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CIUDAD DE MÉXICO

SECRETARÍA DE EDUCACIÓN, CIENCIA,
TECNOLOGÍA E INNOVACIÓN



Best practices in data visualization

Guillermo Aguilar & Carlos Cernuda

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

Mexico City, ASPP LATAM 2023

Plan

18:00 Principles of data visualization

Hands-on Exercise 1: mastering matplotlib

19:00

Tomorrow

09:00 (cont). Exercise 1

Types of visualizations - Use of color - Common pitfalls

Hands-on Exercise 2: which visualization should I use?

+ Review of your solutions as PR

10:30 END

(*) Hands-on Exercise 3: images

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

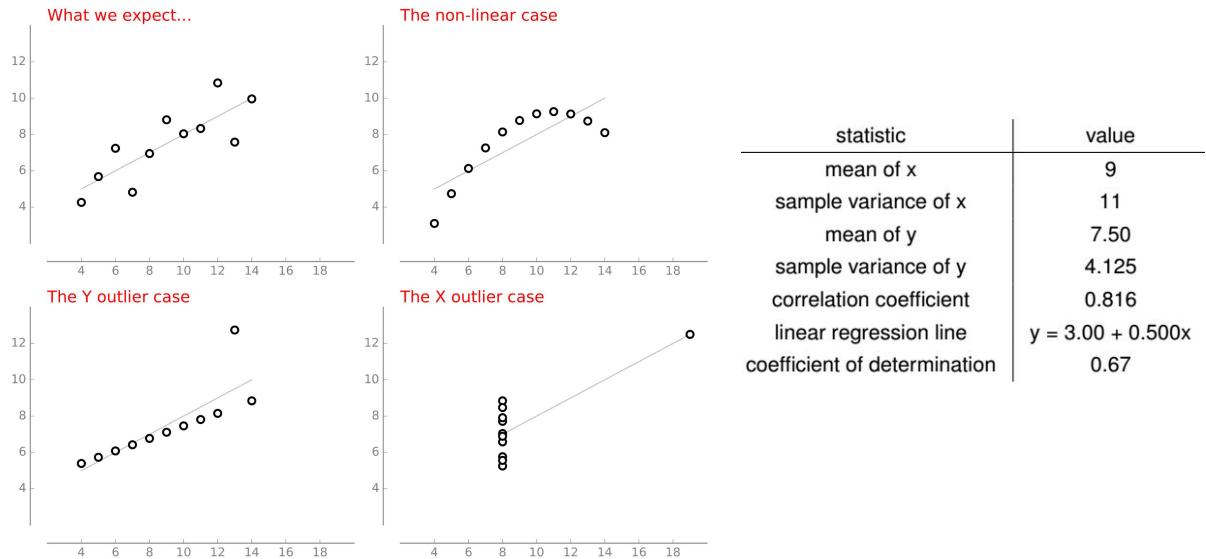
statistic	value
mean of x	9
sample variance of x	11
mean of y	7.50
sample variance of y	4.125
correlation coefficient	0.816
linear regression line	$y = 3.00 + 0.500x$
coefficient of determination	0.67

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. So for a computer or an algorithm that only looks at these numbers, these four datasets would be identical.

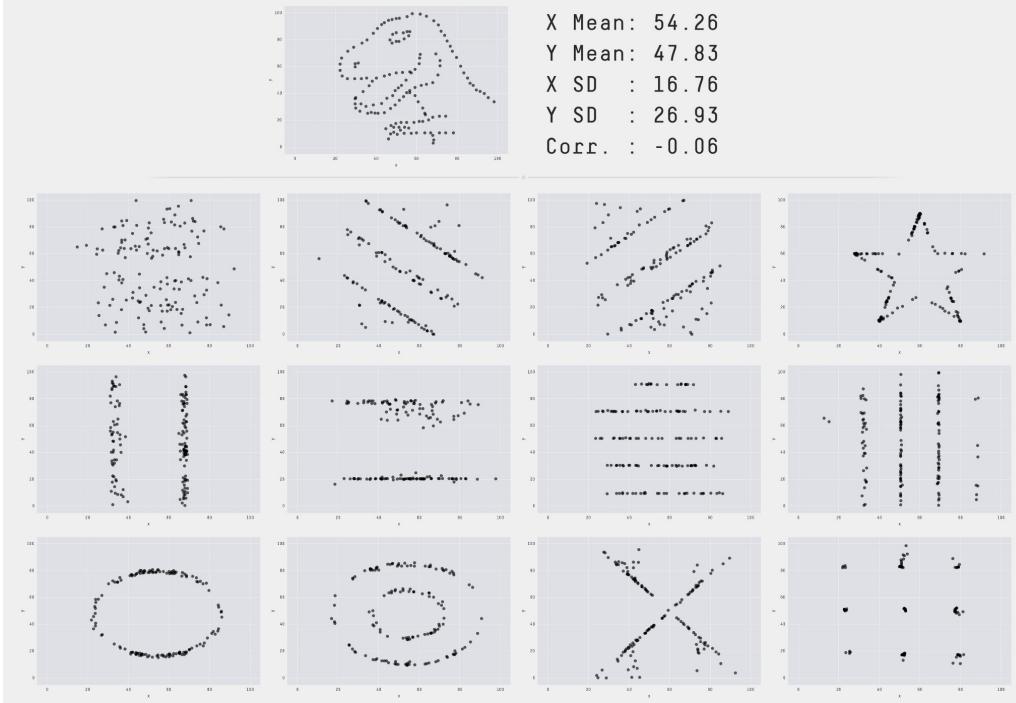
Classical example: Anscombe's quartet



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>

And you will read this last

You will read this first

And you will read this

Then this one

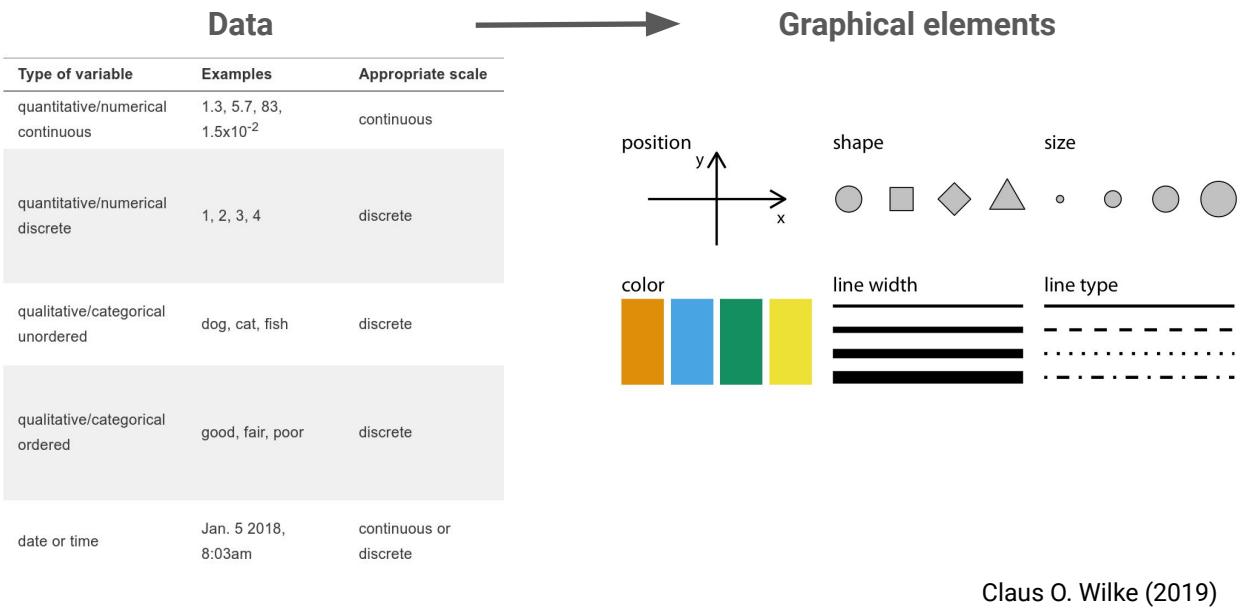
So although you might think that numbers are just numbers and you just need statistics, that's not the whole story.

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 this 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 on data visualization: the **mapping from..**



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, 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. You probably know that a continuous variable can be assigned to x and y axis.

But for example a categorical variable, dog, cat, fish, cannot be assigned to say, 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.

Editorial

Ten Simple Rules for Better Figures

Nicolas P. Rougier^{1,2,3*}, Michael Droettboom⁴, Philip E. Bourne⁵

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 of 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

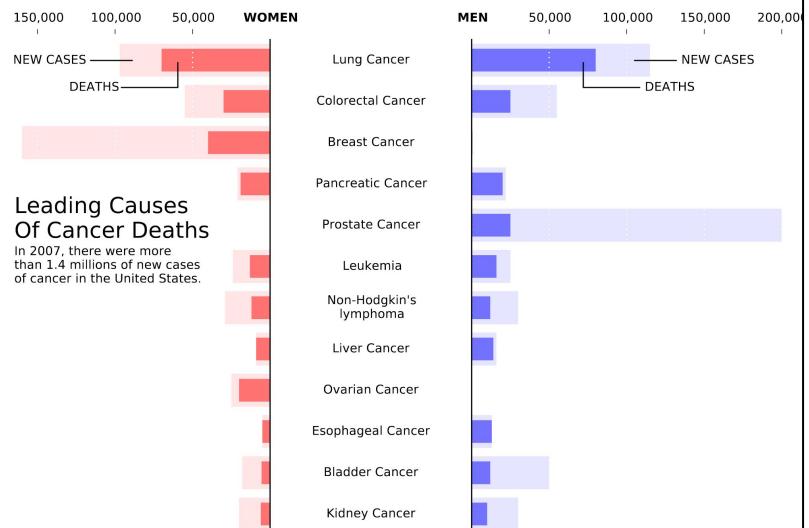
Complexity
+
-

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.

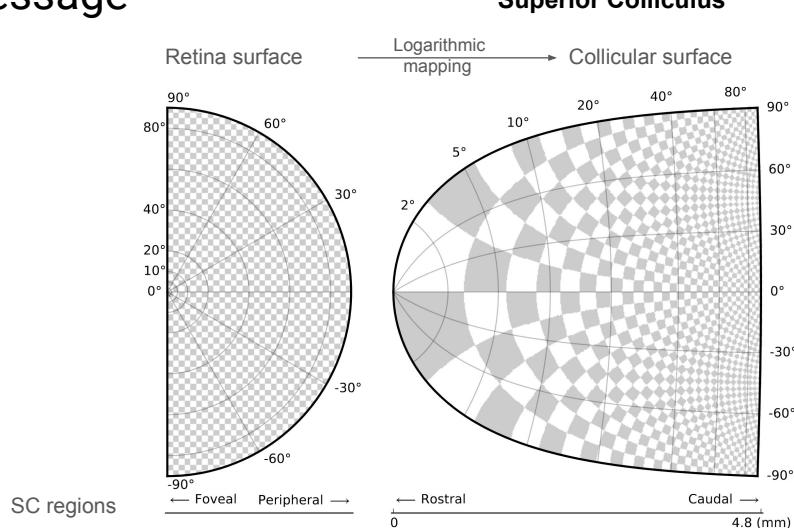
Focus of this figure:

- Audience: general public
- Qualitative (you can't tell the exact numbers)
- Main message in the center: cancer
- New cases always higher than deaths and deaths part of cases, so we 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 as 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

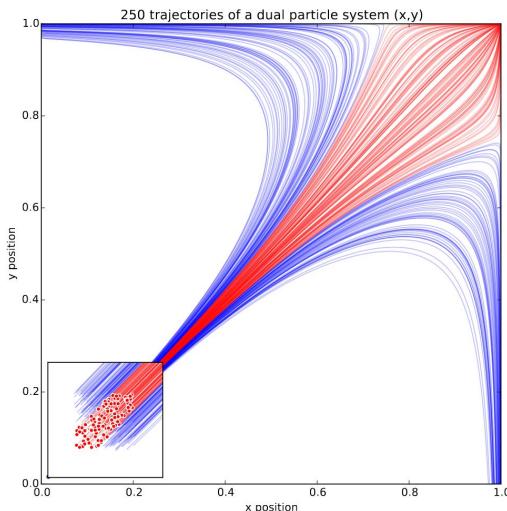
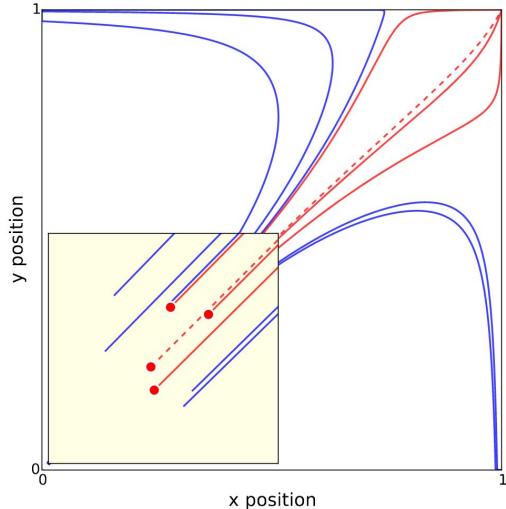


Figure for a Talk



Each media is different. Seeing a figure in a printed poster on a conference is different than having it digitally in a computer, and different than 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 used to 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

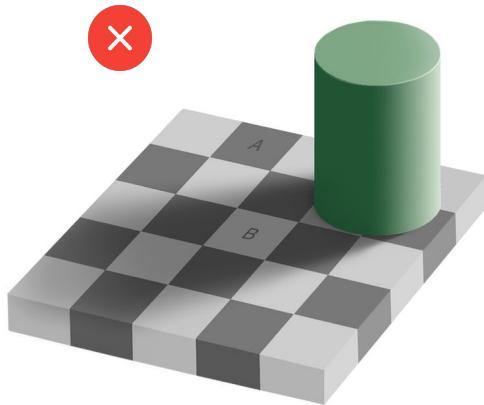
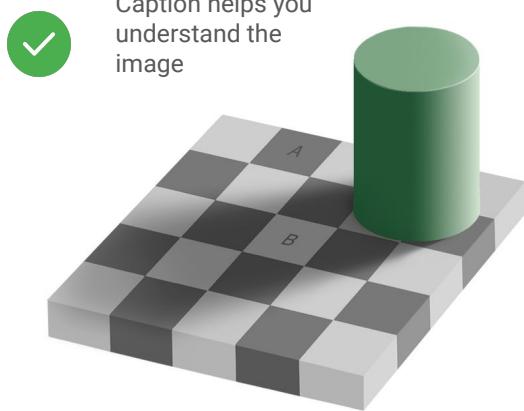


Figure 1. Optical illusion



Caption helps you understand the image

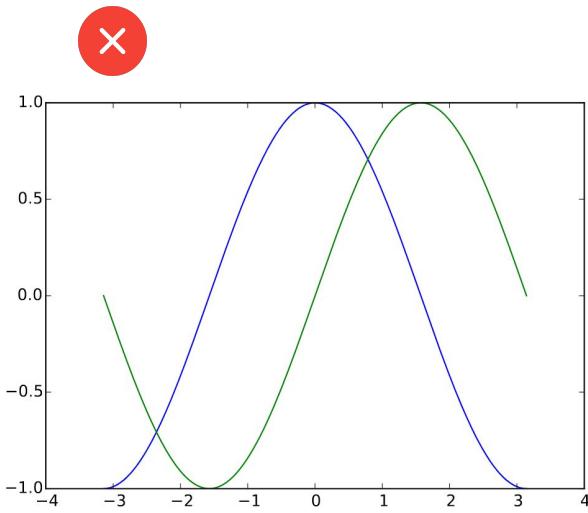
Figure 1. A and B patches are actually the same color even though we perceive them at being different color

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

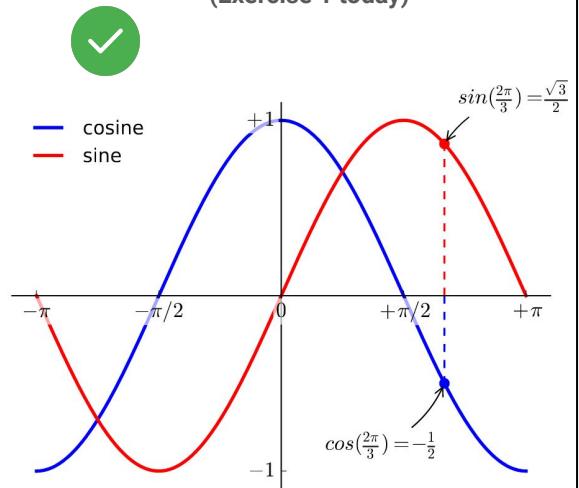
Be concrete and explicit in the caption. Describe all what is going on, if there are different panels, colors, line types, you should mention what they all mean.

5) Do not trust the defaults

Matplotlib defaults



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



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.

6) Use color effectively → [more on this later](#)

7) Do not mislead the reader



Using full range bars shows a more realistic comparison among them

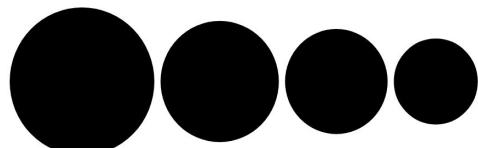


Relative size using full range

Relative size using partial range



Using the **disc area** shows a more proportional sizes

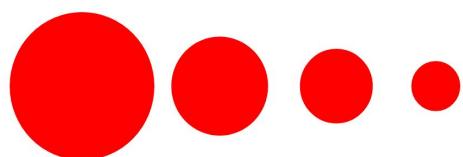


Relative size using disc area

Relative size using disc radius



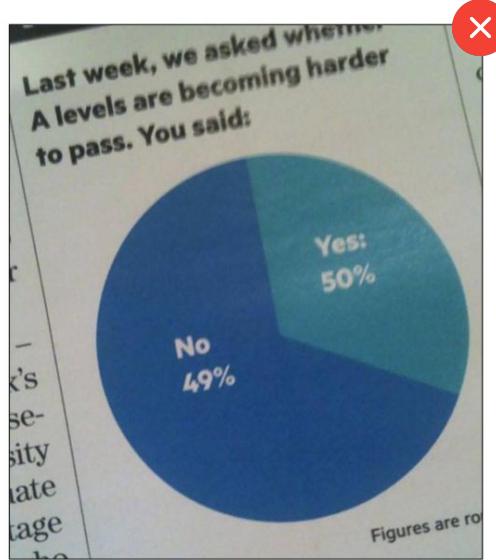
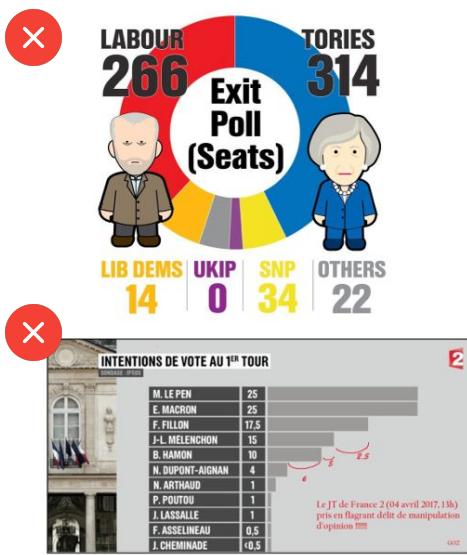
Using **partial range bars** misleads the reader to think the difference is bigger



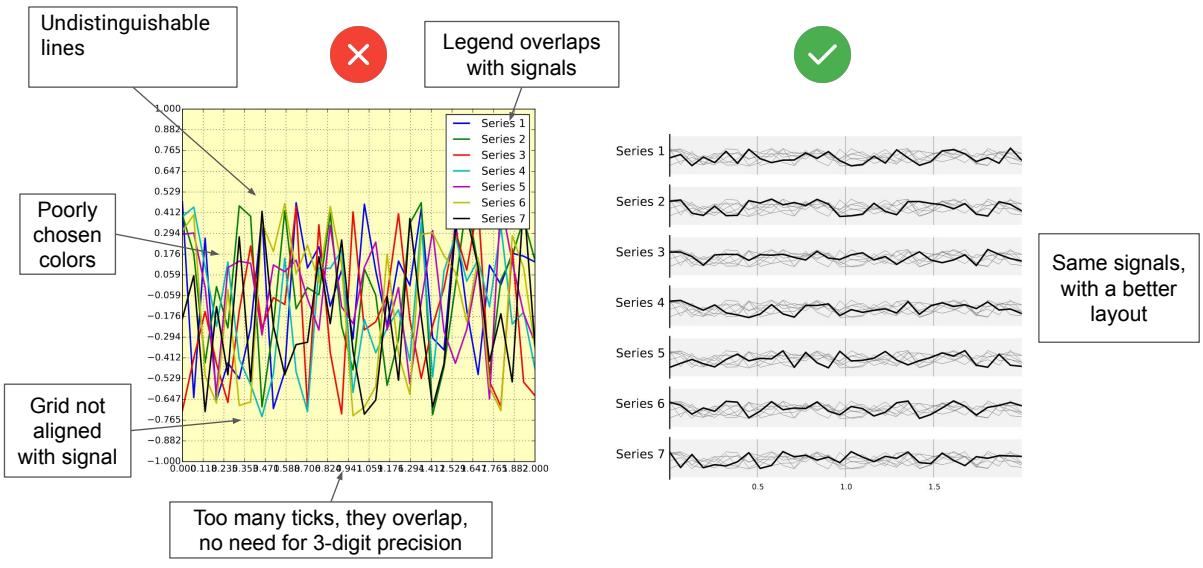
Using the **disc radius** misleads the reader to think the difference is bigger

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.



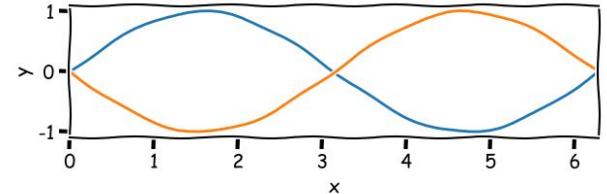
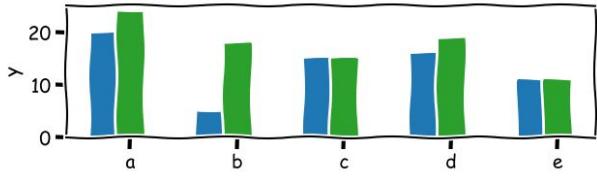
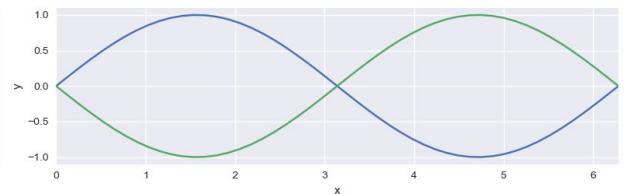
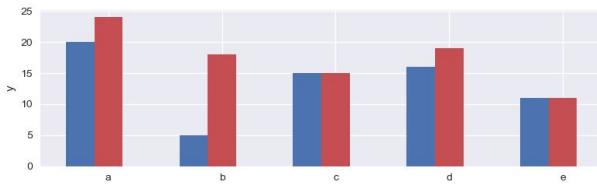
8) Avoid chartjunk



Chartjunk refers to all the unnecessary or confusing visual elements found in a figure that 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.

9) Message trumps beauty:

To convey an idea, sometimes a 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

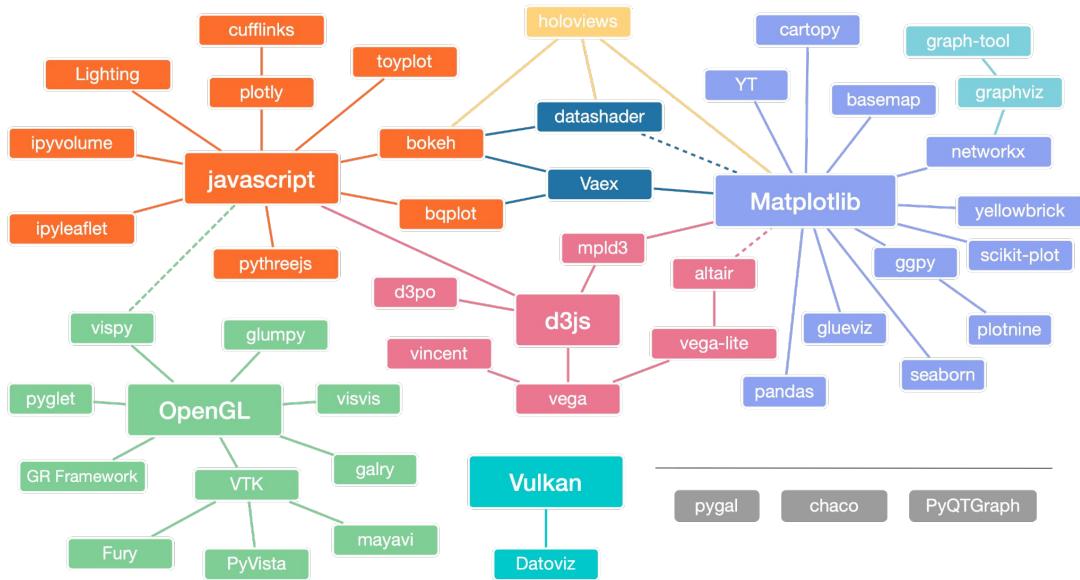


Tikz for scripted vector art



And many, many, many others...

Overview of visualization libraries



A jungle of visualization libraries. Here we will focus on the most used one:
matplotlib.

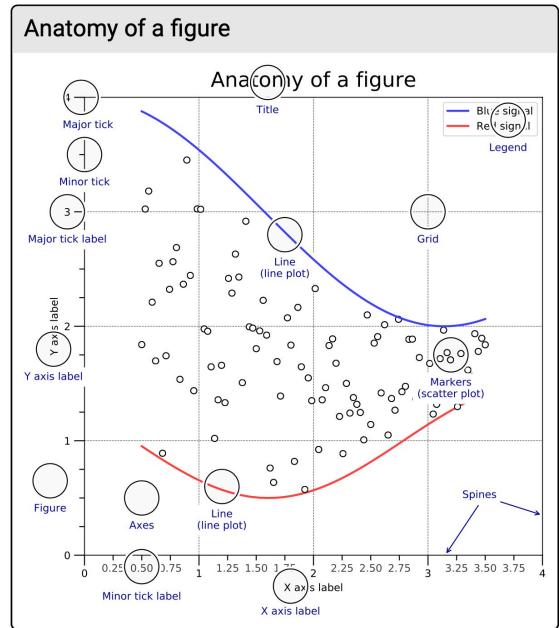
After today's session feel free to expand your knowledge of other libraries, seaborn, plotnine, etc. Check out the Repo's README for links to further resources.

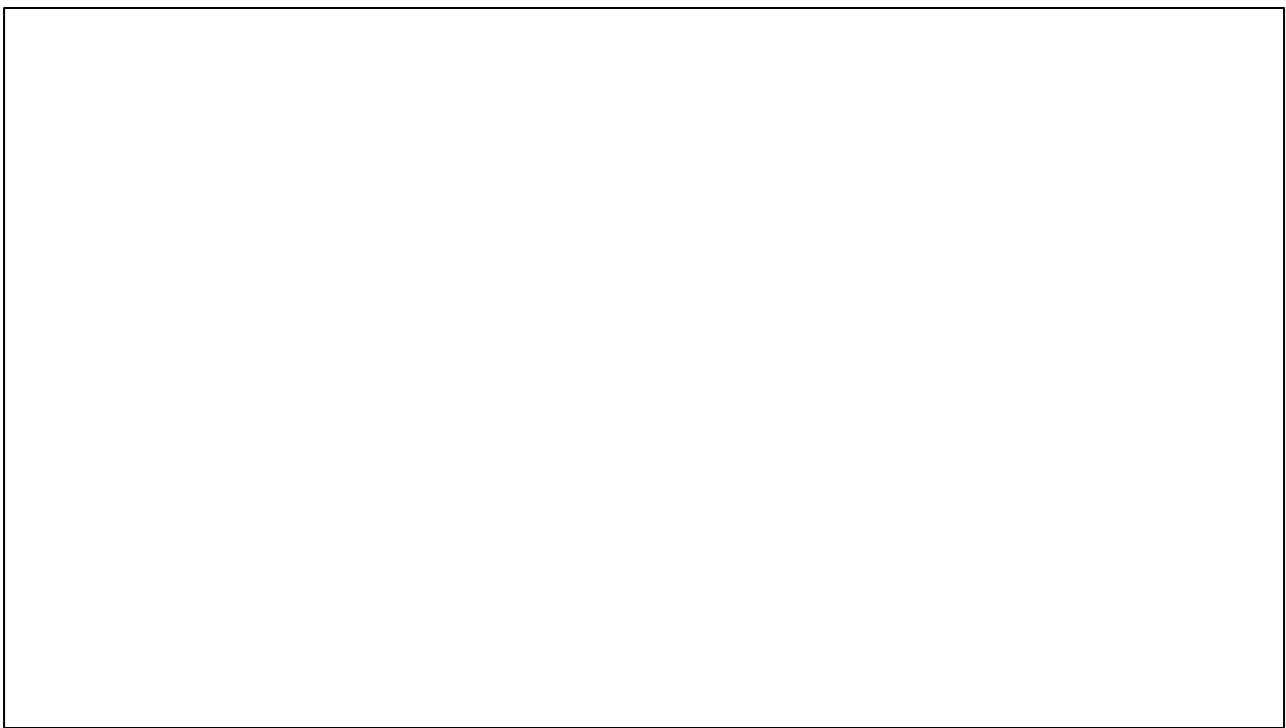
Time for hands-on exercises!

Exercise 1: Mastering matplotlib

Have your cheatsheet at hand!:

<https://matplotlib.org/cheatsheets/>





An useful tool:

datavizcatalogue.com

The Data Visualisation Catalogue

About • Blog • Shop • Resources

What do you want to show?

Here you can find a list of charts categorised by their data visualization functions or by what you want a chart to communicate to an audience. While the allocation of each chart into specific functions isn't a perfect system, it still works as a useful guide for selecting chart based on your analysis or communication needs.

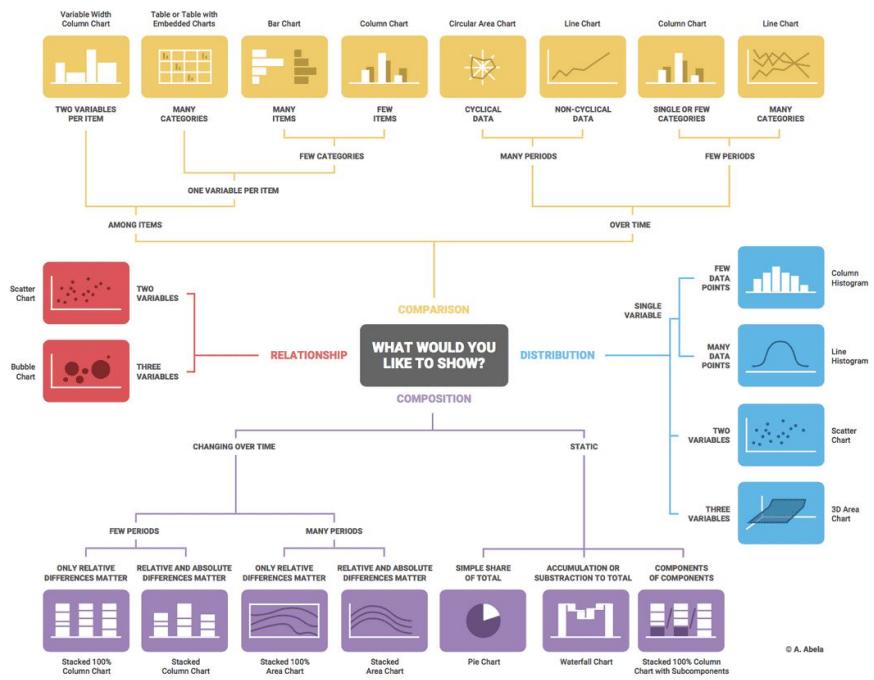


<https://datavizcatalogue.com/search.html>

<https://datavizcatalogue.com/blog/chart-selection-guide/>

Another,
older tool

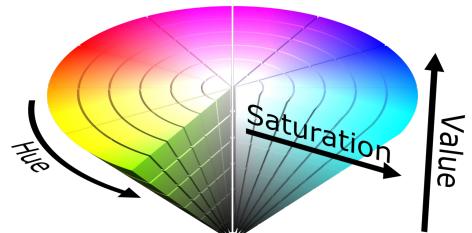
Chart suggestions by Abela



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

Colormaps

API

`plt.get_cmap(name)`

Uniform



Sequential



Diverging

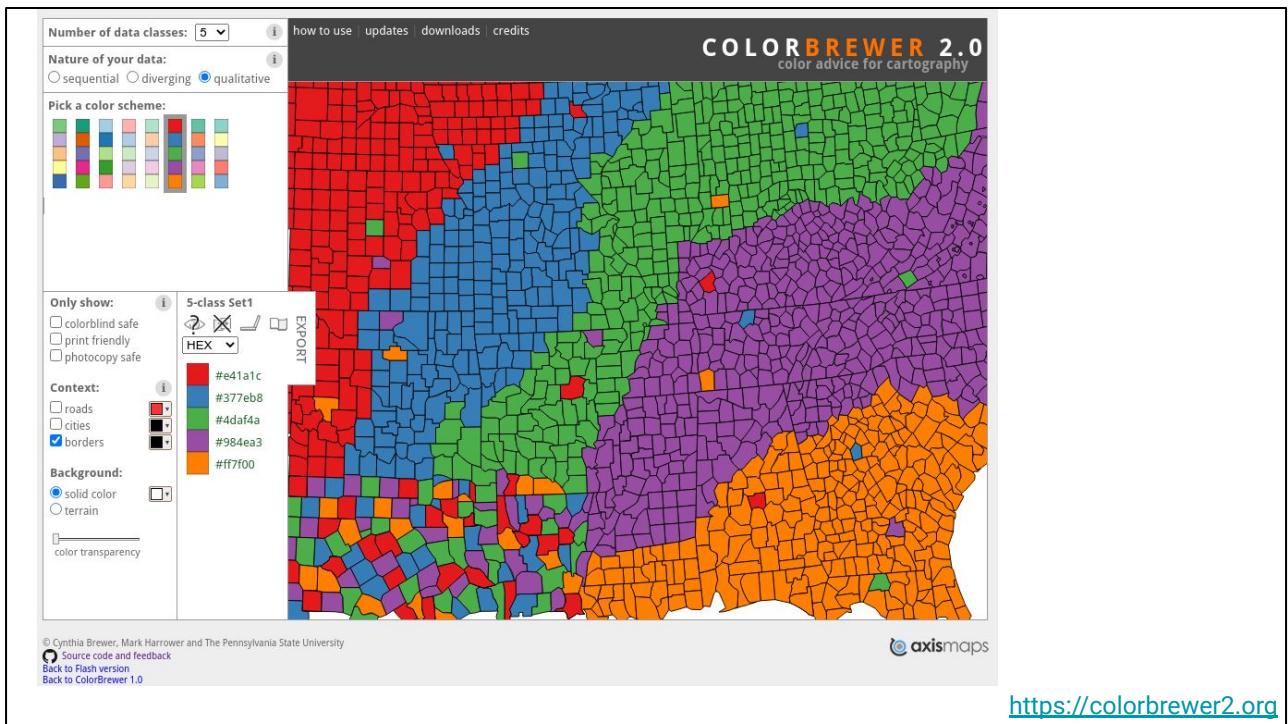


Qualitative



Cyclic





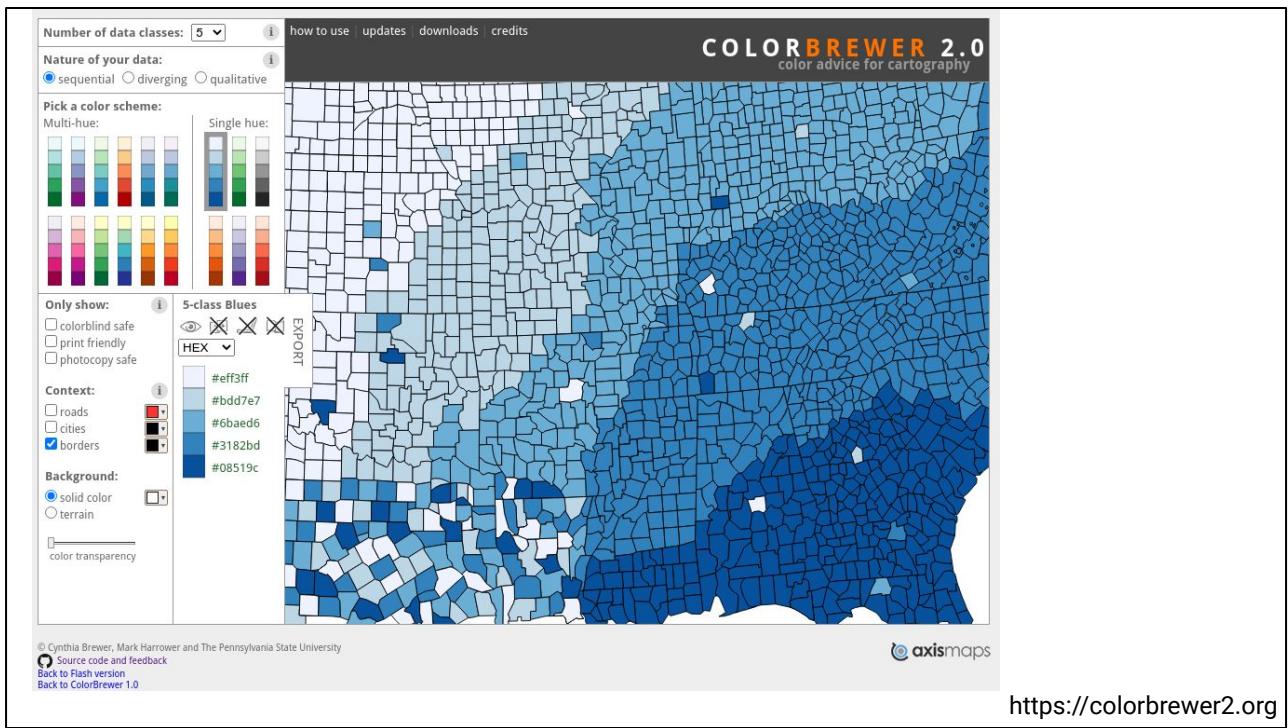
<https://colorbrewer2.org>

Colorbrewer is a tool developed by cartographers, which know a lot color in maps and visualizations.

This tool allows you to get color palettes, depending on the nature of your 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.



Consider colorblindness

original



deuteranomaly



protanomaly



tritanomaly



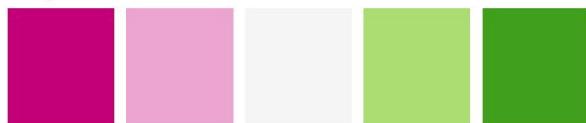
A red–green contrast becomes indistinguishable under red–green color vision deficiency (deuteranomaly or protanomaly) From Wilke (2019)

10 % population have some kind of color anomaly.

You should design visualizations for them

Consider colorblindness

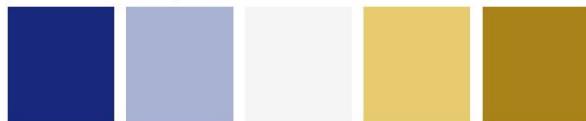
original



deuteranomaly



protanomaly



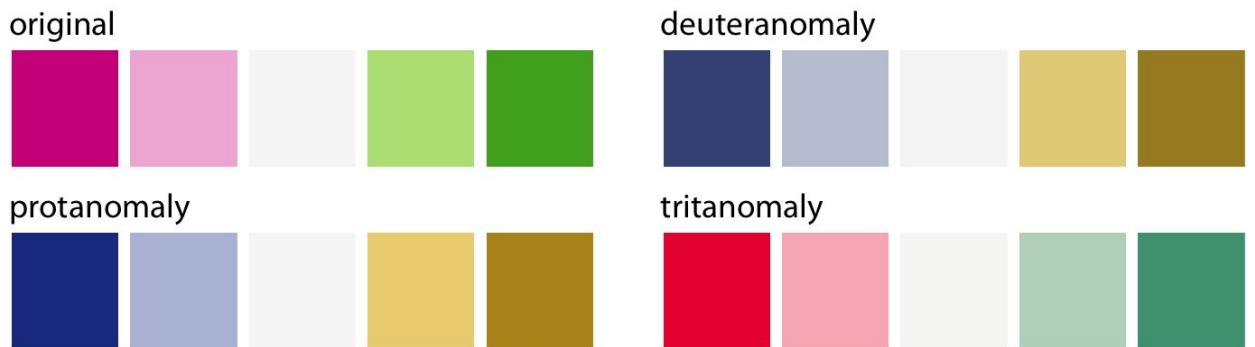
tritanomaly



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)

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.

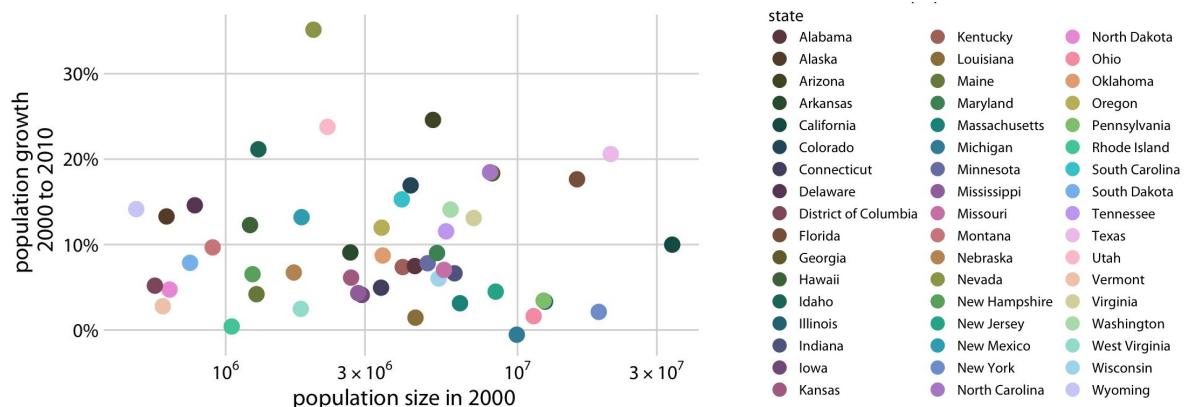
From Wilke (2019)

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 - F)
- 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

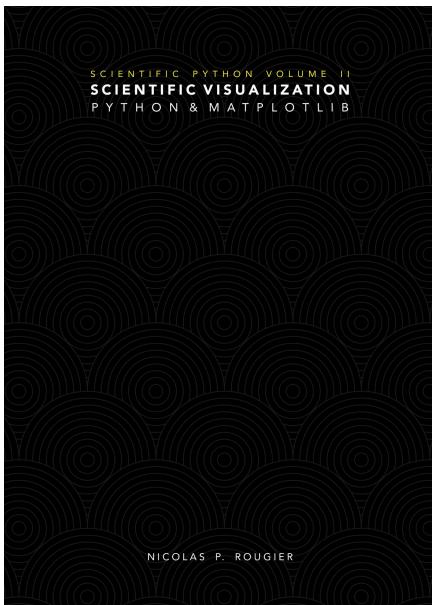
At the conceptual level :

- [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 thought-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](#)

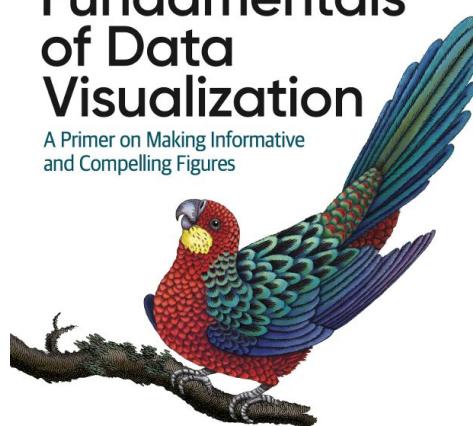
Selected further resources



O'REILLY®

Fundamentals of Data Visualization

A Primer on Making Informative
and Compelling Figures



Claus O. Wilke

Resources:

<https://github.com/rougier/2021-Dataviz>

<https://github.com/rougier/2021-Dataviz/blob/master/Lesson/dataviz.pdf>

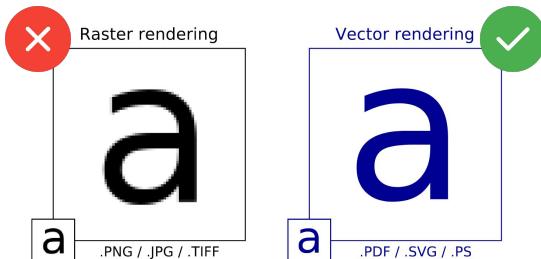
<https://hal.inria.fr/hal-03427242/document>

<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

A text rendered at 10pt size using 50 dpi X
A text rendered at 10pt size using 100 dpi
A text rendered at 10pt size using 300 dpi
A text rendered at 10pt size using 600 dpi ✓

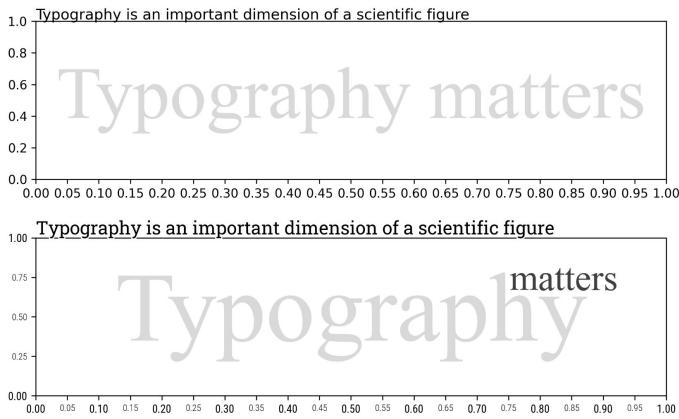
Text rendered in matplotlib and saved
using different dpi

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

Serif

RobotoSlab-Regular.ttf

Serif

SourceSerifPro-Regular.otf

Sans

DejaVuSans.ttf

Sans

RobotoCondensed-Regular.ttf

Sans

SourceSansPro-Regular.ttf

Monospace

DejaVuSansMono.ttf

Monospace

RobotoMono-Regular.ttf

Monospace

SourceCodePro-Regular.ttf

Cursive

Apple Chancery.ttf

Cursive

Merienda-Regular.ttf

Cursive

ITC Zapf Chancery.ttf