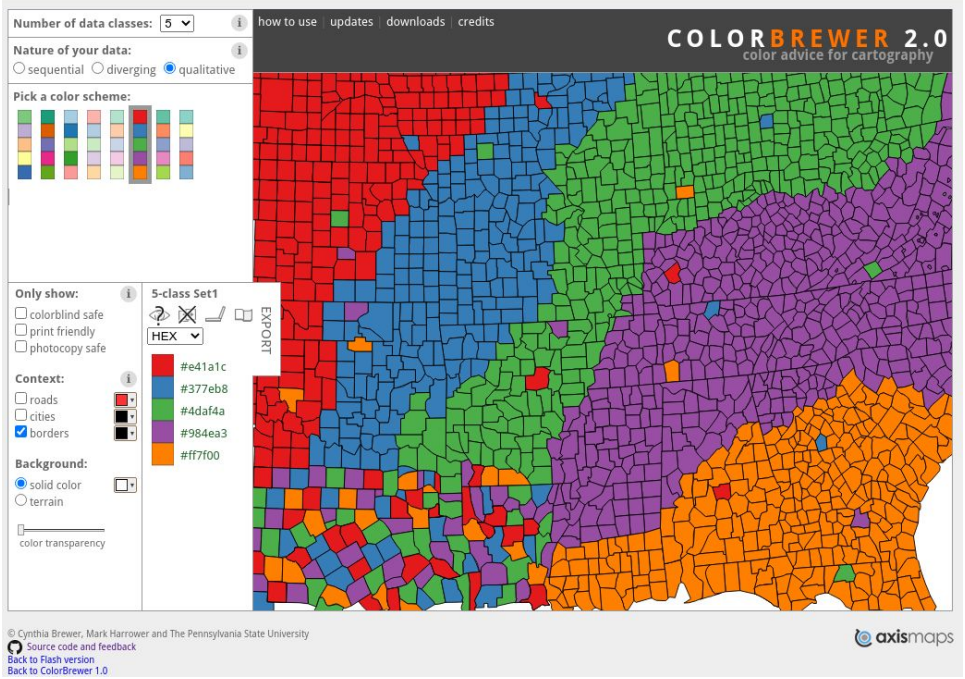
https://lisacharlottemuth.com/
https://blog.datawrapper.de/beautifulcolors/
https://blog.datawrapper.de/colorguide/
https://blog.datawrapper.de/colors/

https://colorizer.org/
https://www.sessions.edu/color-calculator/ -> do not use tetraedric

Types of color scales

- **Qualitative/categorical**: data with no order
  - e.g. cities, countries
- **Sequential**: increasing or decreasing data
  - e.g. year
- **Diverging**: data with a natural zero
  - e.g. % change, temperature
- **Circular**
  - e.g. orientation, direction



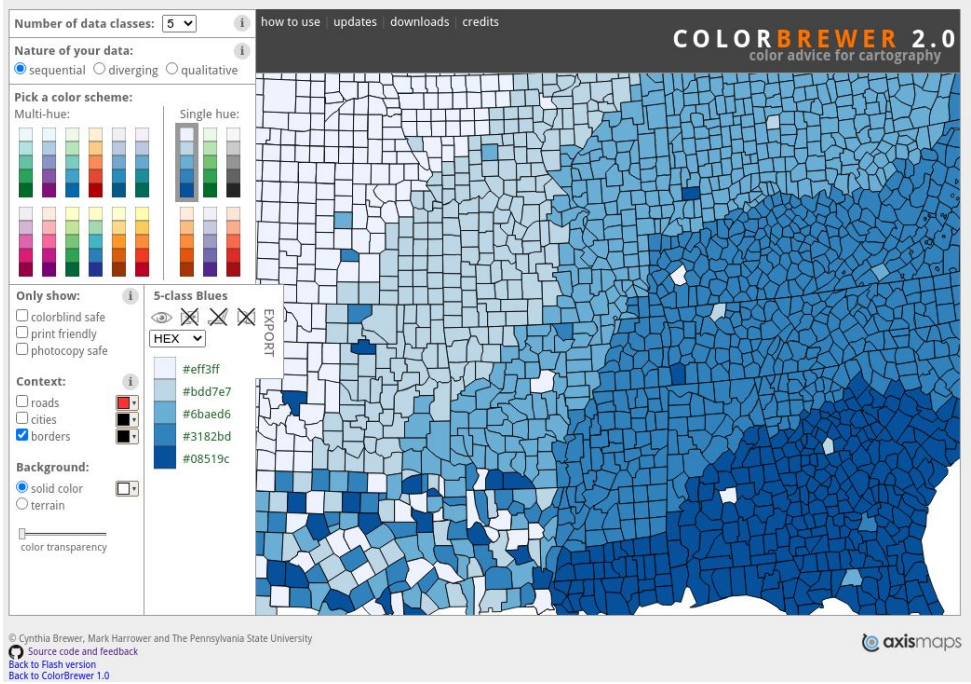


https://colorbrewer2.org

Colorbrewer is a tool developed by carthographers, which know a lot color in maps and visualizations.
This tool allowsyou to get color palettes, depending on the nature of you data (above).

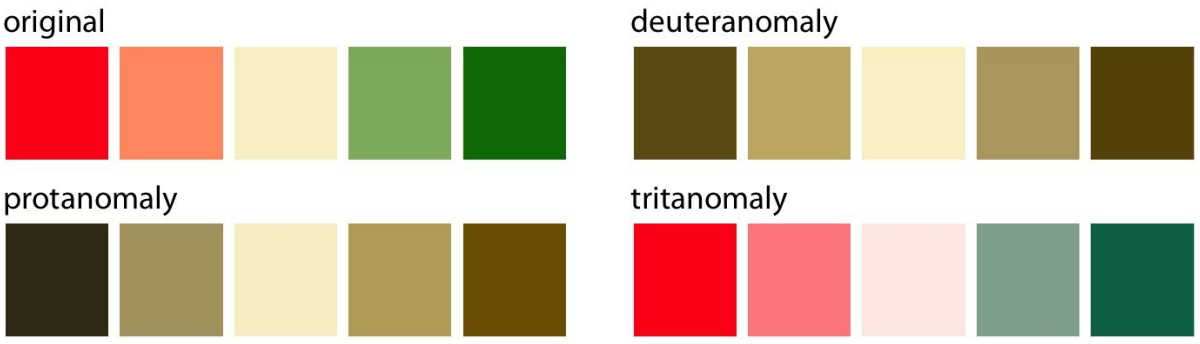
For example, if your data is sequential, clicking above will give you options that you can export as HEX codes.

Notice that you can also use the ‘colorblind safe’ option, which restricts the palette options but it’s designed so that colorblind people can still discriminate the colors you are showing.



https://colorbrewer2.org

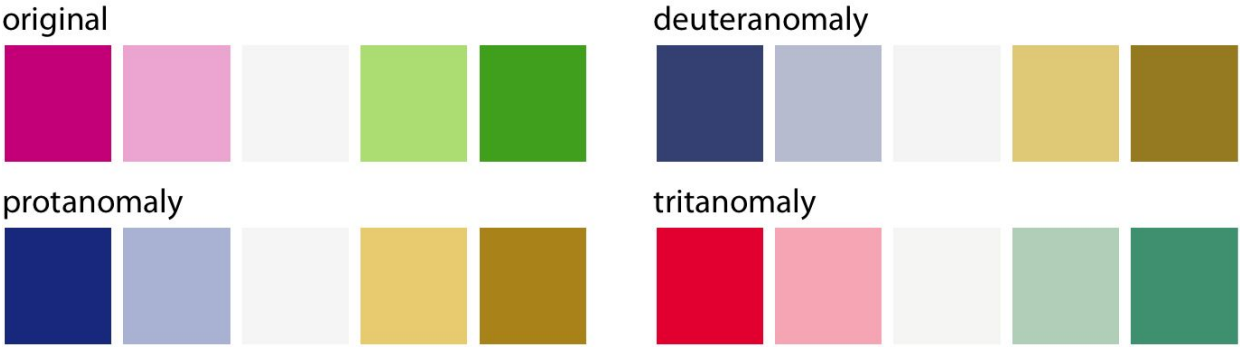
Consider colorblindness



A red–green contrast becomes indistinguishable under red–green color vision deficiency (deuteranomaly or protanomaly) From Wilke (2019)

10 % population have some kind of color anomaly.
You should design visualizations for them

Consider colorblindness



The ColorBrewer PiYG (pink to yellow-green) scale looks like a red–green contrast to people with regular color vision but works for all forms of color-vision deficiency.

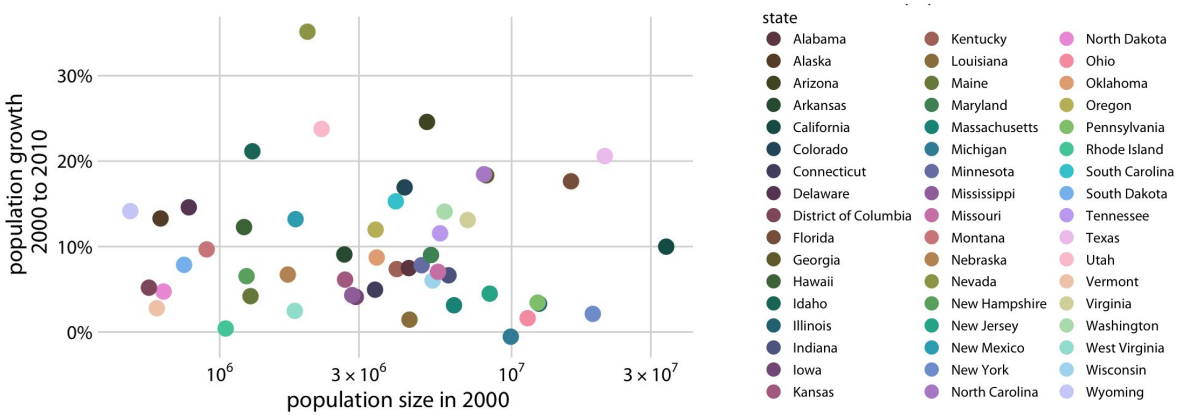
From Wilke (2019)

Try to use colorblind friendly palettes.

In case of doubt, you can also simulate a color deficiency:

https://github.com/DaltonLens/DaltonLens-Python

Common pitfall: encoding too much information



Claus O. Wilke (2019)

Common pitfall: using the wrong color scale

rainbow scale

rainbow converted to grayscale

The jet/rainbow color scale is **NOT a sequential** colormap,

→ our perception of it is NOT linear but **circular!**

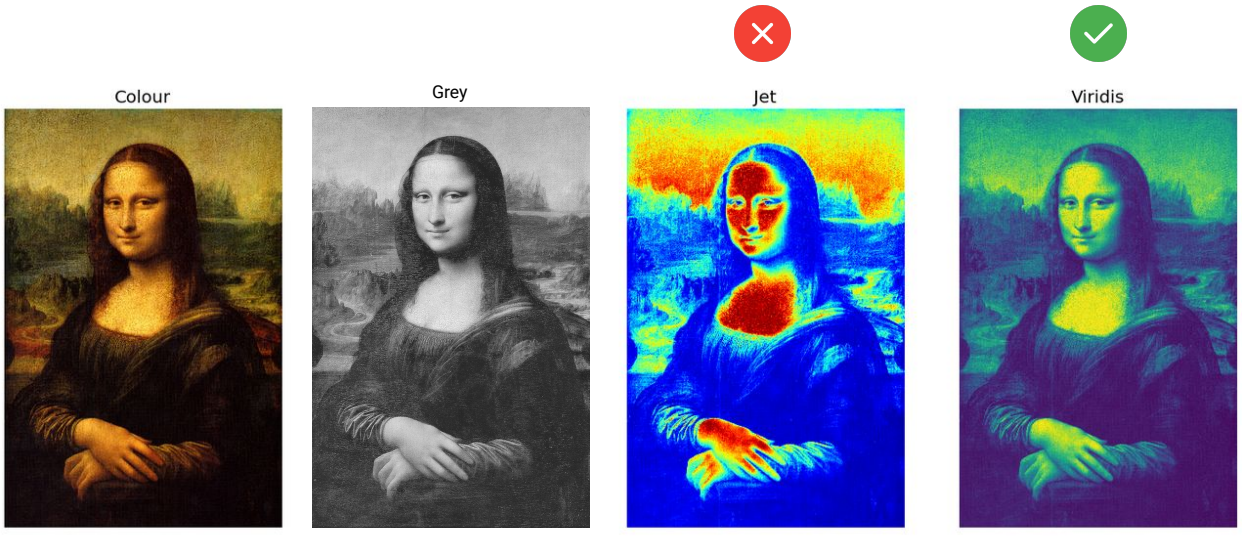
So do not use it for data that is not circular.

We perceived the rainbow / jet color scale as not linear!

Differences in hue are not related to difference in light intensity. This becomes clear when we render a grayscale version of it. We tend to see the yellow green part as lighter as the blue.

So we cannot map increasing or decreasing data to hue! DO NOT USE the rainbow / jet color scale.
It's not a default in matplotlib anymore!

Common pitfall: using the wrong color scale



Exercise 2: which visualization should I use?

- Work in paris, develop in your fork
- Do only 1 exercise (A - E)
- Goal: a visualization that is *publication-ready*
- Do a Merge request when ready.
- We'll review your visualizations together and comment them together

Have your cheatsheet at hand!: https://matplotlib.org/cheatsheets/

Extra-Material (from ASPP-2021)

- **Scales & projections** (**notebook**). Tutorial on different type of scales (log scale, symlog scale, logit scale) and projections (polar, 3D, geographic).
- **Animation** (**notebook**). Animation with matplotlib can be created very easily using the animation framework. This notebook shows how to create an animation and save it as a movie.

Further Resources

At the implementation level (code, galleries and how-tos):

- **Seaborn library**, a library for statistical data visualization. Very recommended as a next step in your learning journey.
- **Matplotlib Cheatsheets**, Nicolas P. Rougier (2020)
- **Scientific Visualization – Python & Matplotlib**, open-source book from Nicolas P. Rougier (2021)
- **Python Graph Gallery**, Yan Holtz (2017)
- **Matplotlib Gallery**, Matplotlib team

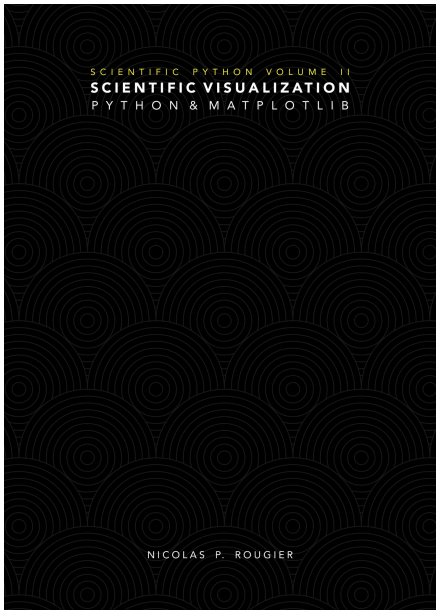
At the conceptual level :

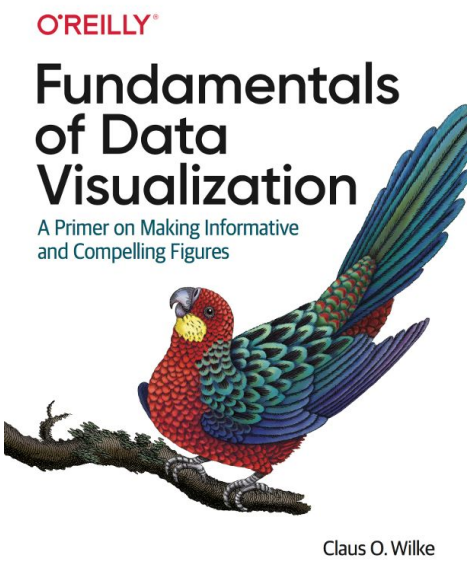
- **Ten simple rules for better figures**, Nicolas P. Rougier, Michael Droettboom, Philip E. Bourne (2014)
- **Fundamentals of Data Visualization**, book by Claus O. Wilke (2019)
- **Chart Suggestions - a though-starter** by A. Abelas.
- **Data Visualization Catalogue**
- **Edward Tufte**'s series of books: The Visual Display of Quantitative Information (1983), Envisioning Information (1990), Beautiful Evidence (2006), etc.

Interactive visualizations:

- **Widgets in Jupyter notebook**
- **Plotly**

Selected further resources



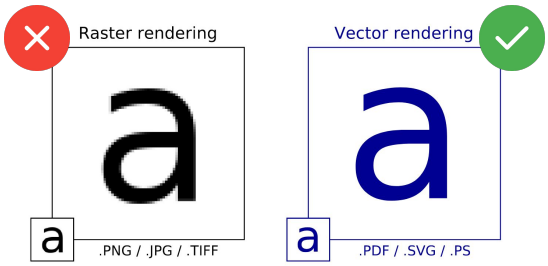


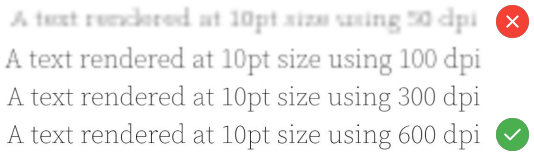
Resources:
https://github.com/rougier/2021-Dataviz
https://github.com/rougier/2021-Dataviz/blob/master/Lesson/dataviz.pdf
https://hal.inria.fr/hal-03427242/document
https://datavizcatalogue.com

Some extra tips

Exporting a figure: vector format!

As a rule of thumb: Save in vector format and with enough DPI (dots per inch)





Bitmap formats

PNG: Portable Network Graphics (lossless)
JPG: Joint Photographic Experts Group (lossy)

Vector formats

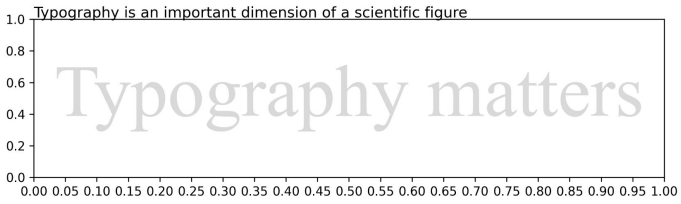
PDF: Portable Document Format
SVG: Scalable Vector Graphics

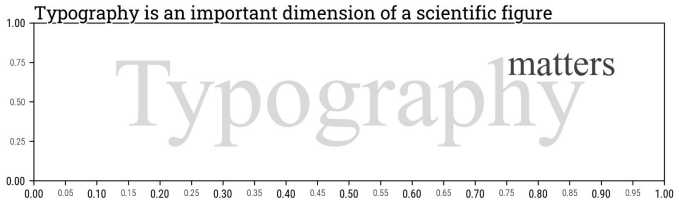
Text rendered in matplotlib and saved using different dpi

Format of a figure: lossy/lossless compression, what is DPI, how to create a figure with text of same size as paper text…
Script to modify a figure that was already done (after review), generic label

Font stack choice

Influence of typography on the perception of a figure. Choose the right font for you.





Serif DejaVuSerif.ttf	Sans DejaVuSans.ttf
Serif RobotoSlab-Regular.ttf	Sans RobotoCondensed-Regular.ttf
Serif SourceSerifPro-Regular.otf	Sans SourceSansPro-Regular.ttf
Monospace DejaVuSansMono.ttf	*Cursive* Apple Chancery.ttf
Monospace RobotoMono-Regular.ttf	*Cursive* Merienda-Regular.ttf
Monospace SourceCodePro-Regular.ttf	*Cursive* ITC Zapf Chancery.ttf