A 2h30 crash-course on

Scientific visualisation

Nicolas P. Rougier

Advanced Scientific Programming in Python, University of Reading, 2016

What is scientific visualisation ?

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

Visualisation in Scientific Computing, NSF report, 1987

“For example, about 50 percent of the cerebral cortex of primates is devoted exclusively to visual processing, and the estimated territory for humans is nearly comparable.”

The MIT Encyclopedia of the Cognitive Sciences

Anscombe's quartet, 1973

The purpose of computing is insight, not numbers
Richard Hamming, 1962

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

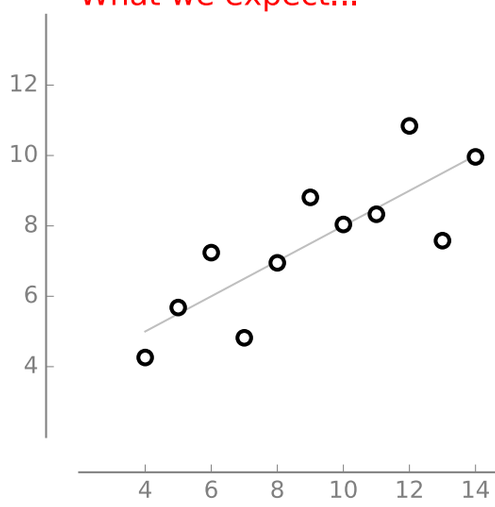
What is **common** to these data sets?

Mean of x:	9
Sample variance of x:	11
Mean of y:	7.50
Sample variance of y:	4.12
Linear regression:	y=3.00+0.500*x
R squared:	0.666
p value	0.0021

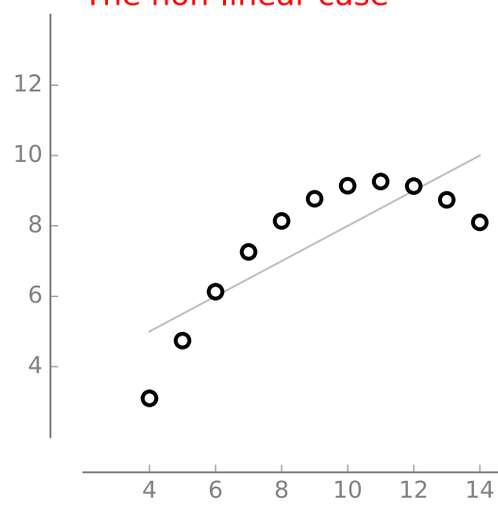
But having a **closer look** at the data…

Anscombe's quartet, 1973

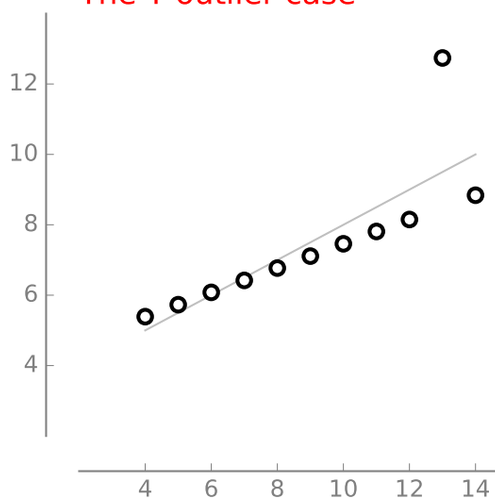
What we expect...



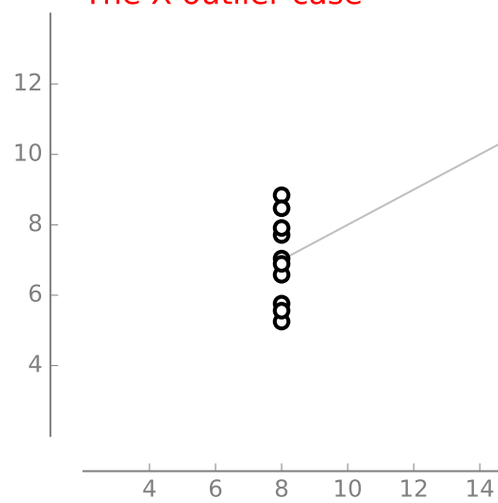
The non-linear case



The Y outlier case



The X outlier case



*"A computer should make both calculations **and** graphs"*

Francis Anscombe (1918-2001)

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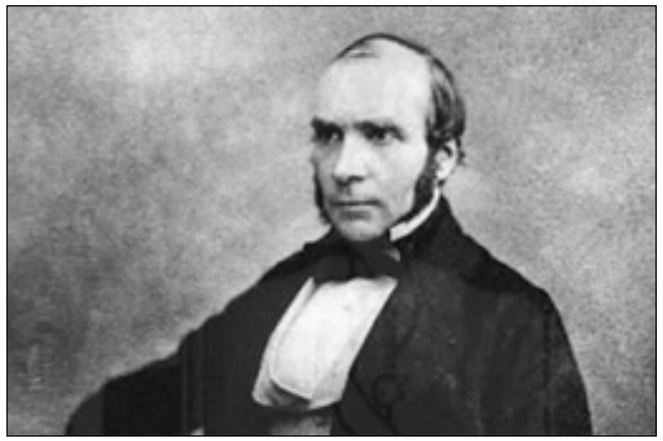
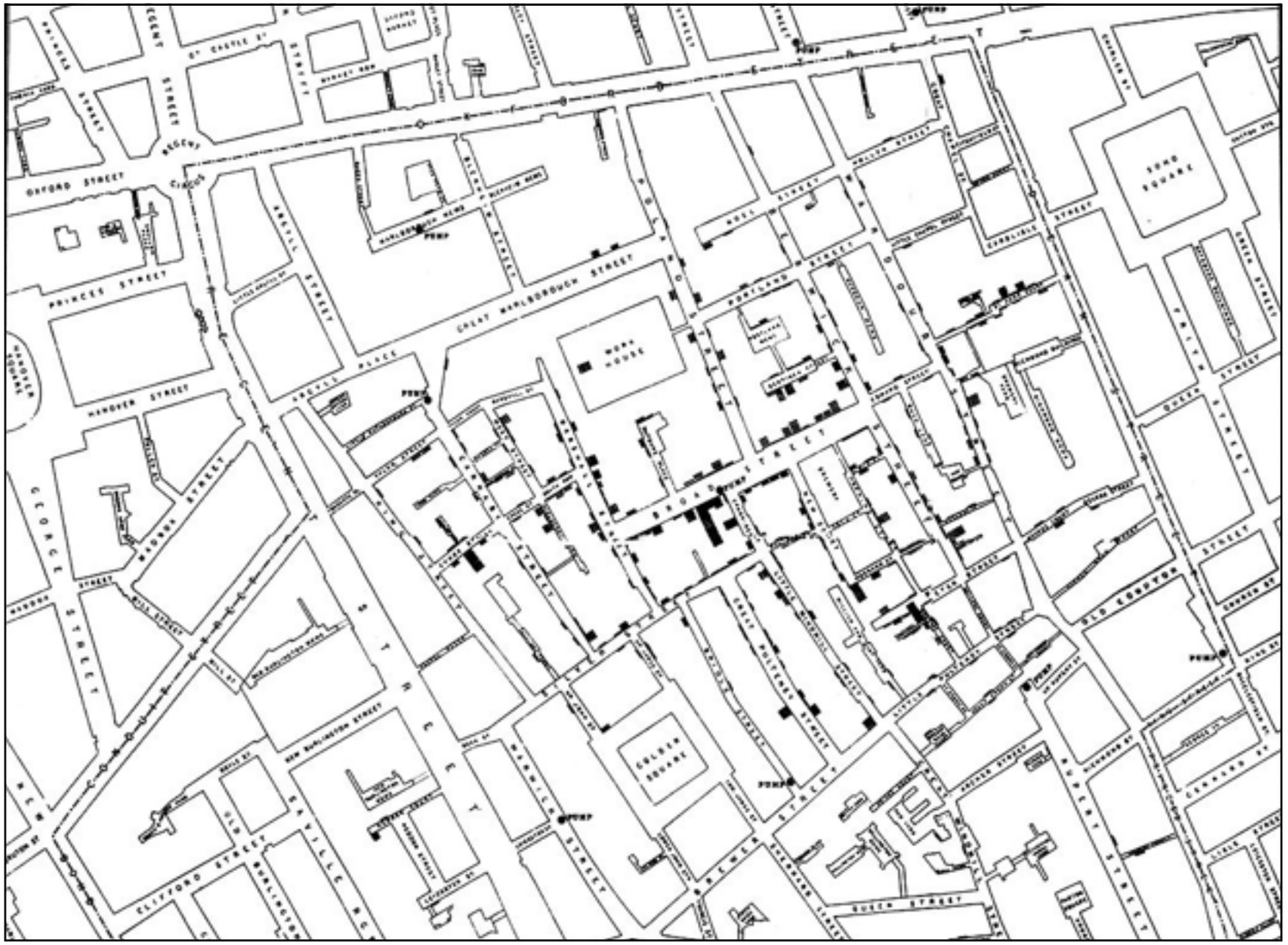
Cholera epidemic, London, 1854

The most terrible outbreak of cholera which ever occurred in this kingdom (J. Snow)

John Snow (1813-1858)





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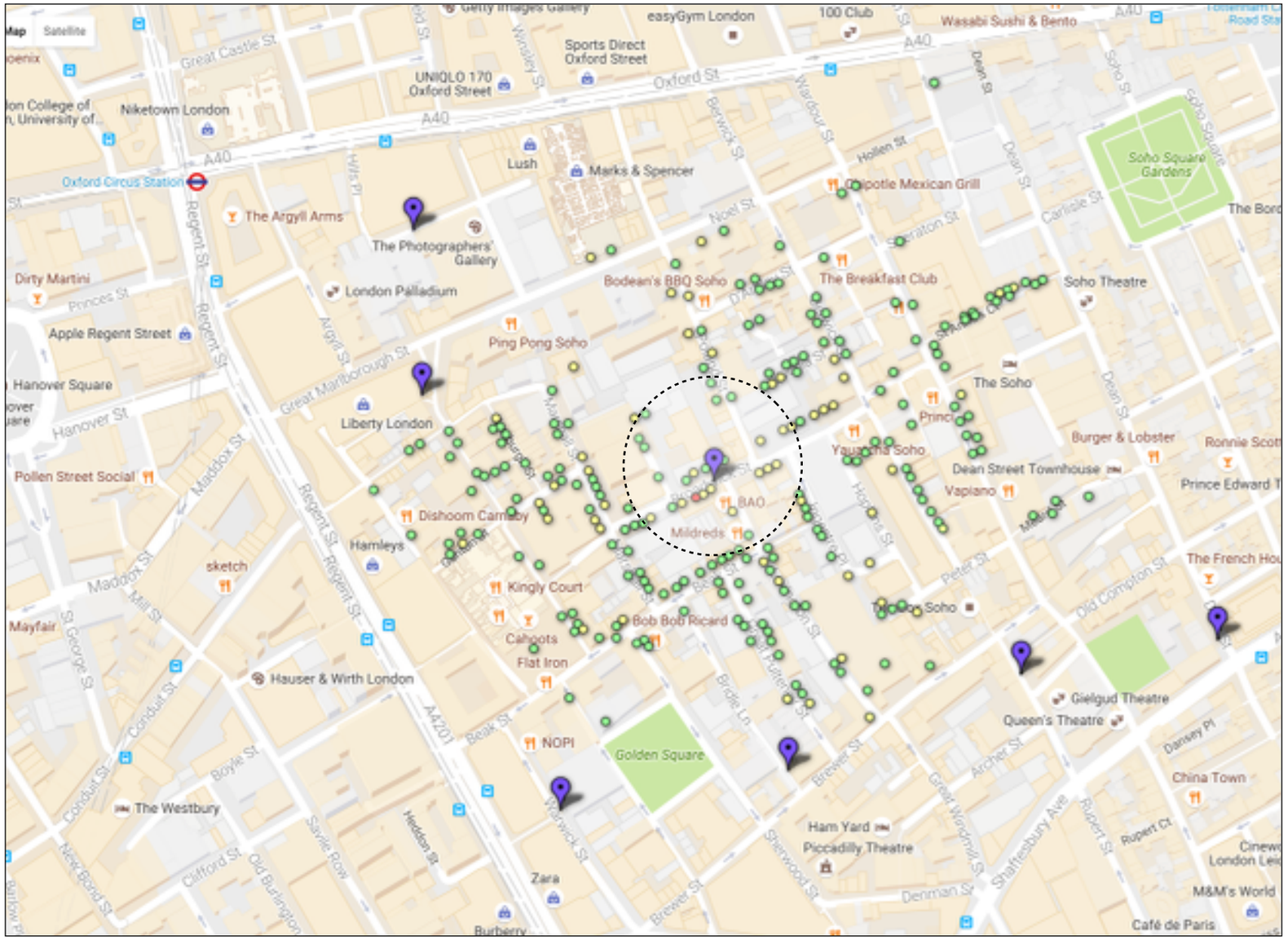
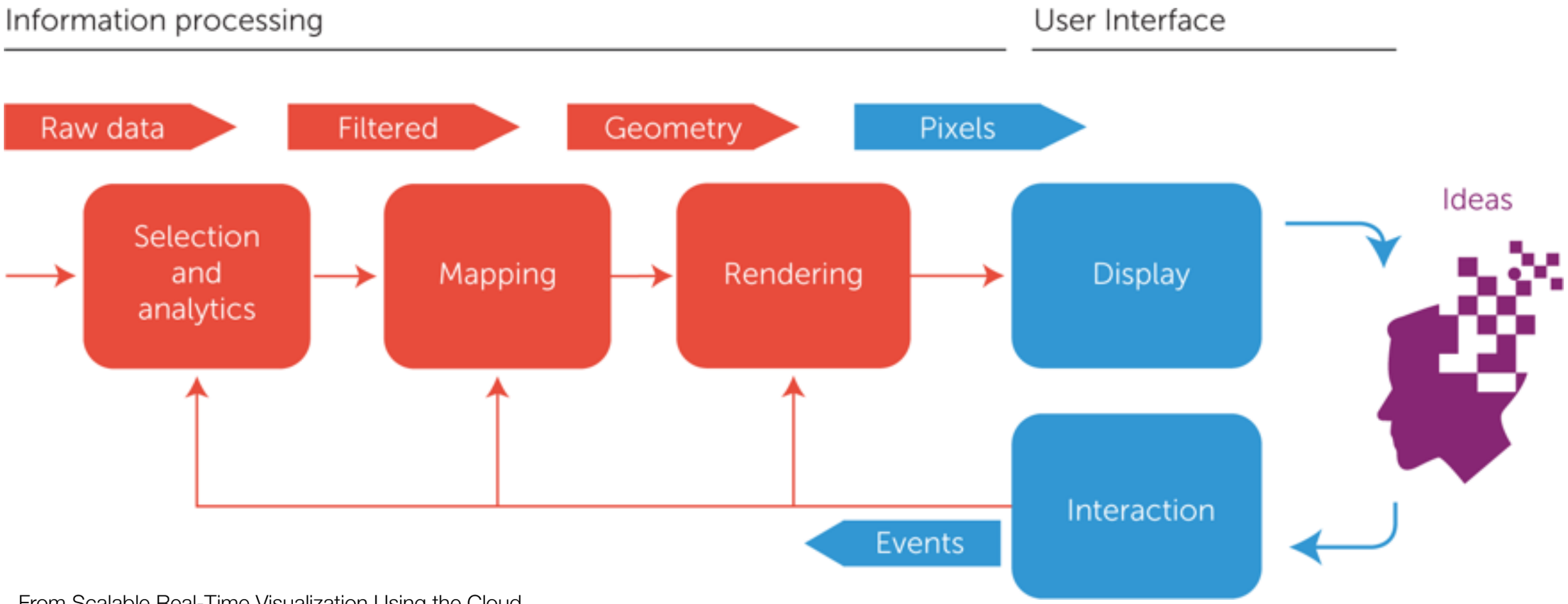


Jon Snow (no connection at all)

The visualisation pipeline



From Scalable Real-Time Visualization Using the Cloud
Issue No.06 - Nov.-Dec. (2015 vol.2)
Nick Holliman , Newcastle University, UK
Paul Watson , Newcastle University, UK
DOI Bookmark: http://doi.ieeecomputersociety.org/10.1109/MCC.2015.131

Data type

Quantitative vs. Categorical Data: A Difference Worth Knowing (S.Few)

Quantitative → values or observations that can be measured

- Continuous *(e.g. temperature)*
- Discrete *(e.g. number of inhabitants)*

Categorical → values or observations that can be sorted into groups or categories

- Nominal *(e.g. nationality)*
- Ordinal *(e.g. months)*
- Interval *(e.g. age groups)*

Graphical elements

A scientific figure can be fully described by a set of graphic primitives with different attributes:

- Points, markers, lines, areas, …
- Position, color, shape, size, orientation, curvature, …
- Helpers, text, axis, ticks, …
- Interaction, animation, …

But who want to describe each individual elements? Describing a figure in terms of such graphic primitives would be a very tedious and complex task.

This is exactly where visualization libraries are useful because they will automatize most of the work (more or less depending on the library).

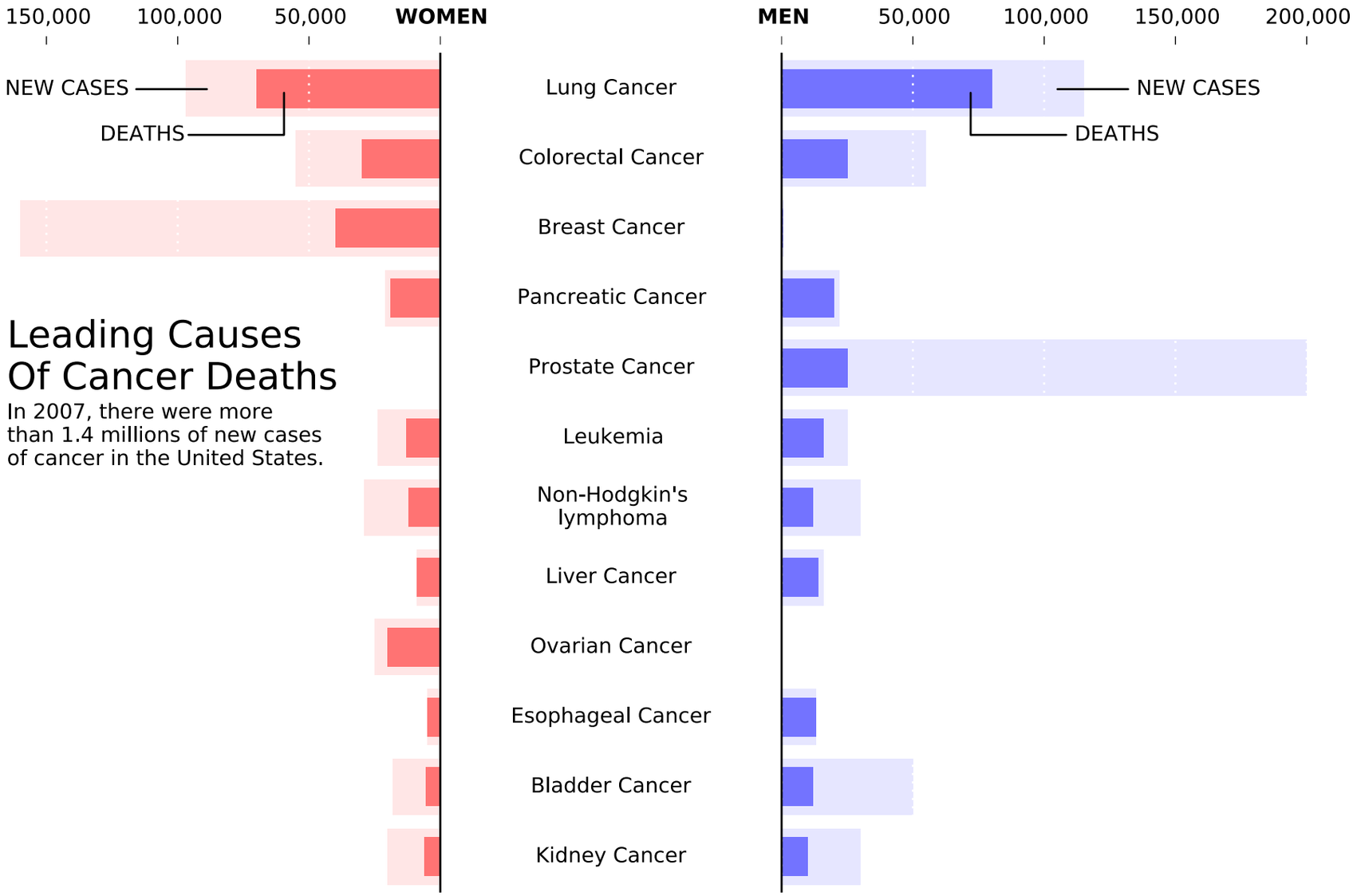
Visualization type

Data Visualisation catalogue by S. Rebecca

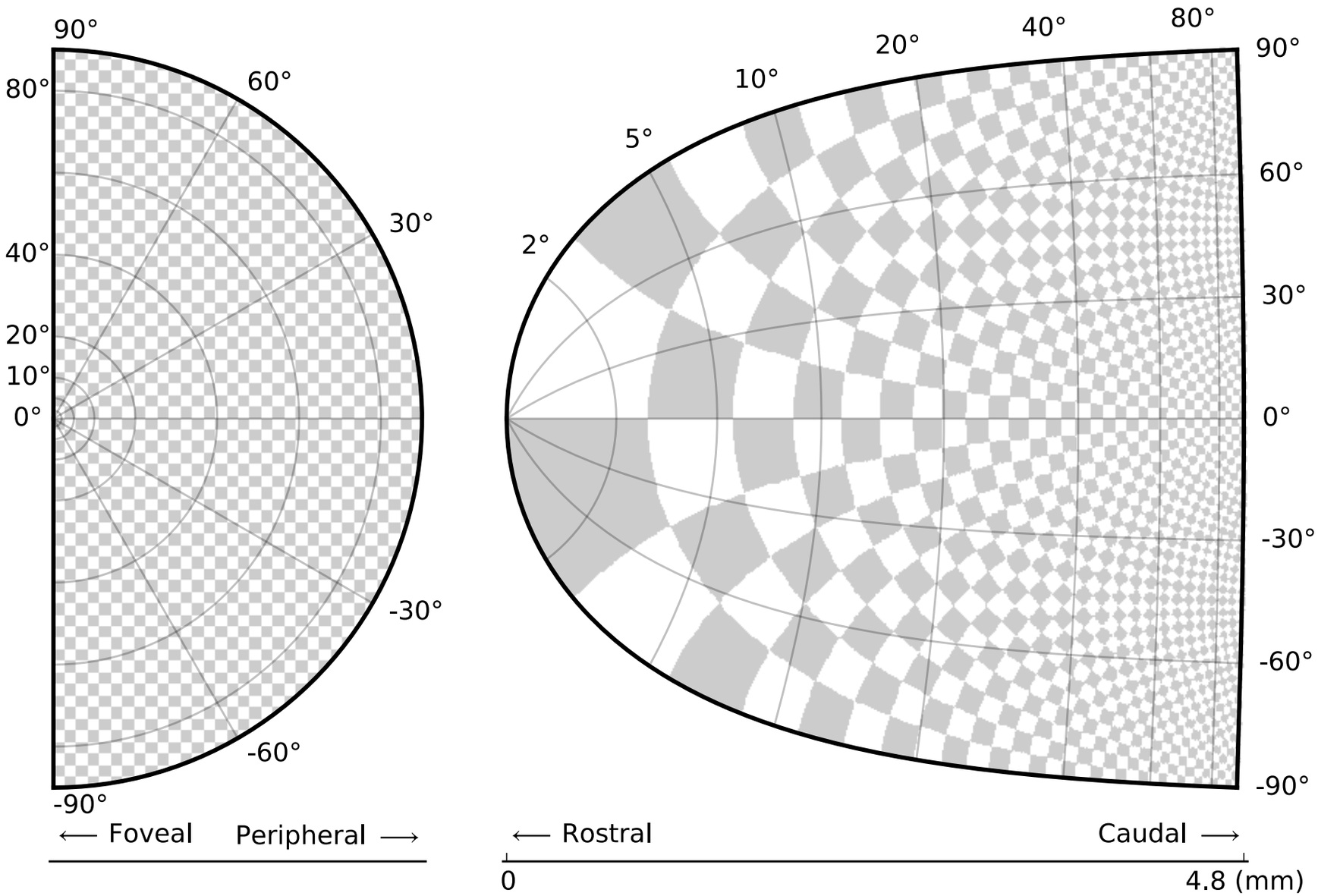
10 Simple Rules for Better Figures

CRASH COURSE ON SCIENTIFIC VISUALISATION

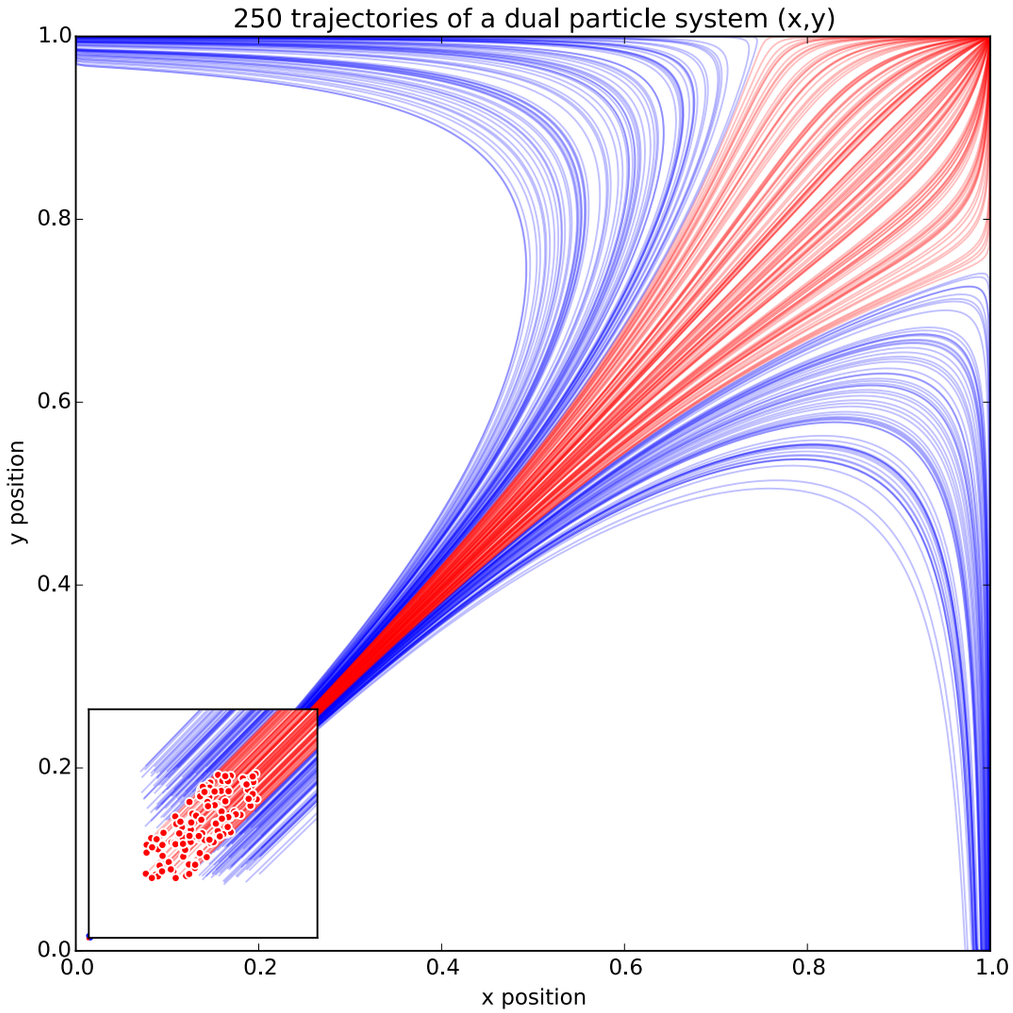
Rule 1: Know your audience

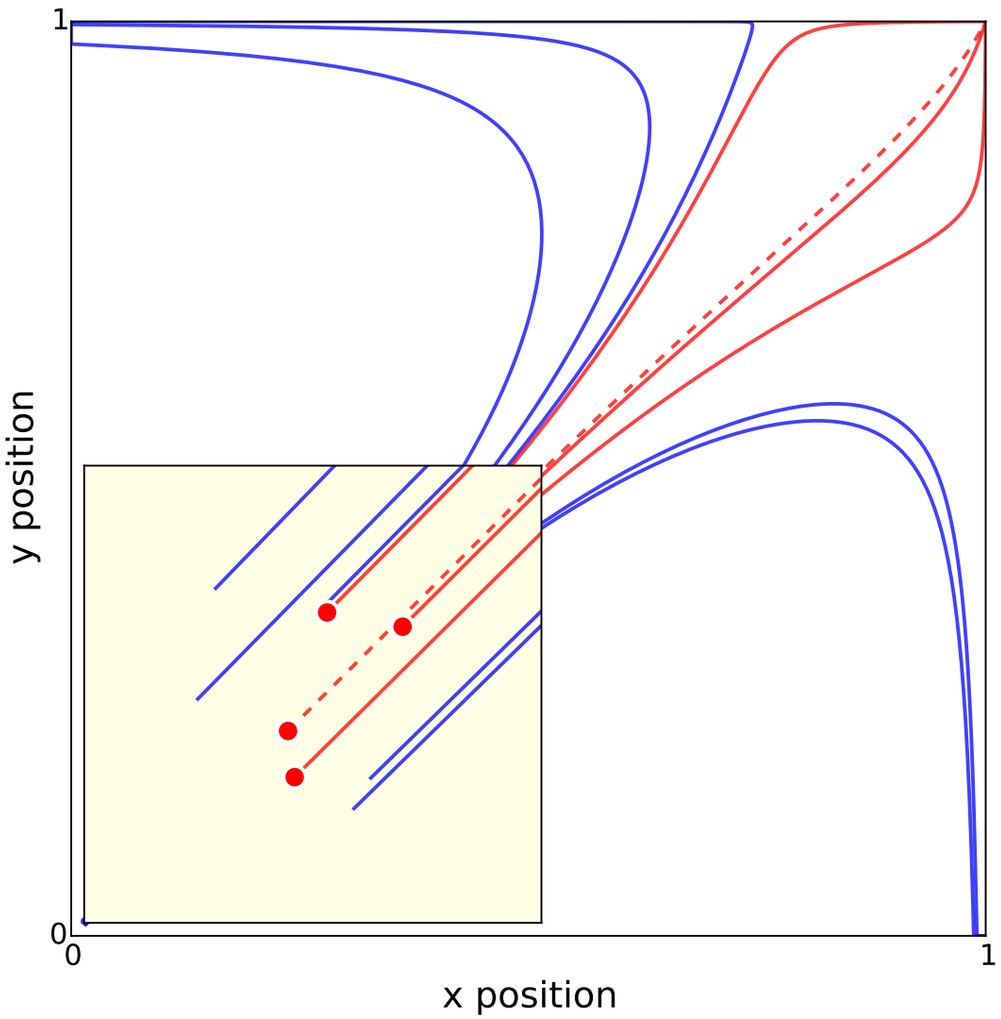


Rule 2: Identify your message



Rule 3: Adapt the figure





Rule 4: Captions are not optional

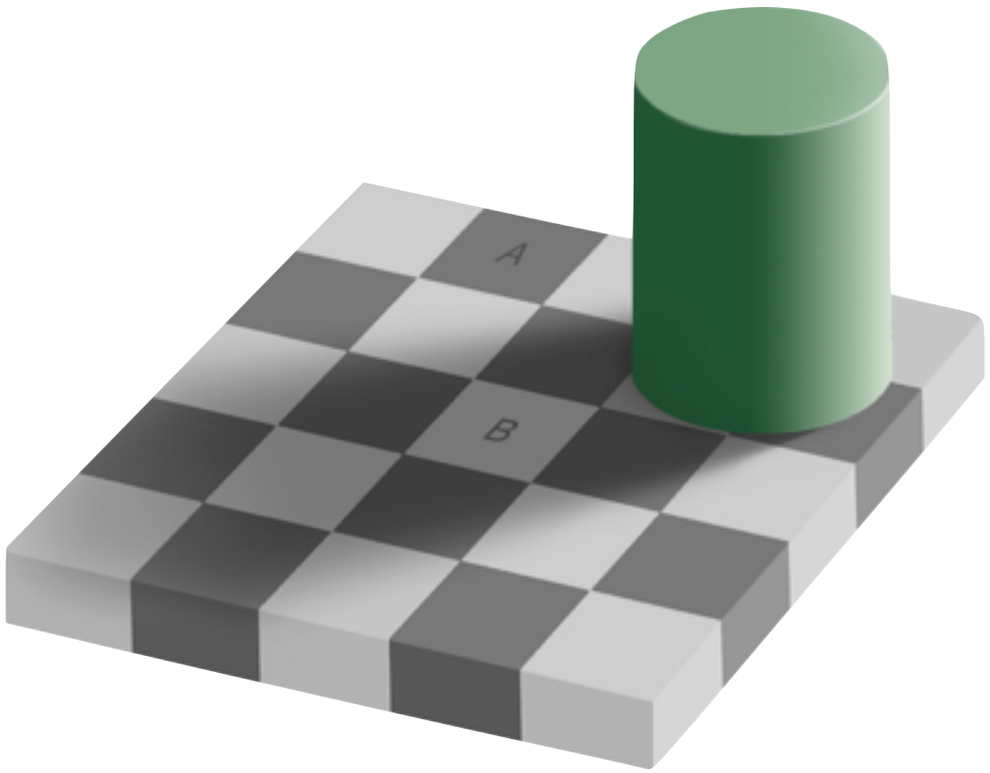


Figure 1. Optical illusion

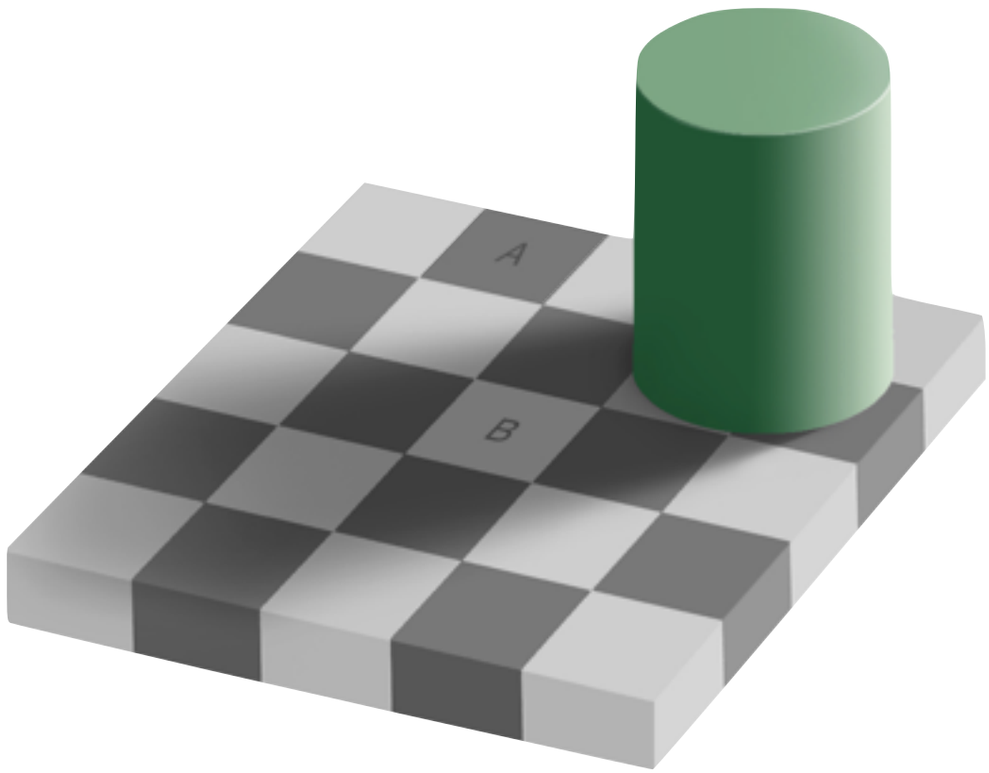
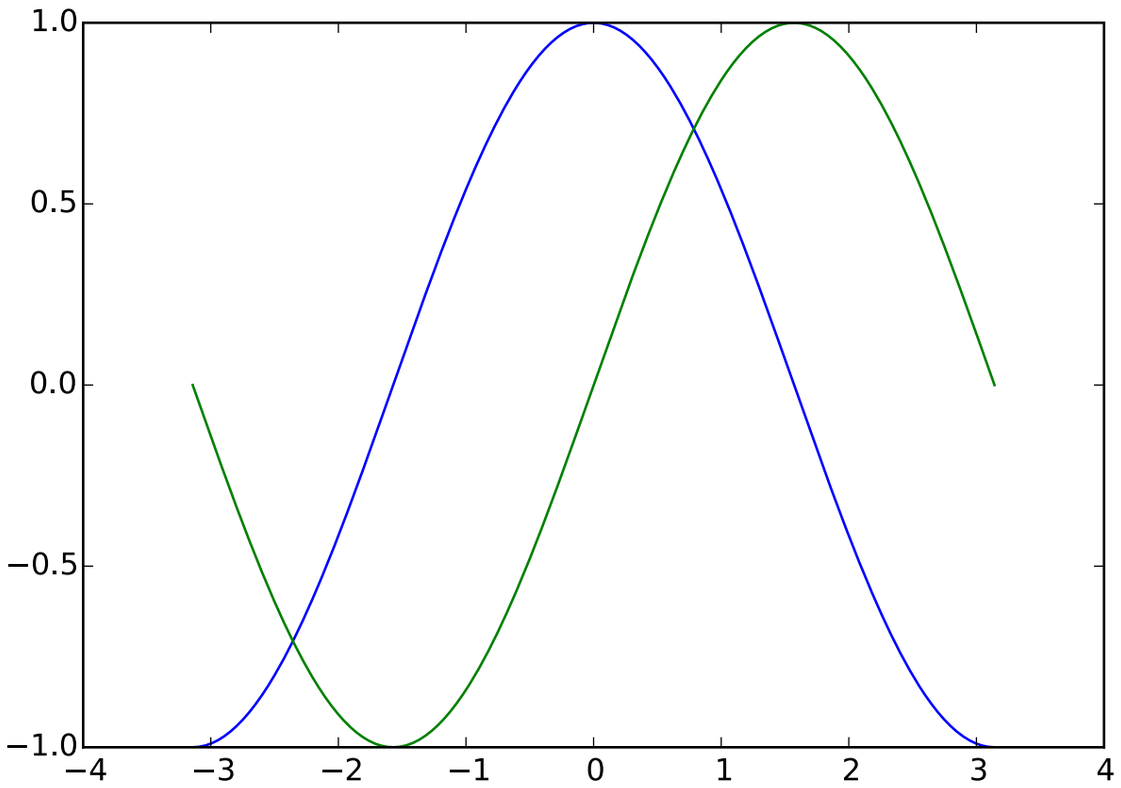
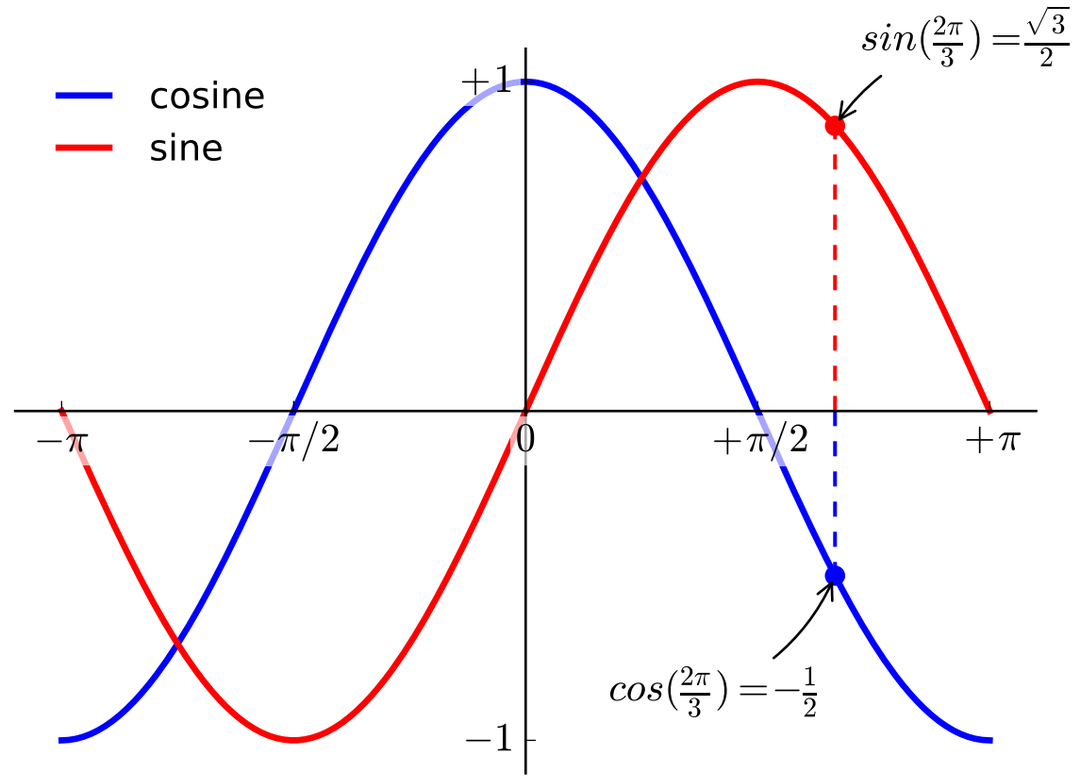


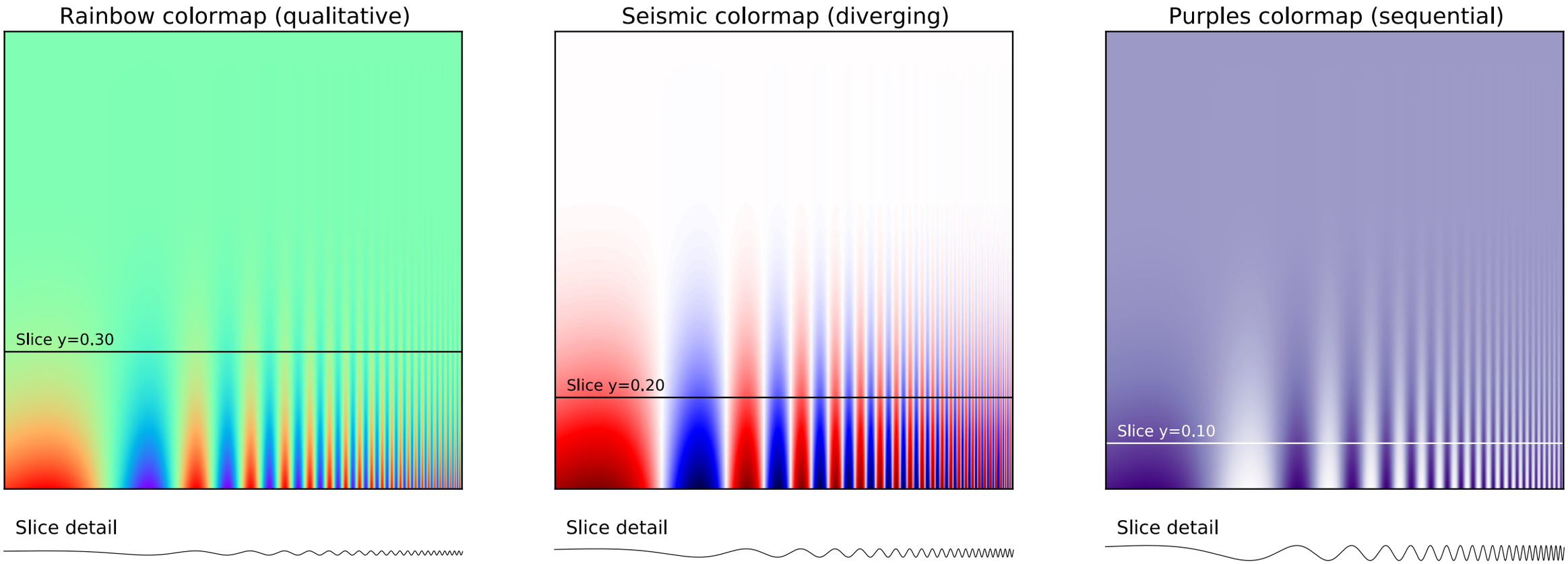
Figure 1. The A and B patches are actually the same color even though we perceived them at being different color.

Rule 5: Do not trust the defaults

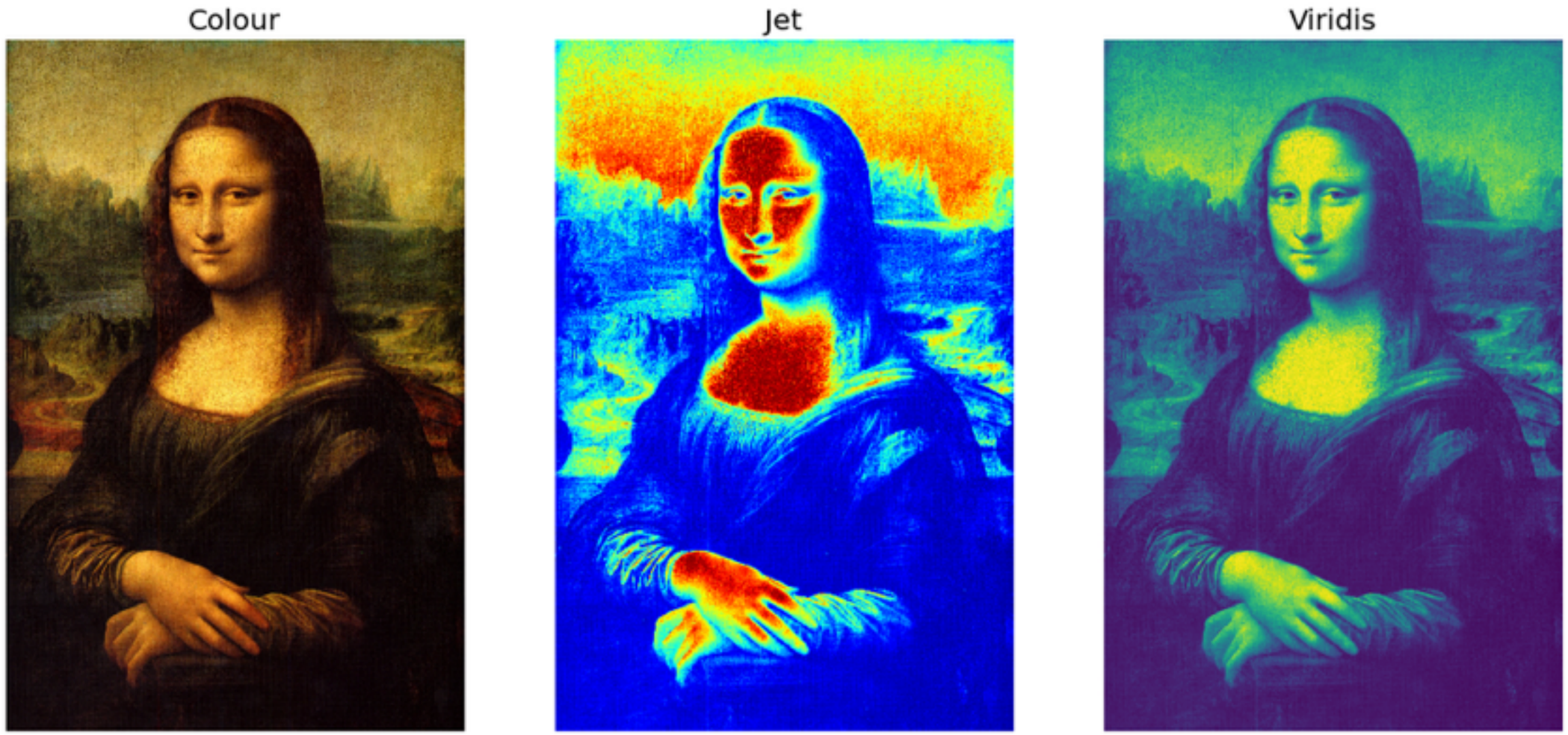




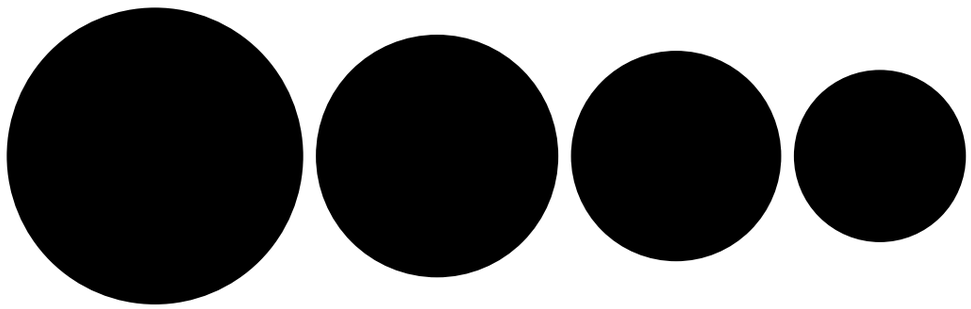
Rule 6: Use color effectively



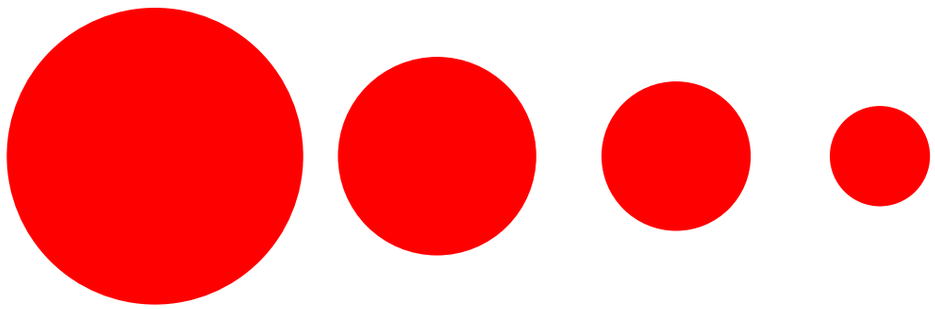
Rule 6 bis: Above all, do no harm (no jet, ever !)



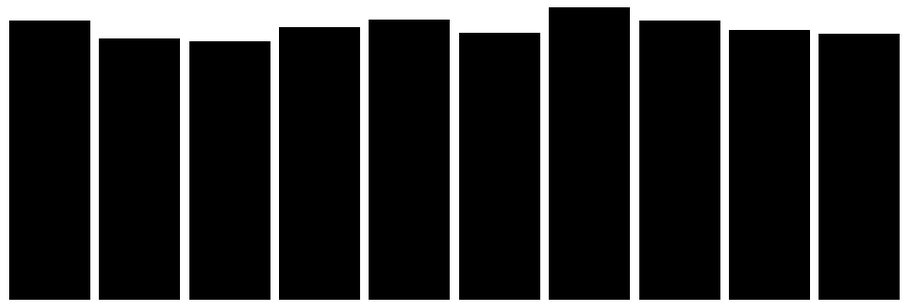
Rule 7: Do not mislead the reader



Relative size using disc area



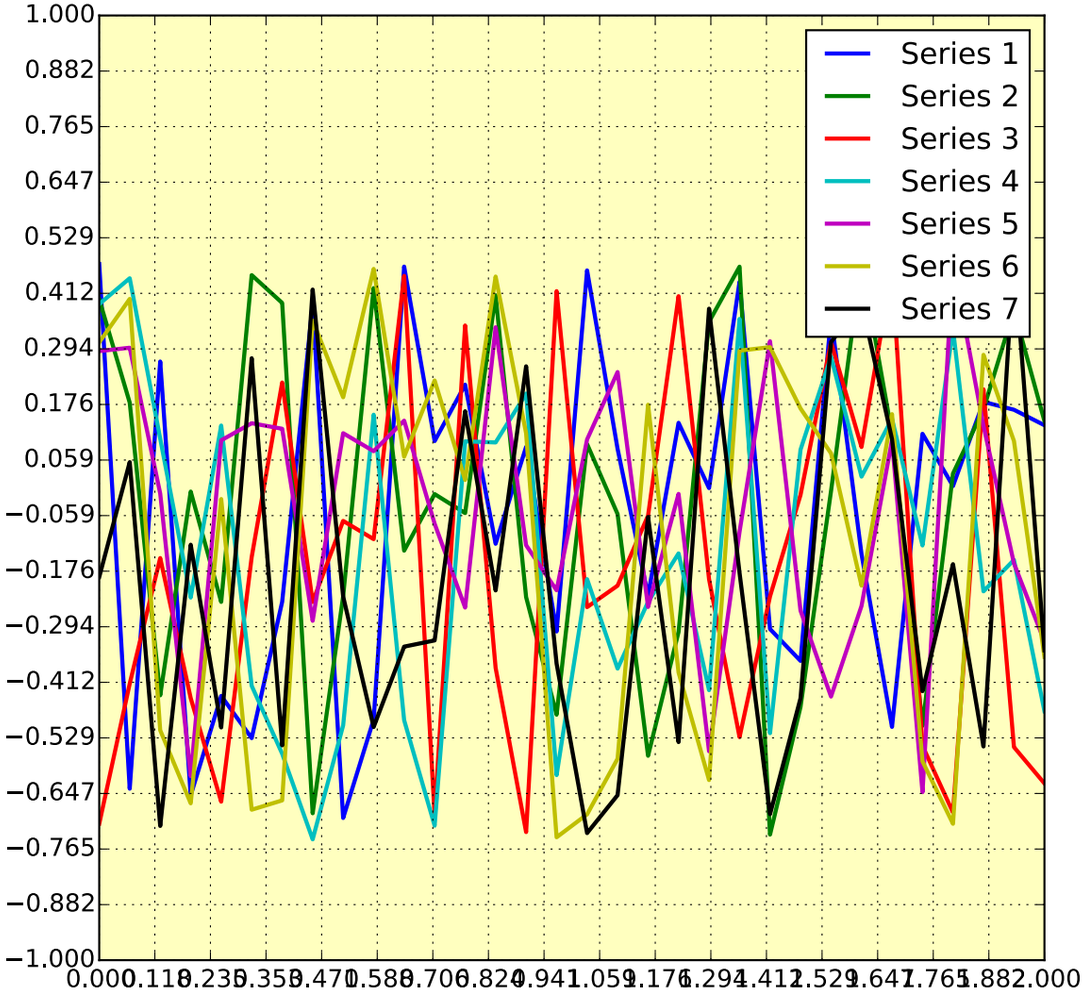
Relative size using disc radius

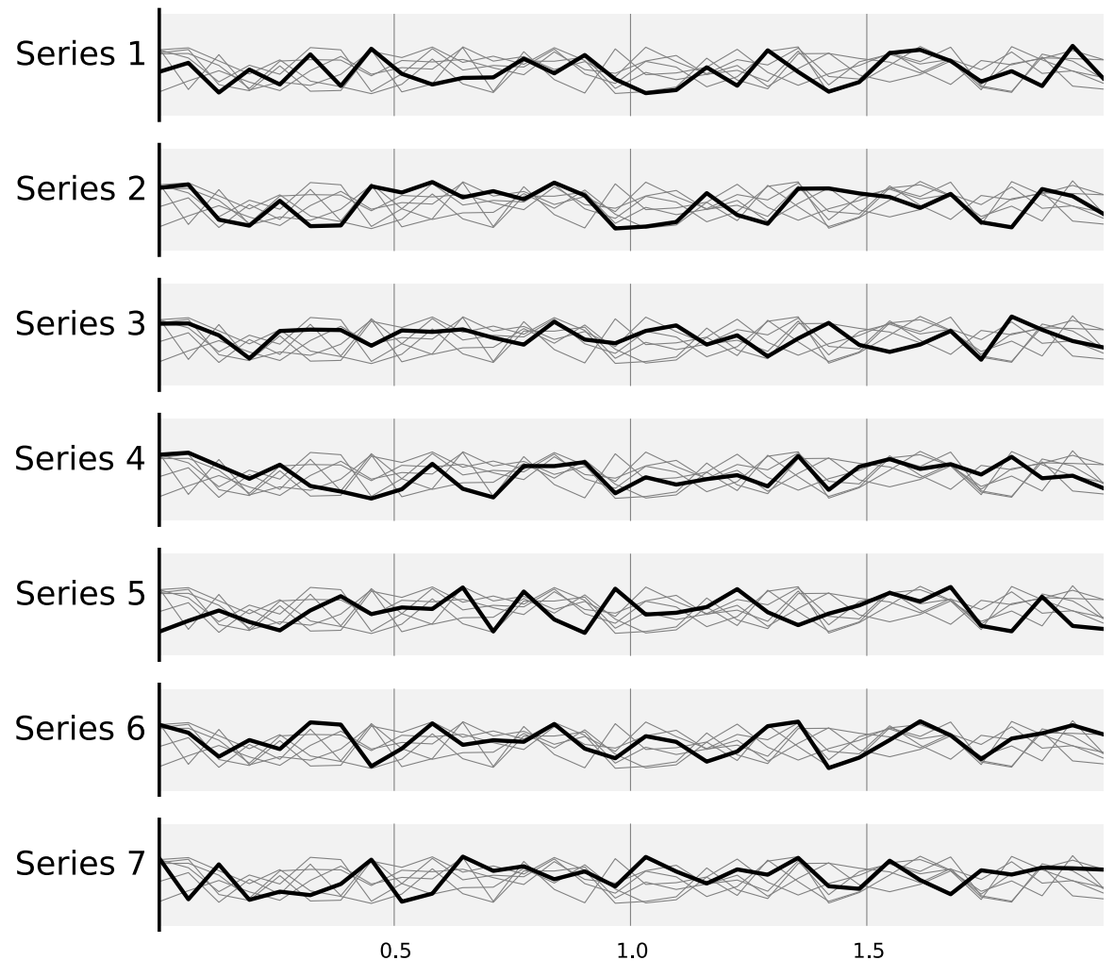


Relative size using full range

Relative size using partial range

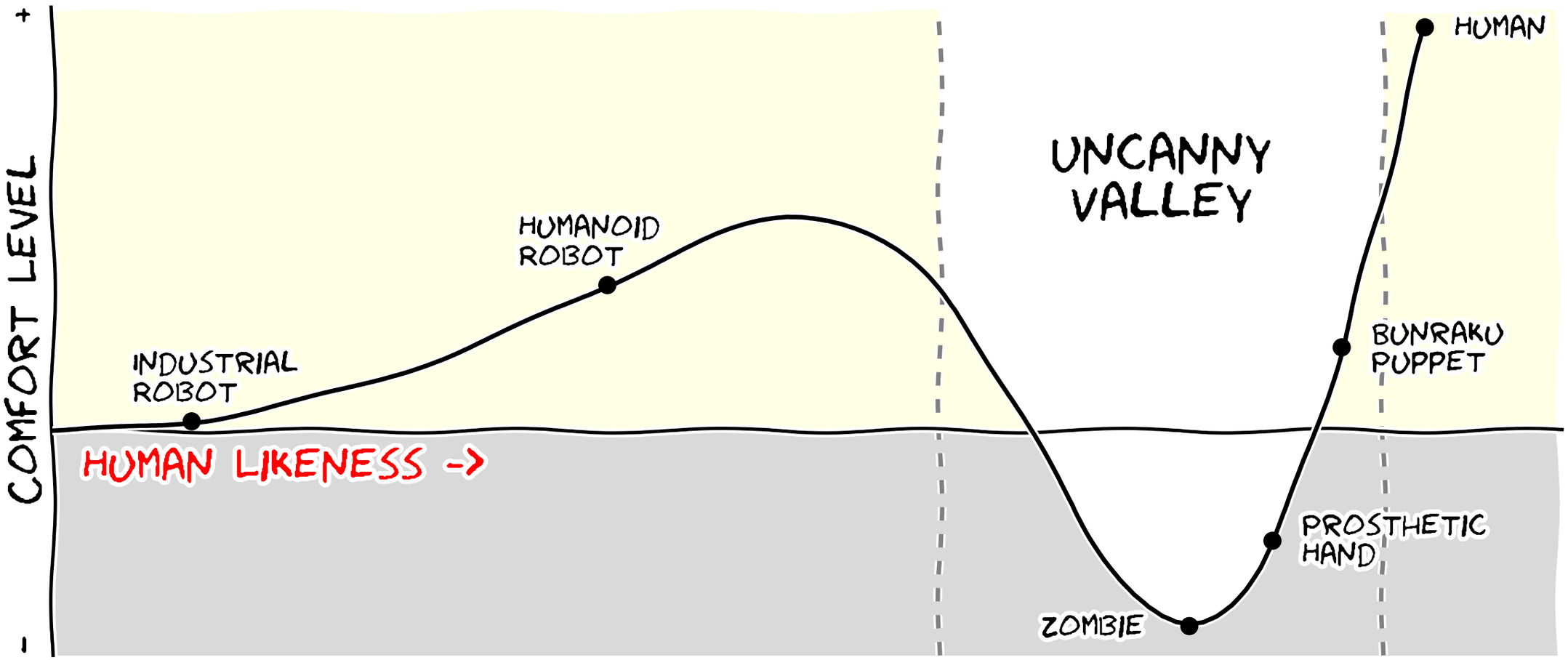
Rule 8: Avoid “Chartjunk”





Rule 8 bis: Less is more

Rule 9: Message trumps beauty



Rule 10: Get the right tool

- PDFCrop (remove white borders)
  http://pdfcrop.sourceforge.net
- GraphViz (easy graph)
  http://www.graphviz.org
- ImageMagick (scripted image processing)
  http://www.imagemagick.org/script/index.php
- Gimp (bitmap image manipulation)
  https://www.gimp.org
- Inkscape (vector image manipulation)
  https://www.inkscape.org
- Tikz (scripted vector art)
  http://www.texample.net/tikz/examples/all/
- And many, many, many others …

Enough, theory, let's practice !

github.com/rougier/ASPP-2016

github.com/rougier/matplotlib-tutorial