Scientific visualization

Nicolas P. Rougier, Python Scientifique, La Rochelle, 2017

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

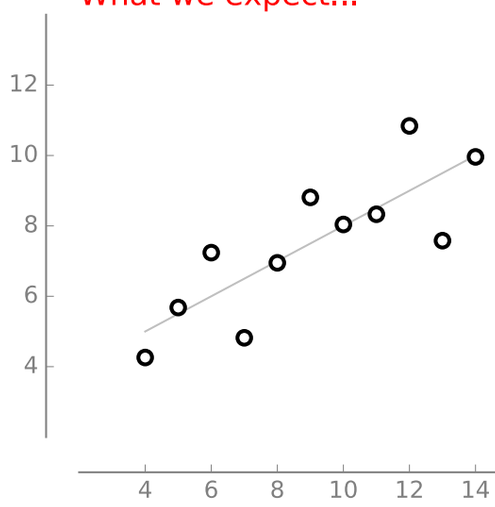
What is **common** to these data sets?

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

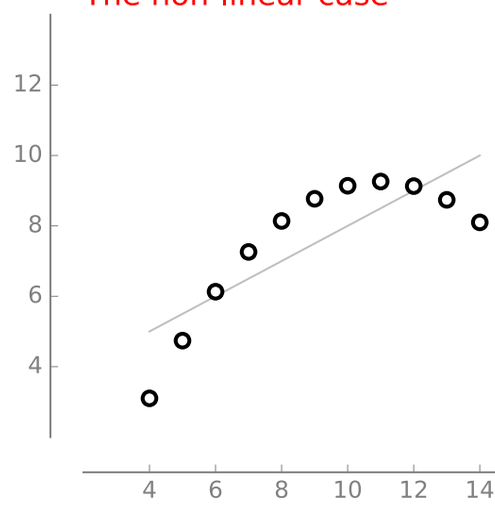
But having a **closer look** at the data…

Anscombe's quartet, 1973

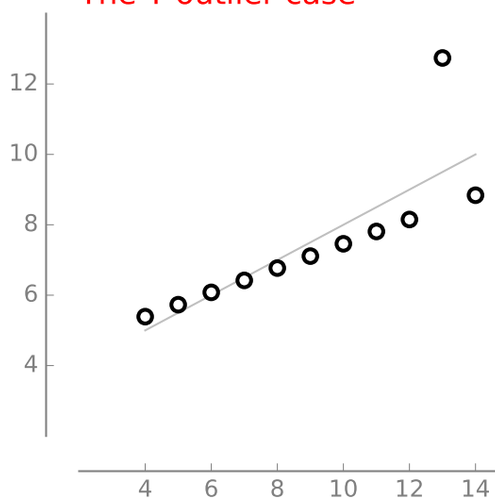
What we expect...



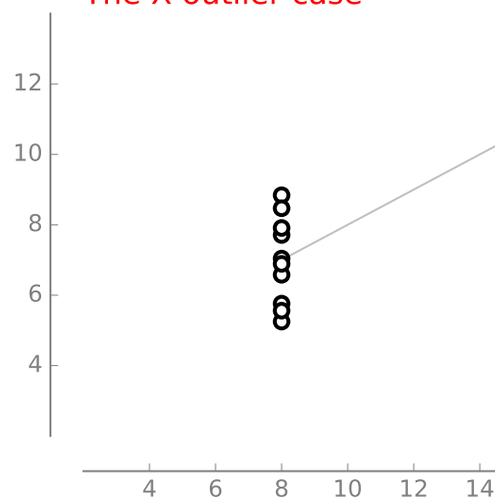
The non-linear case



The Y outlier case



The X outlier case



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

Francis Anscombe (1918-2001)

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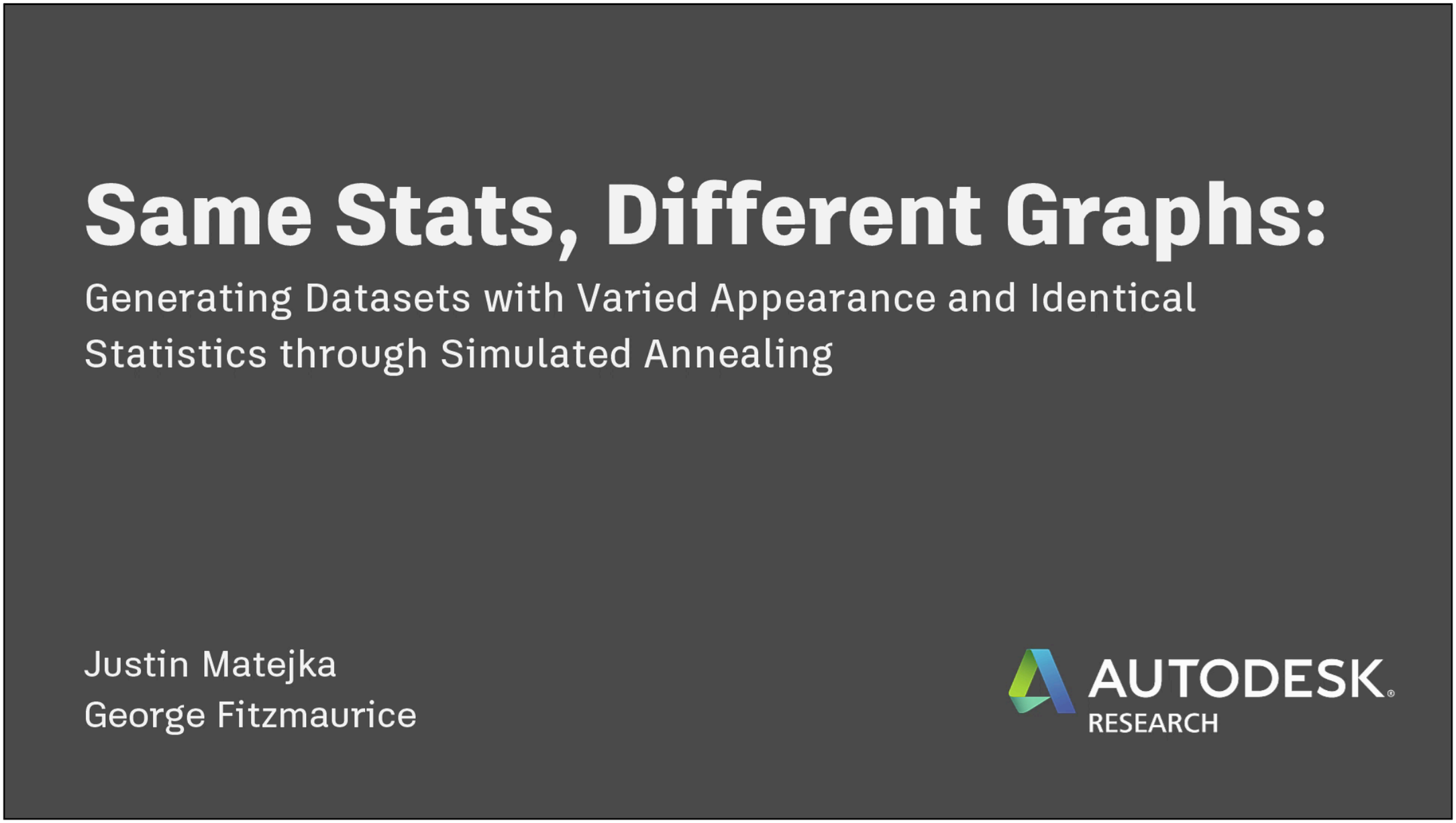
But having a **closer look** at the data…

Same Stats, Different Graphs

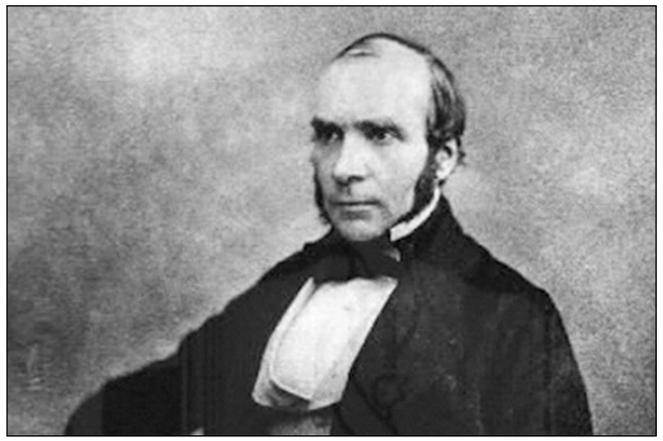
Justin Matejka & George Fitzmaurice, 2017

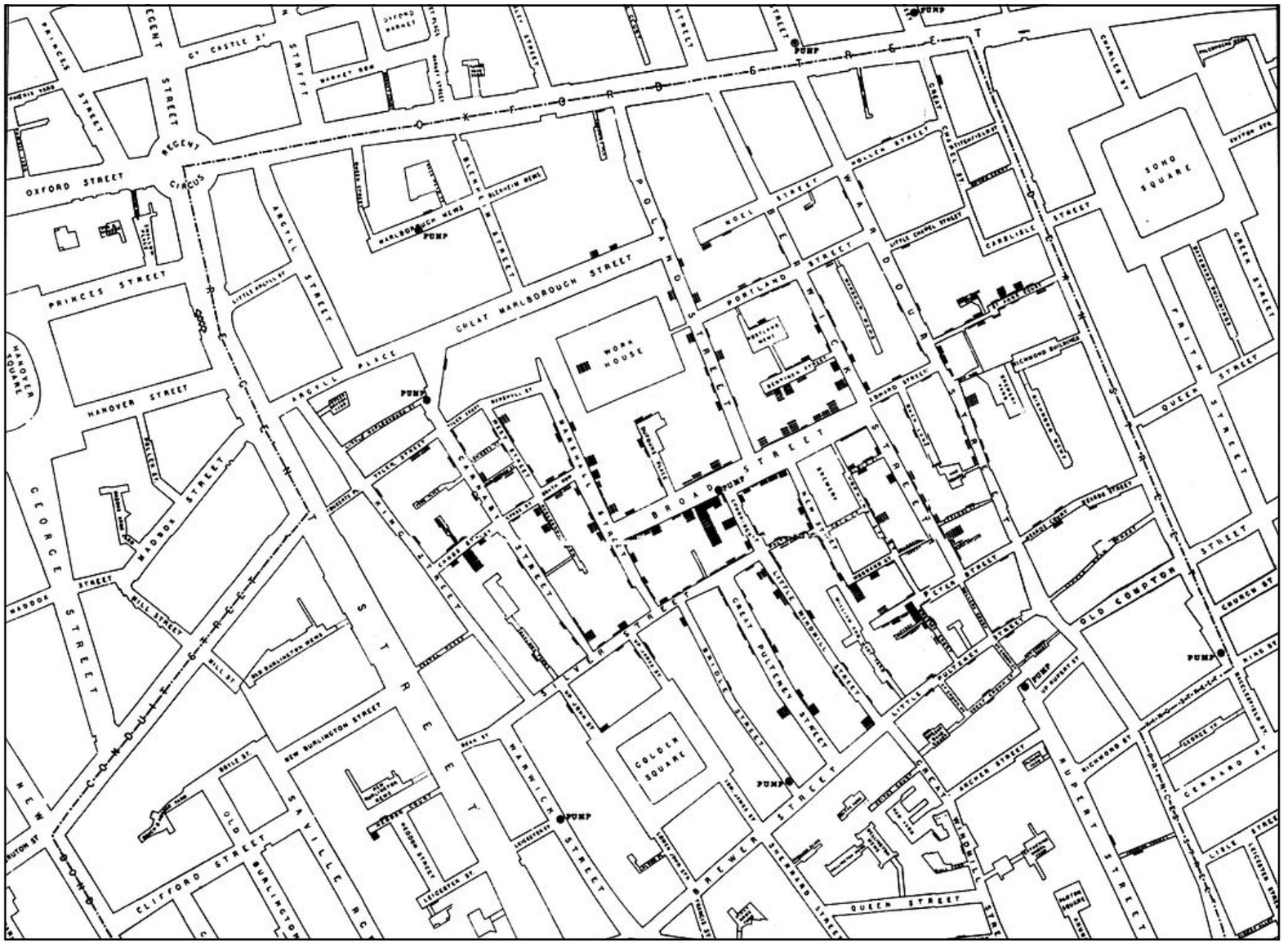


Cholera epidemic, London, 1854

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

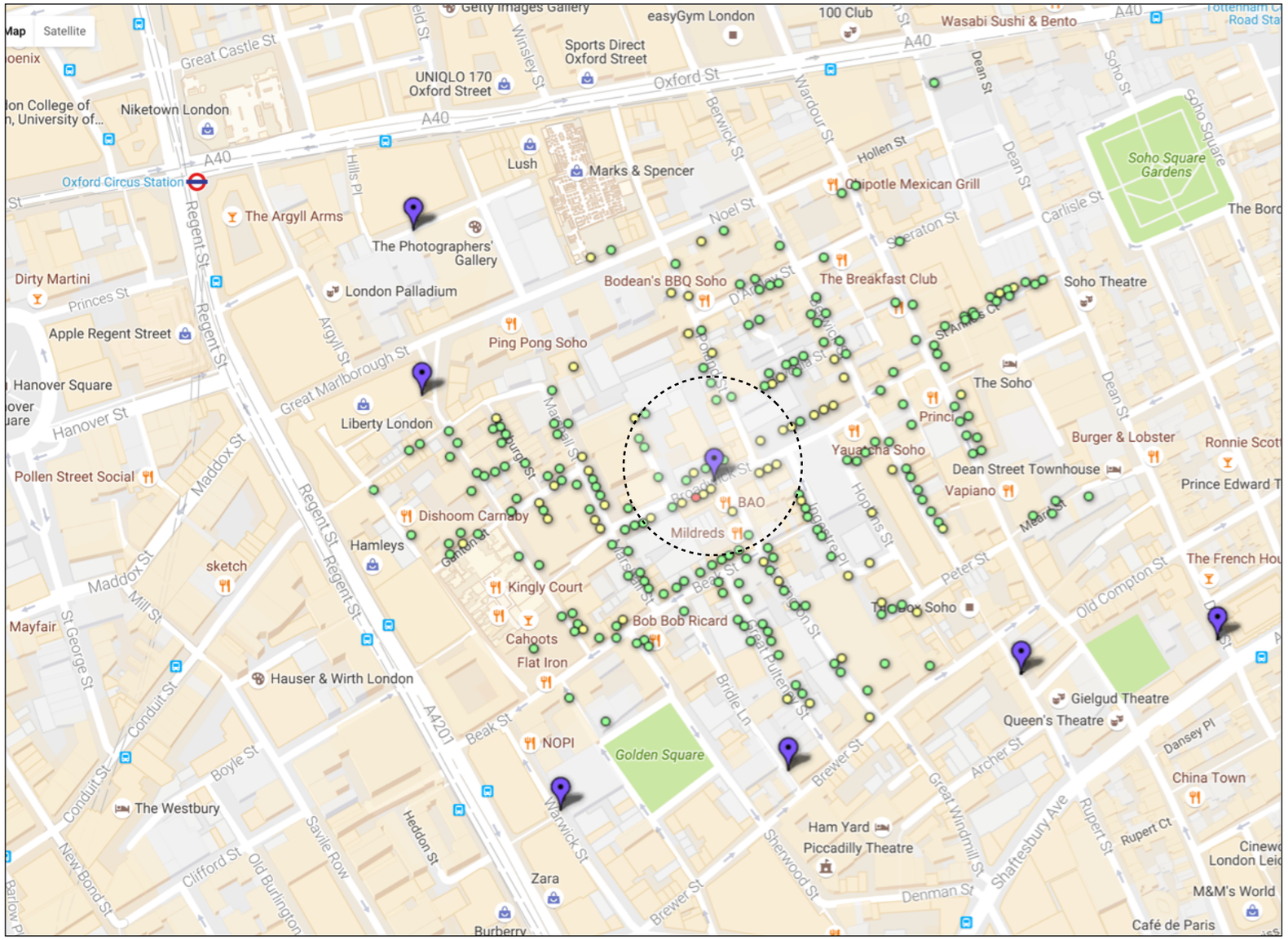
John Snow (1813-1858)





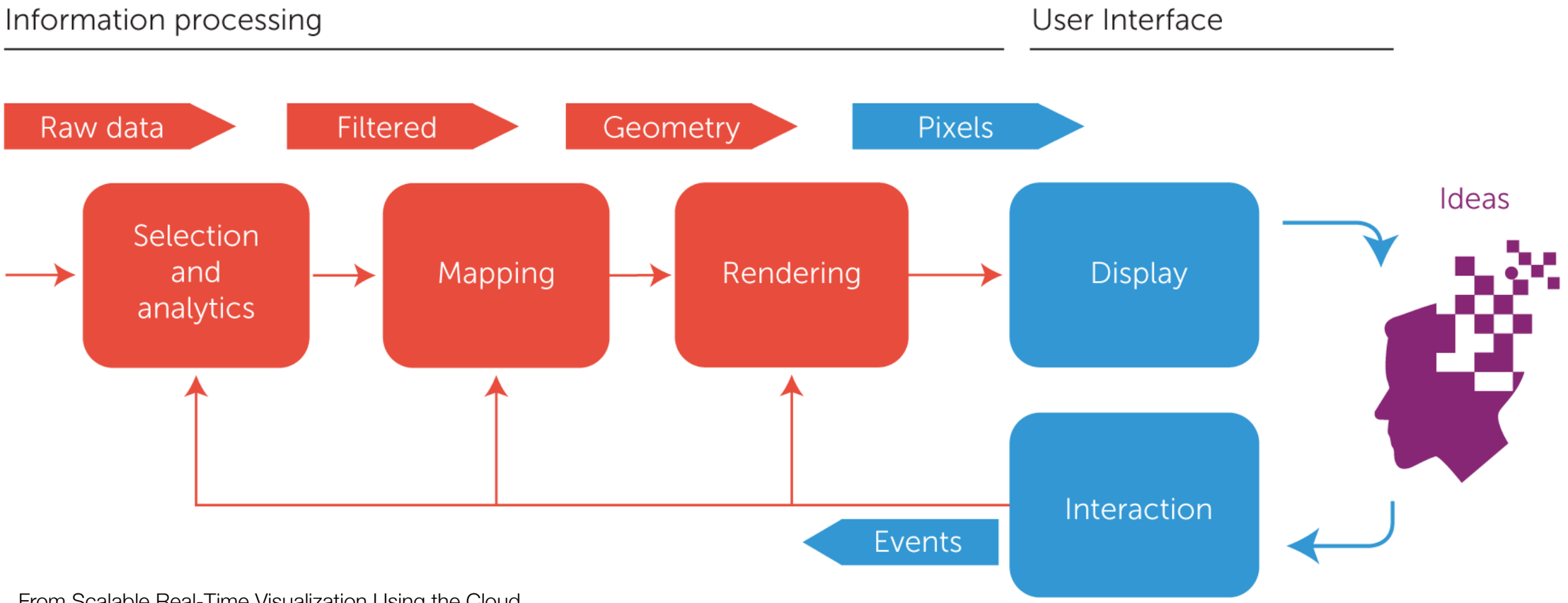
Cholera epidemic, London, 1854

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



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.

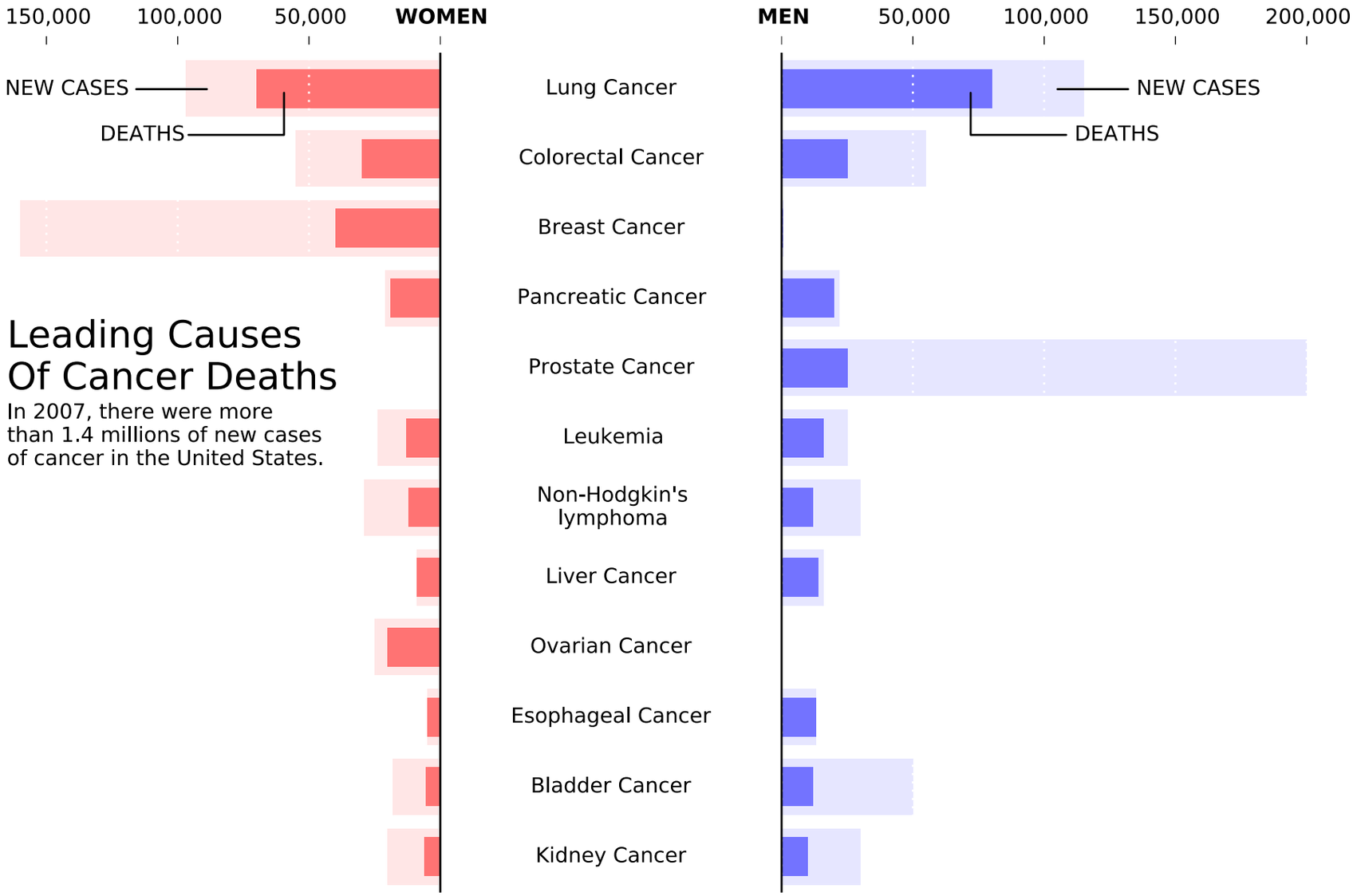
This is exactly where visualization libraries are useful because they will automatize most of the work (more or less depending on the library).

Visualization type

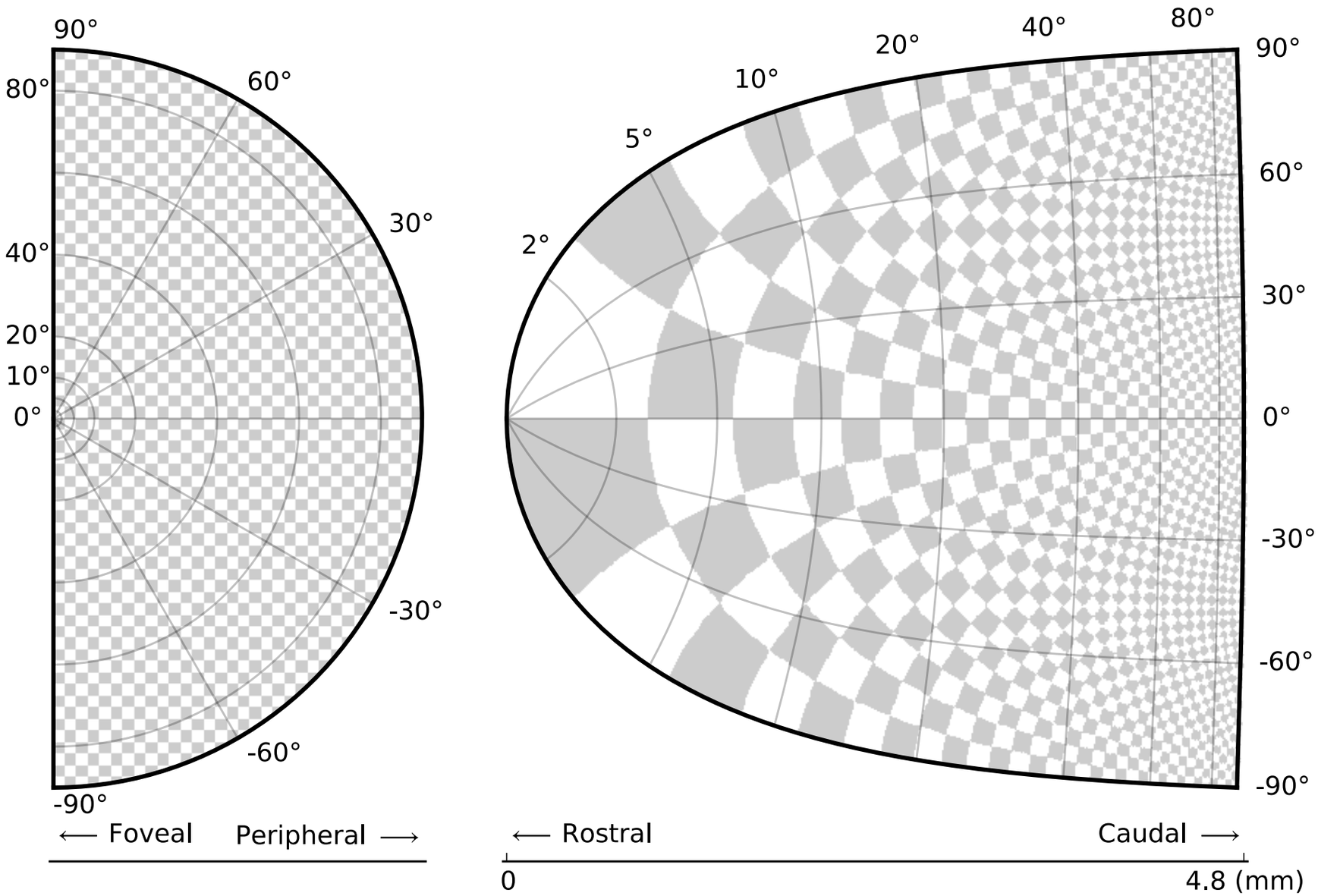
Data Visualisation catalogue by S. Rebecca

10 Simple Rules for Better Figures

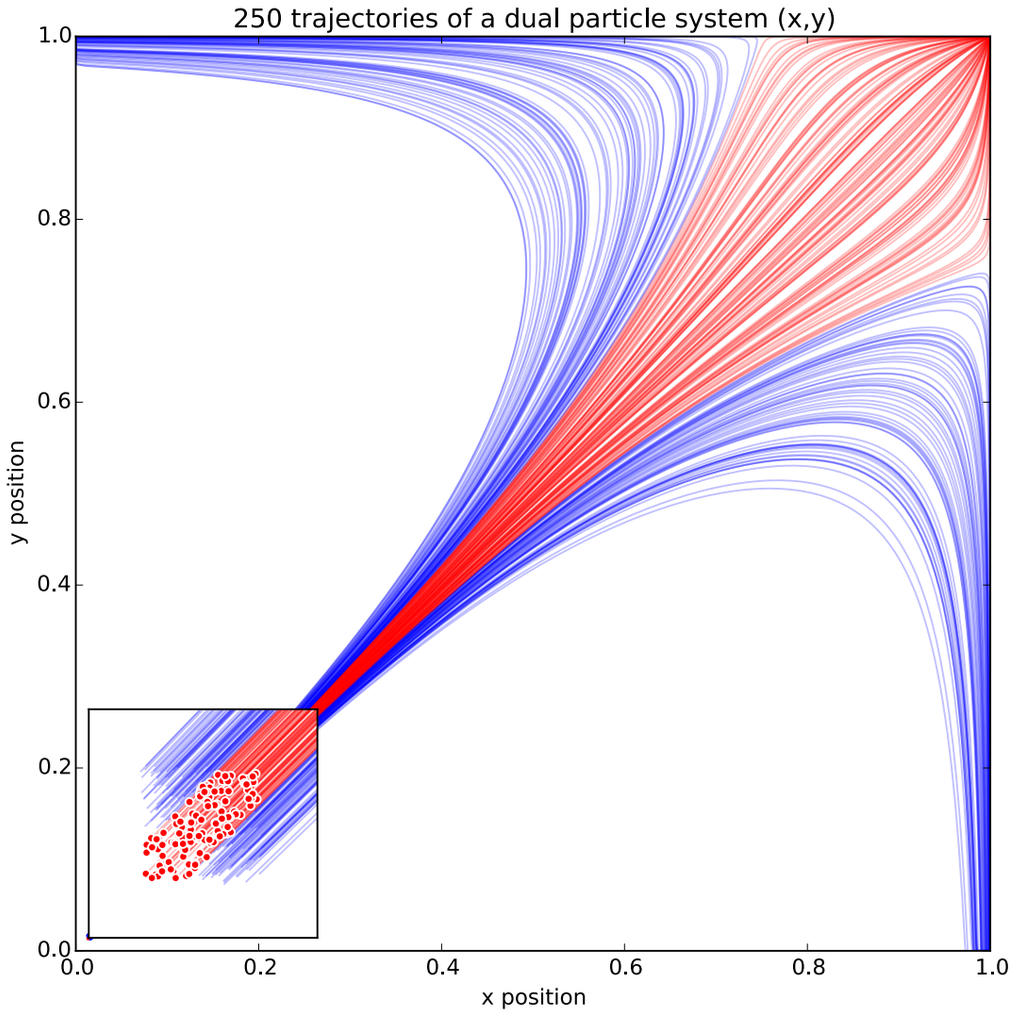
Rule 1: Know your audience

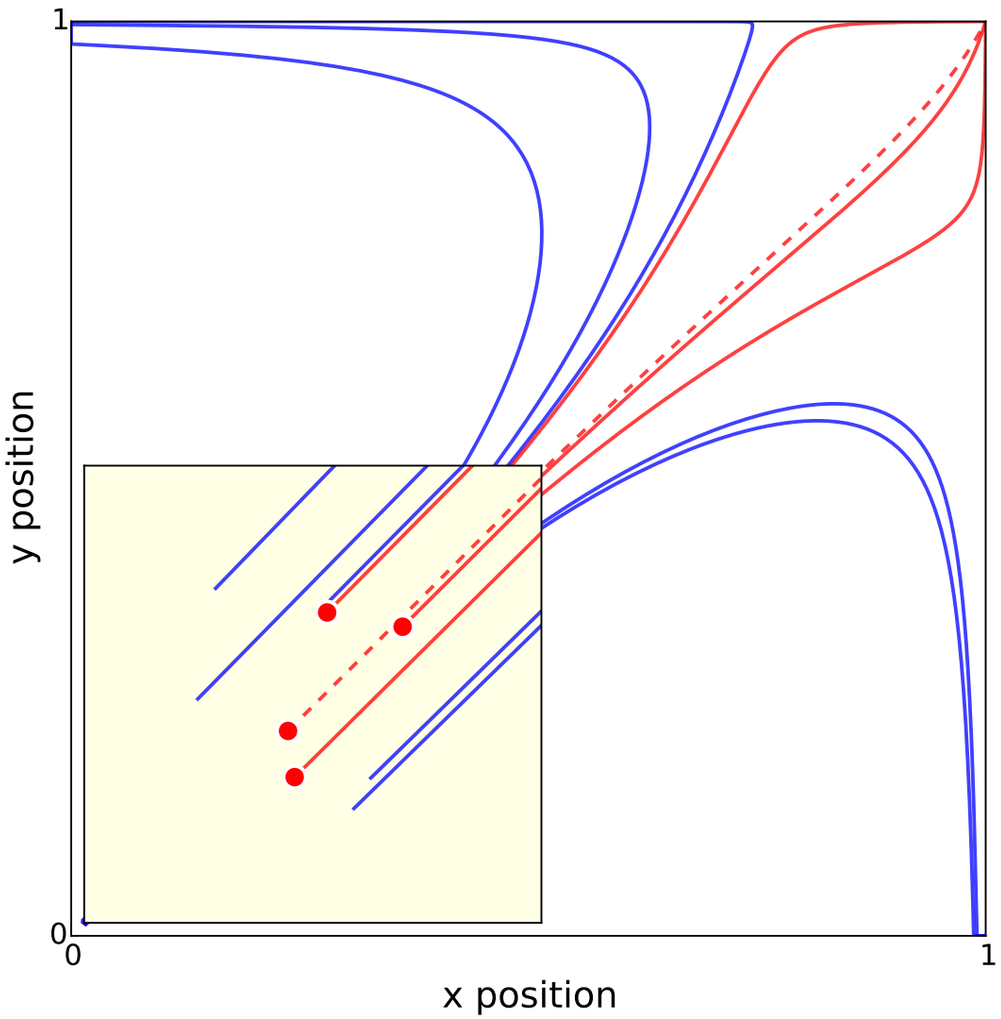


Rule 2: Identify your message



Rule 3: Adapt the figure





Rule 4: Captions are not optional

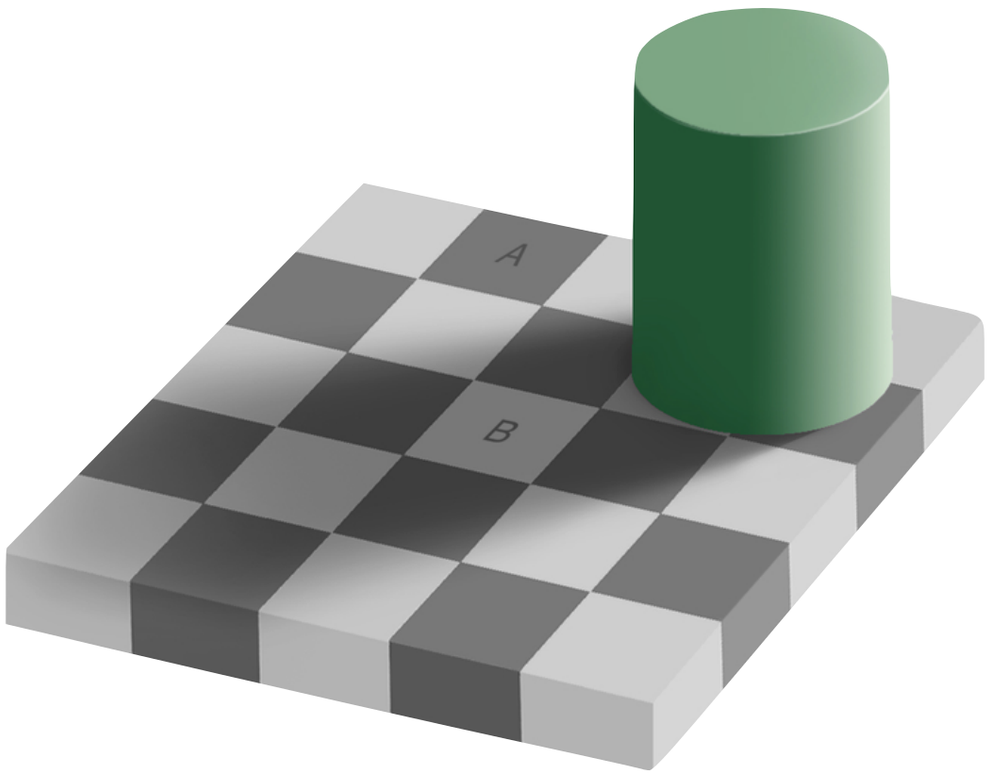


Figure 1. Optical illusion

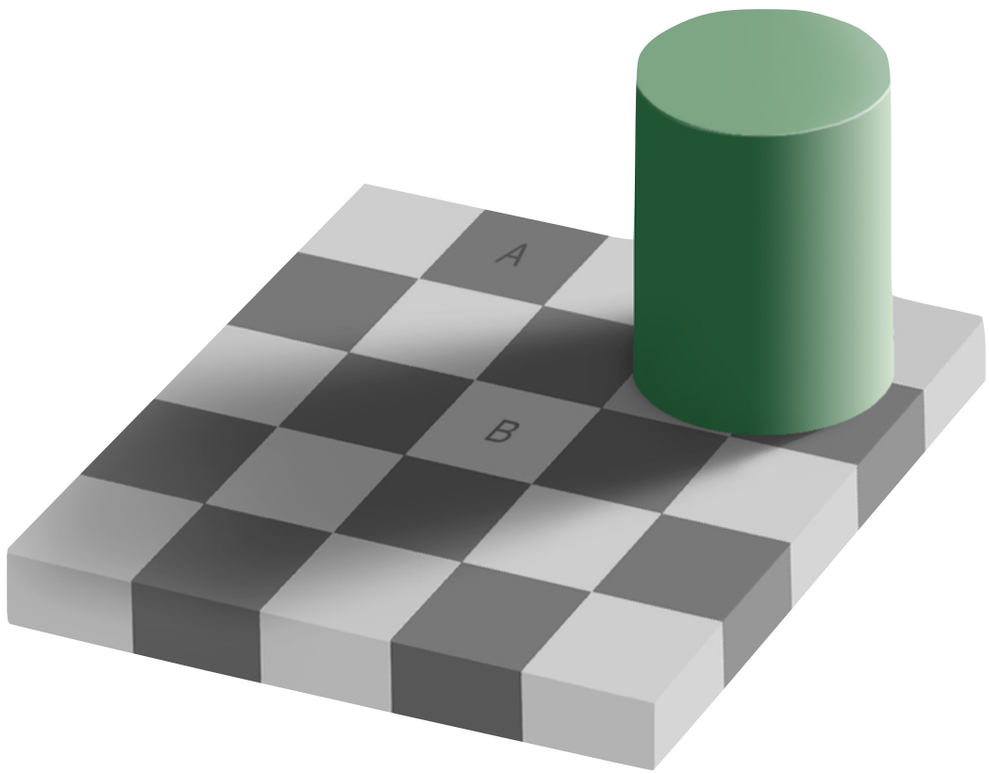
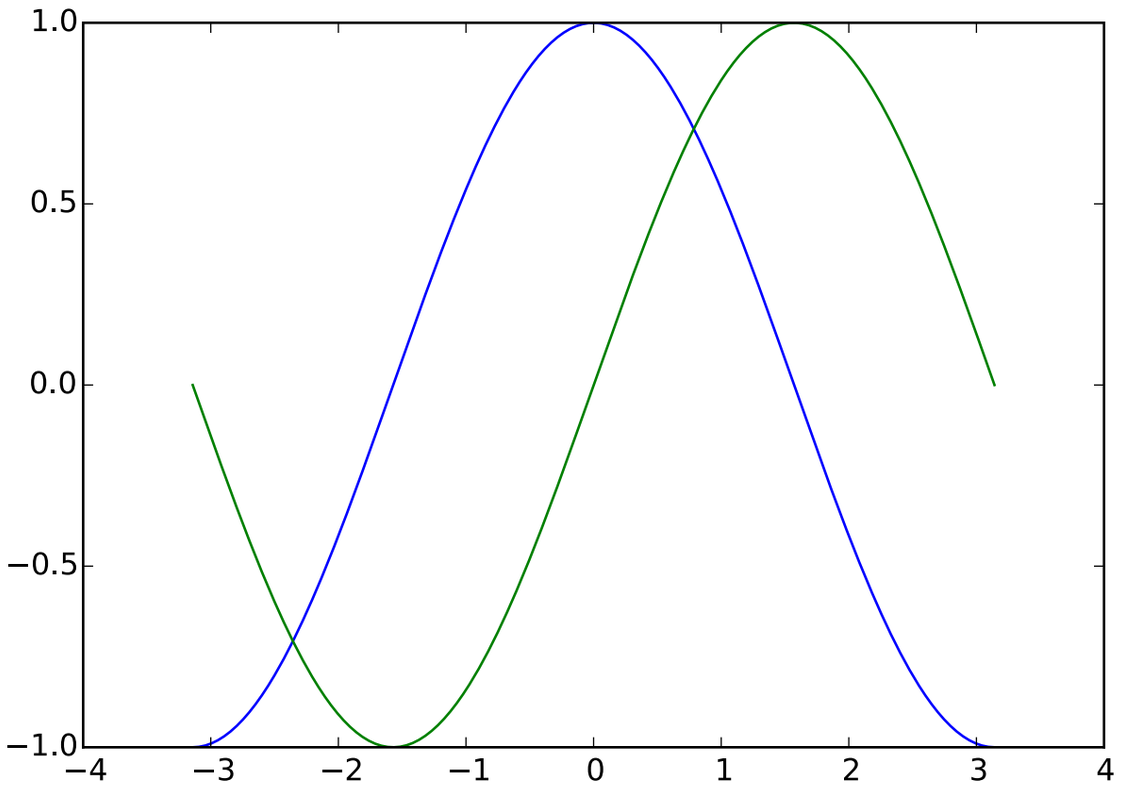
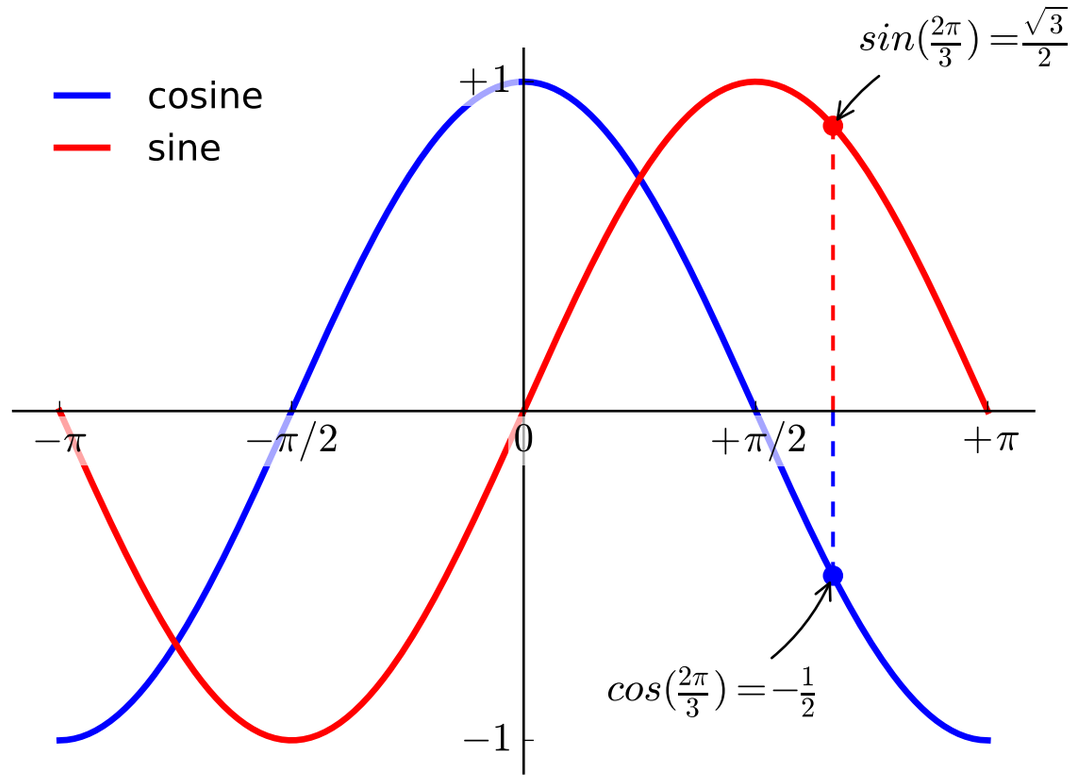


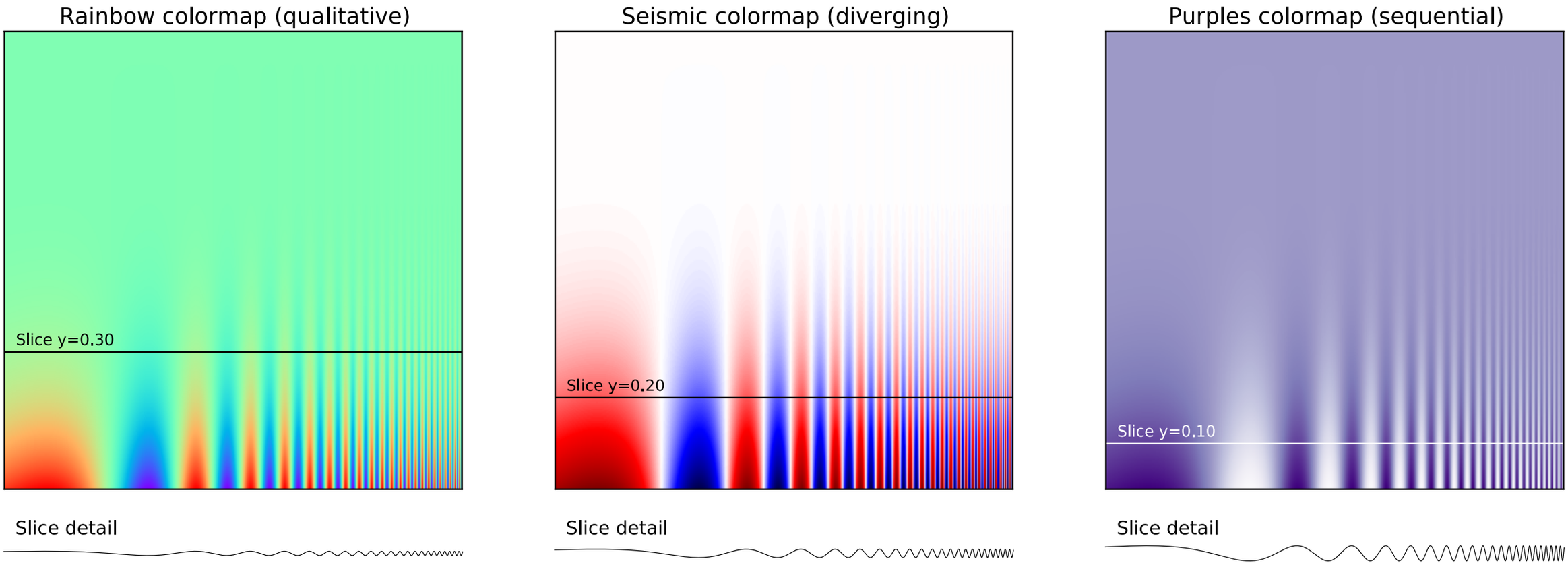
Figure 1. The A and B patches are actually the same color even though we perceived them at being different color.

Rule 5: Do not trust the defaults

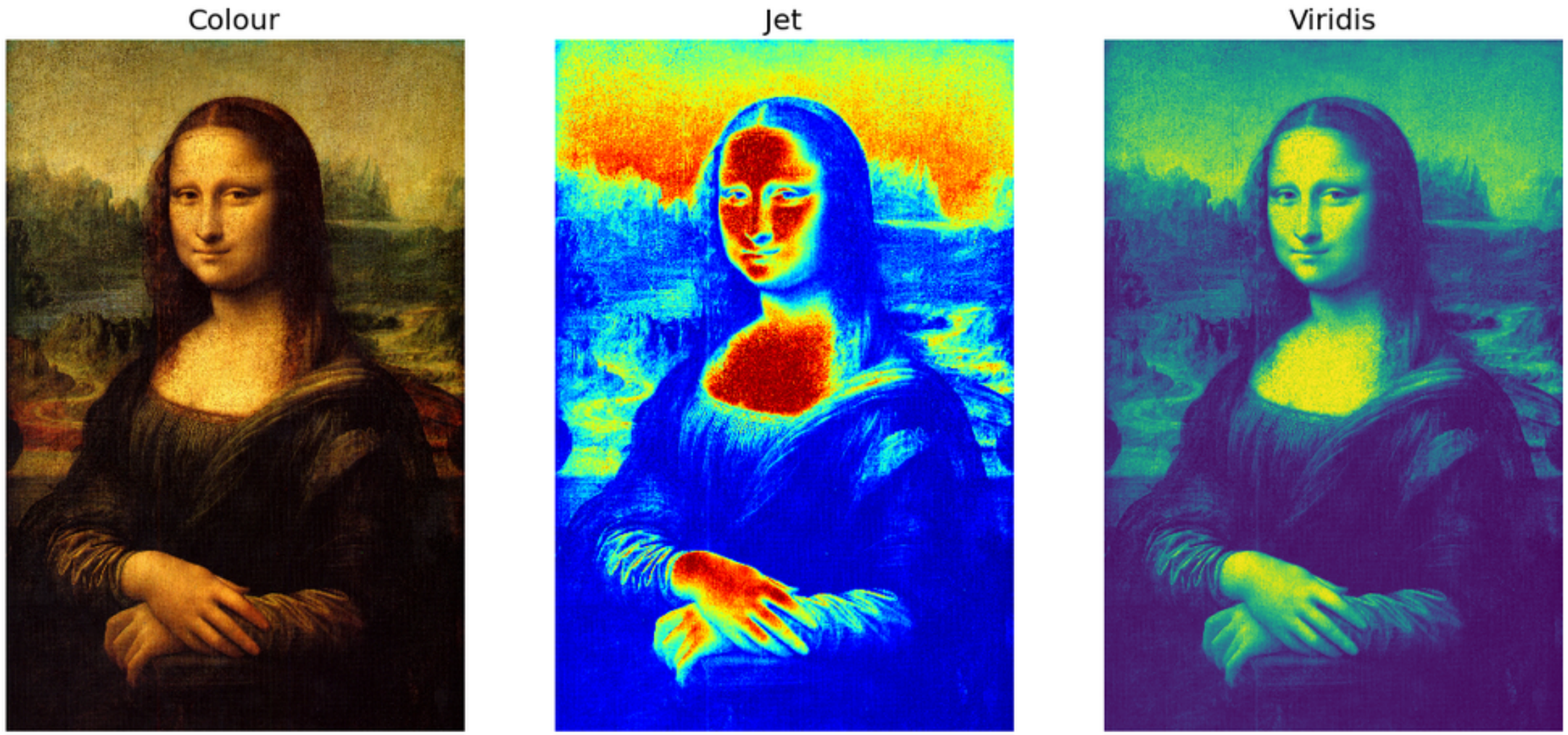




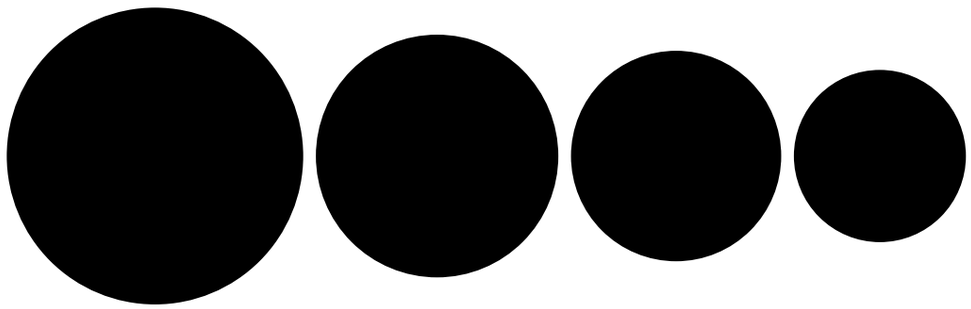
Rule 6: Use color effectively



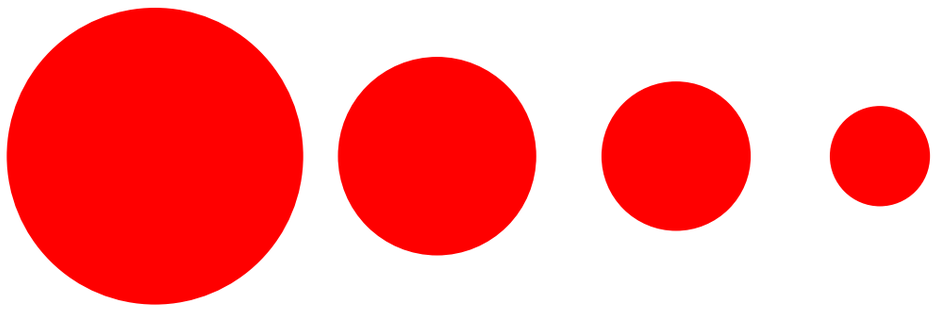
Rule 6 bis: Above all, do no harm (no jet, ever !)



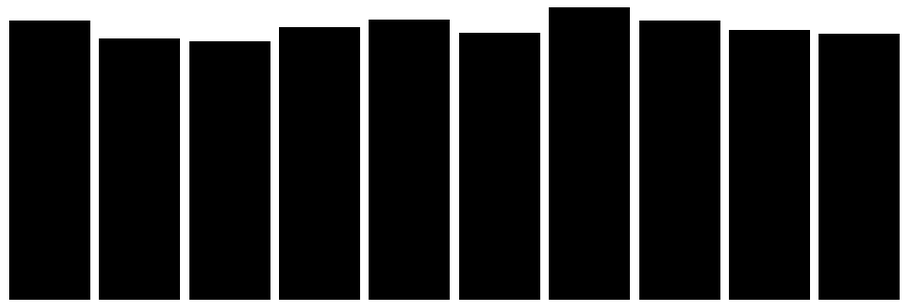
Rule 7: Do not mislead the reader



Relative size using disc area



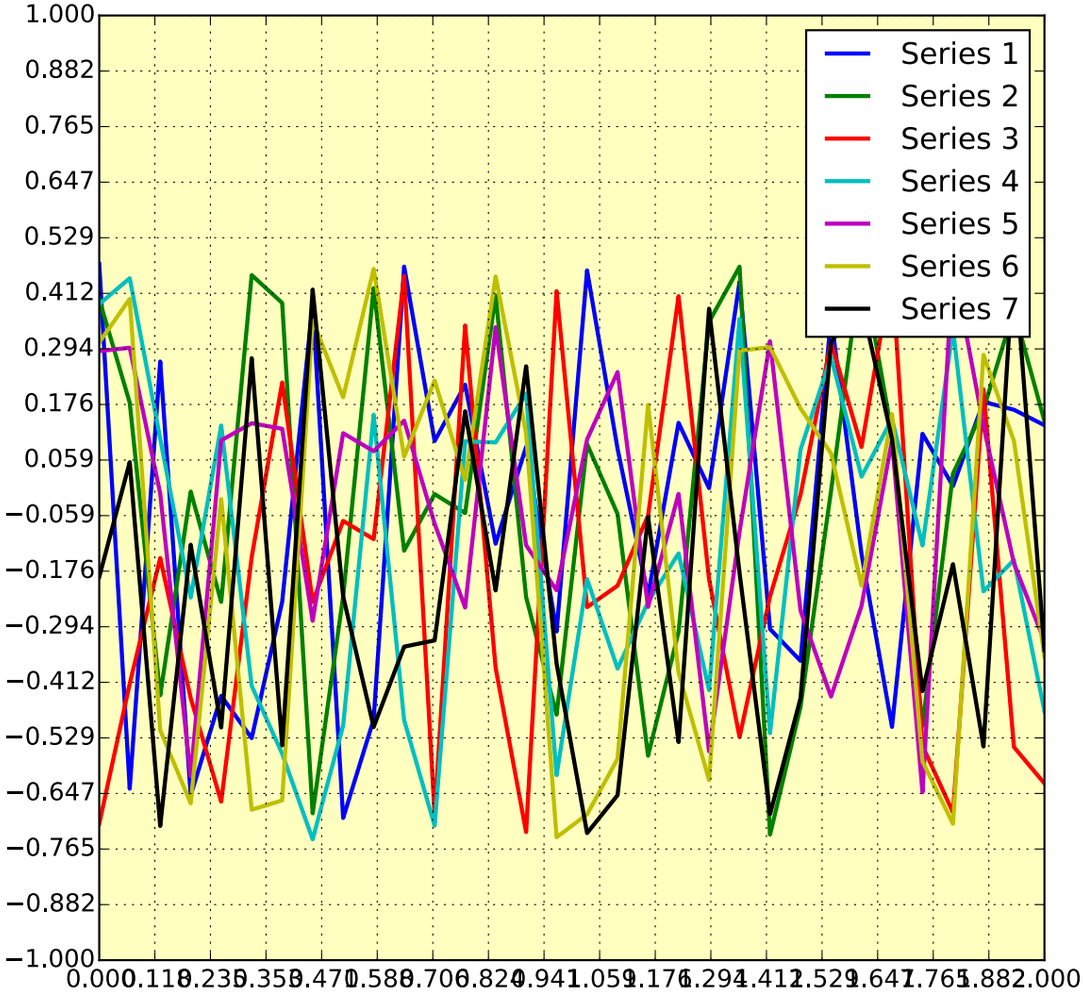
Relative size using disc radius

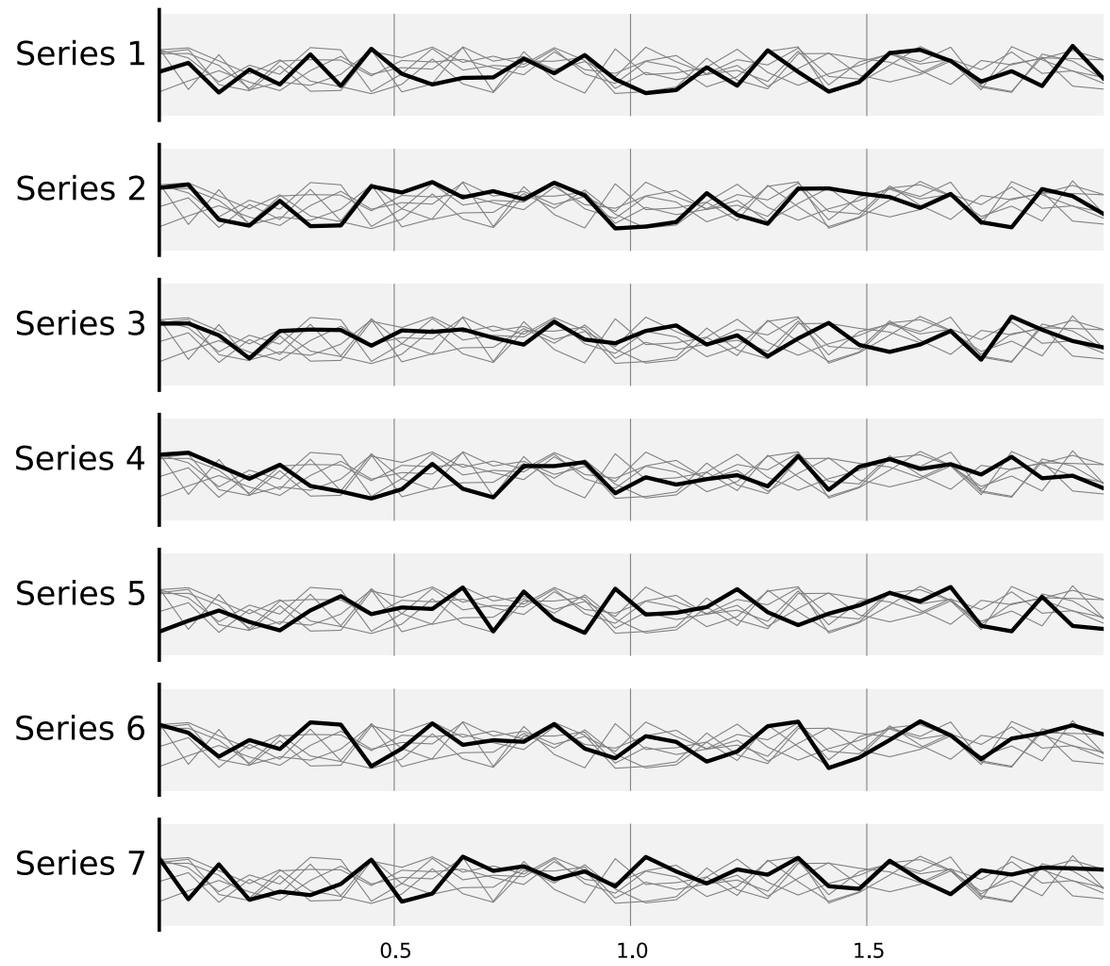


Relative size using full range

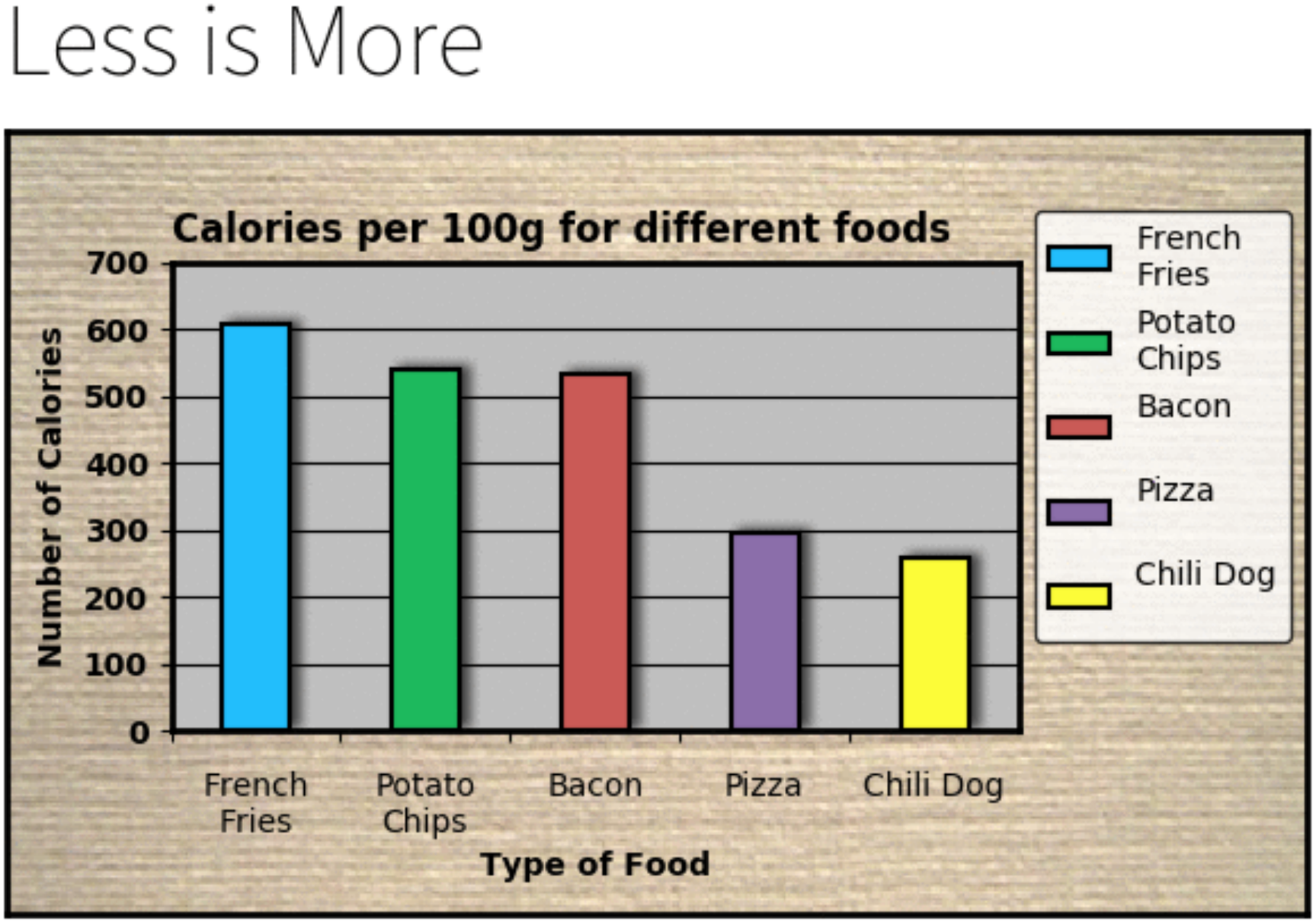
Relative size using partial range

Rule 8: Avoid “Chartjunk”

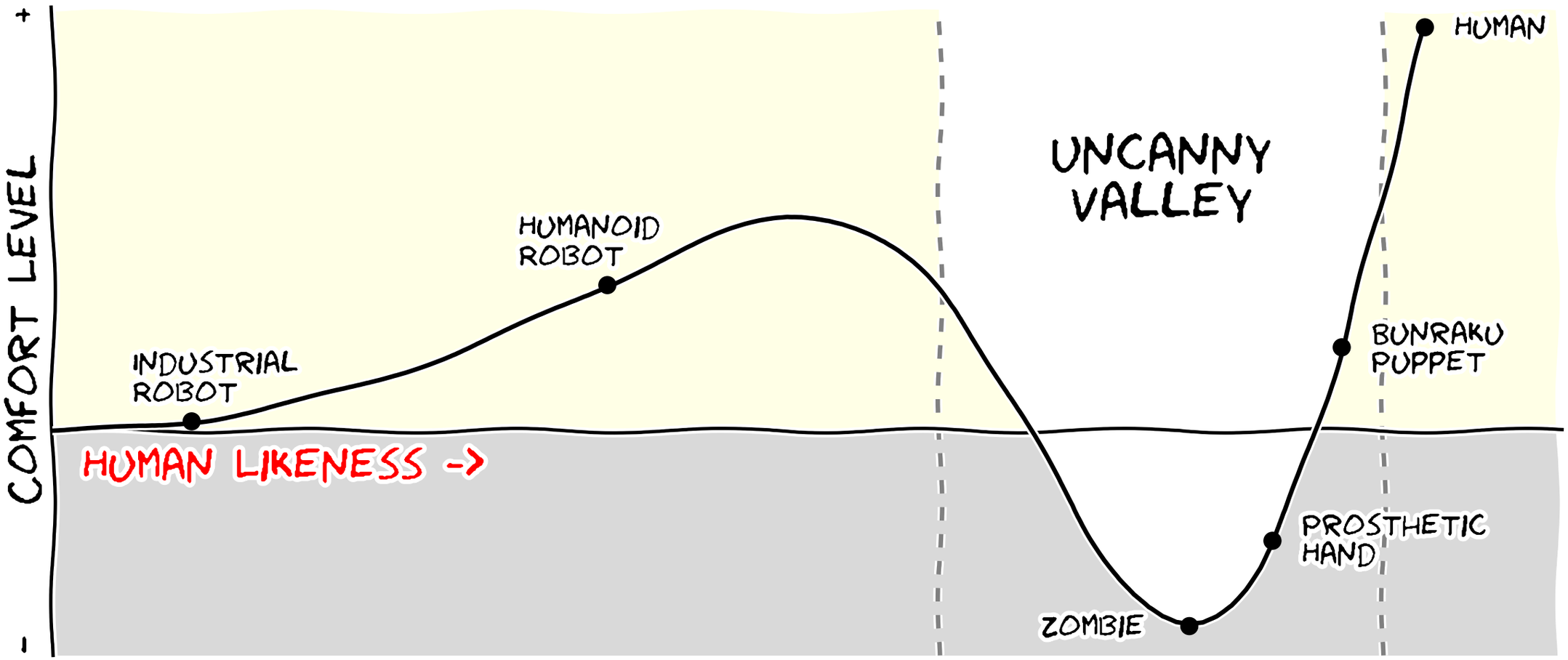




Rule 8 bis: Less is more



Rule 9: Message trumps beauty

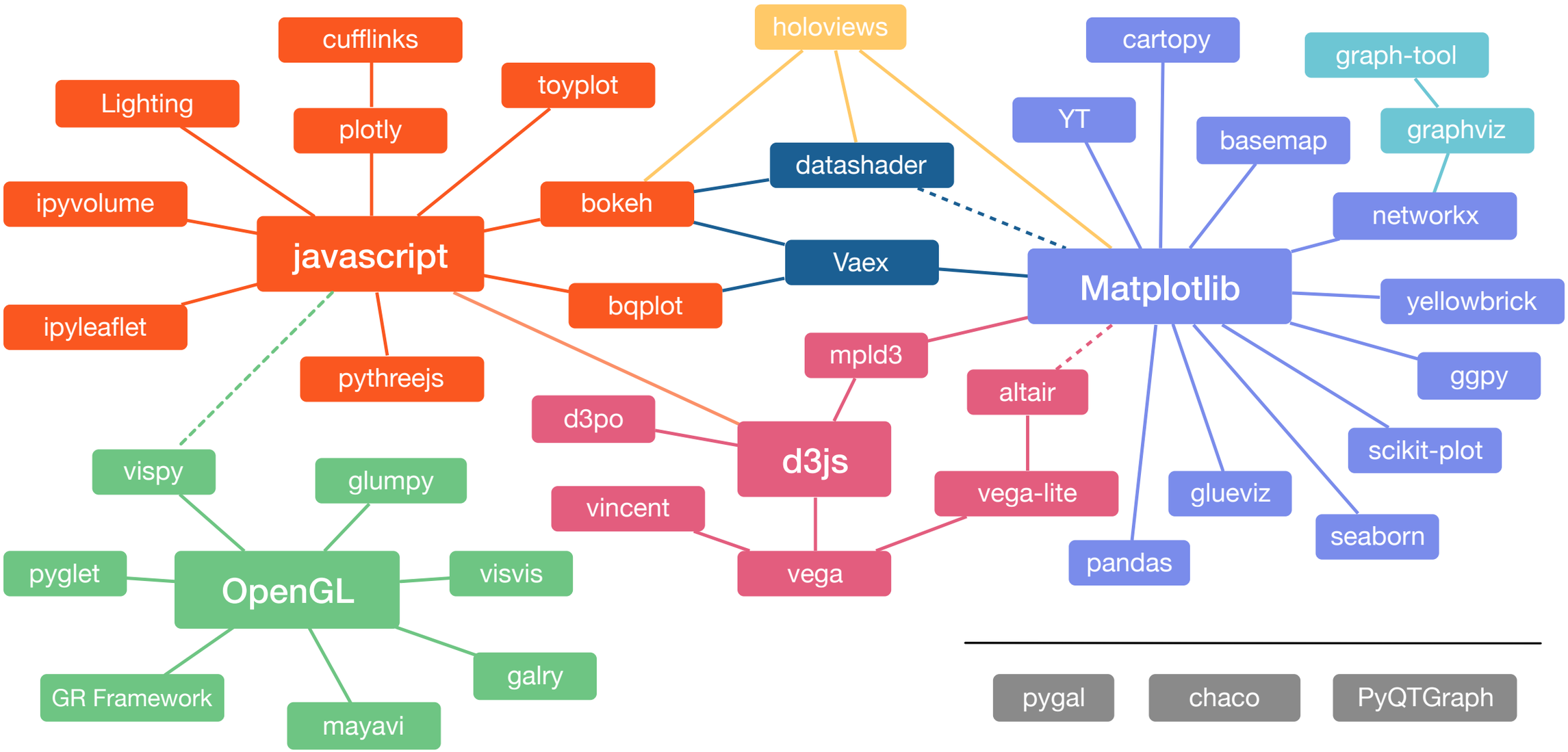


Rule 10: Get the right tool

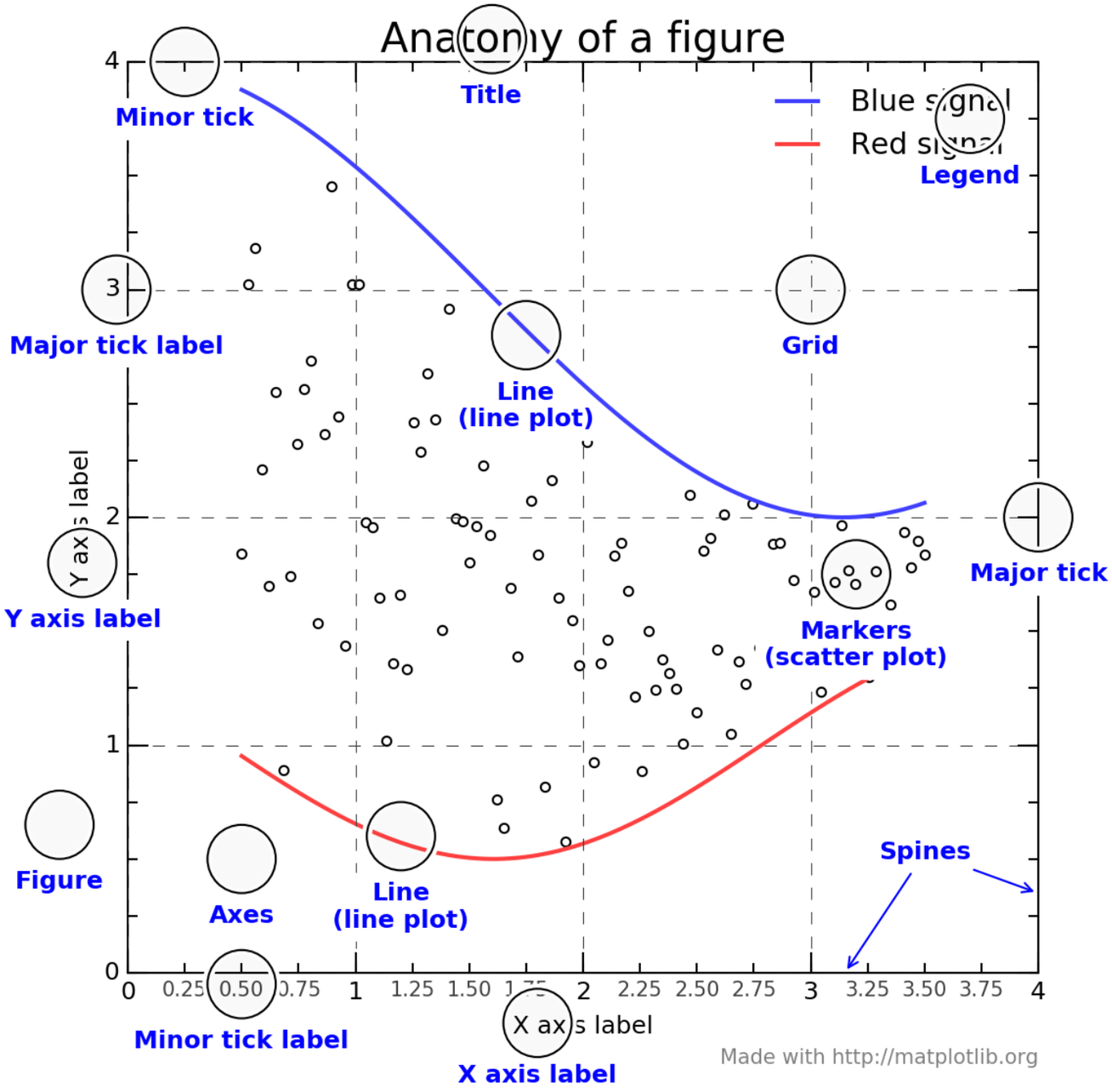
- PDFCrop (remove white borders)
  http://pdfcrop.sourceforge.net
- GraphViz (easy graph)
  http://www.graphviz.org
- ImageMagick (scripted image processing)
  http://www.imagemagick.org/script/index.php
- Gimp (bitmap image manipulation)
  https://www.gimp.org
- Inkscape (vector image manipulation)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

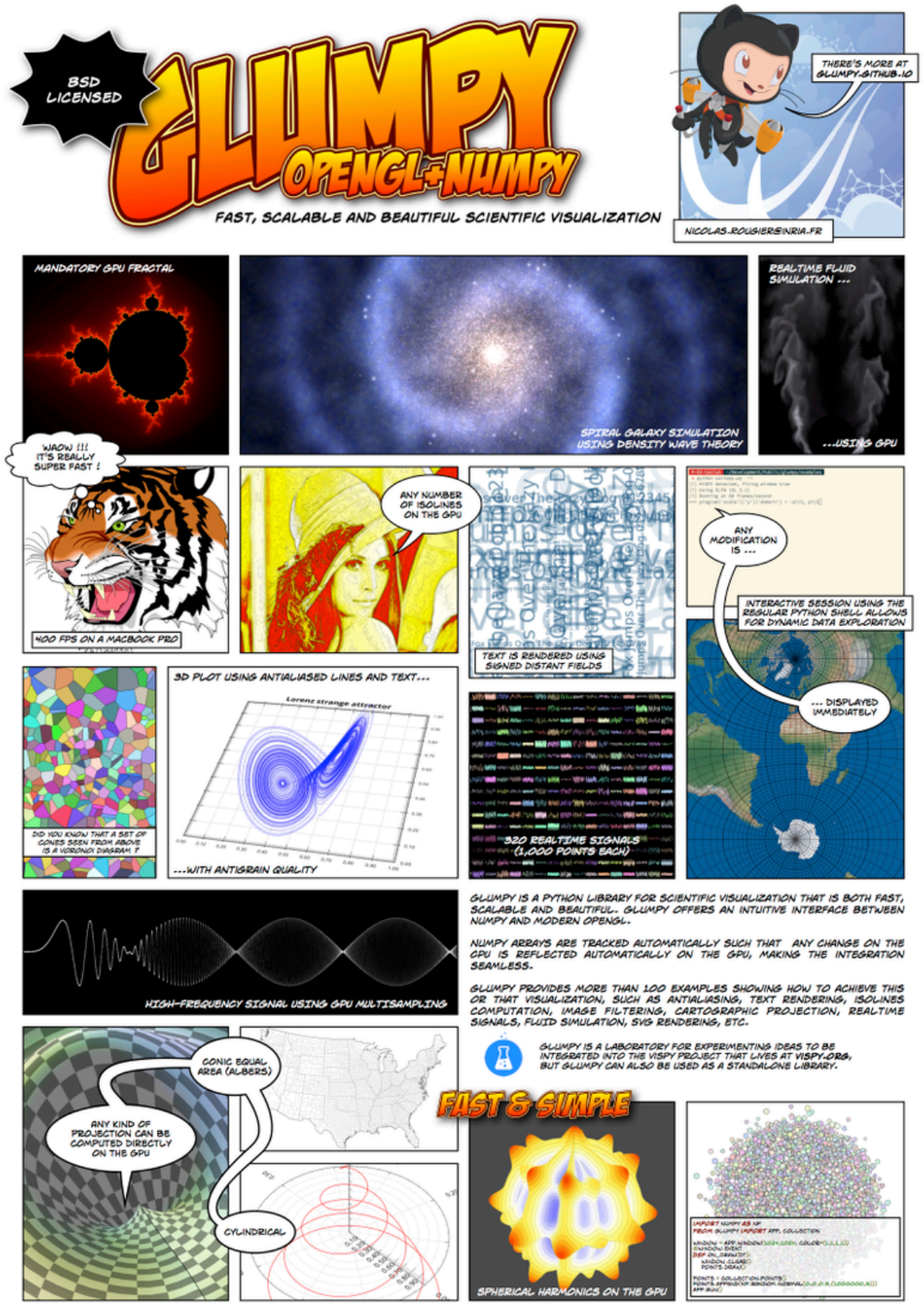
Python Visualization Landscape

Jake VanderPlas, Pycon 2017



Showtime !


Anatomy of a figure
Title
Minor tick
Major tick label
Line
(line plot)
Grid
Blue signal
Red signal
Legend
Y axis label
Markers
(scatter plot)
Major tick
Figure
Axes
Line
(line plot)
Spines
Minor tick label
X axis label
X axis label
Made with http://matplotlib.org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TEXT IS RENDERED USING SIGNED DISTANT FIELDS
ANY MODIFICATION IS ...
INTERACTIVE SESSION USING THE REGULAR PYTHON SHELL ALLOWS FOR DYNAMIC DATA EXPLORATION
... DISPLAYED IMMEDIATELY
3D PLOT USING ANTIALIASED LINES AND TEXT...
Lorenz strange attractor
...WITH ANTIGRAIN QUALITY
DID YOU KNOW THAT A SET OF CONES SEEN FROM ABOVE IS A VORONOI DIAGRAM ?
320 REALTIME SIGNALS (1,000 POINTS EACH)
HIGH-FREQUENCY SIGNAL USING GPU MULTISAMPLING
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NUMPY ARRAYS ARE TRACKED AUTOMATICALLY SUCH THAT ANY CHANGE ON THE CPU IS REFLECTED AUTOMATICALLY ON THE GPU, MAKING THE INTEGRATION SEAMLESS.
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Enough, theory, let's practice !

github.com/rougier/larochelle-2017
github.com/rougier/matplotlib-tutorial
github.com/rougier/ten-rules
github.com/rougier/less-is-more
github.com/rougier/figure-anatomy
github.com/gumpy/glumpy