# Hands-on session: Python

## Research Data Visualisation Workshop

The James Hutton Institute

Leighton Pritchard[1,2,3]
[1]Information and Computational Sciences,
[2]Centre for Human and Animal Pathogens in the Environment,
[3]Dundee Effector Consortium,
The James Hutton Institute, Invergowrie, Dundee, Scotland, DD2 5DA

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# What I do

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- Computational biologist (1996-present)
  - protein sequence-structure-function (1996-1999)
  - yeast metabolism (1999-2003)
  - plant pathology (2003-present)
- Large datasets
  - sequence/genomic
  - metabolomics
  - statistics
  - geographical
- Visualisation as communication to (wet) biologists
  - protein structures
  - metabolic flux
  - comparative genomics/evolution
  - statistical plots

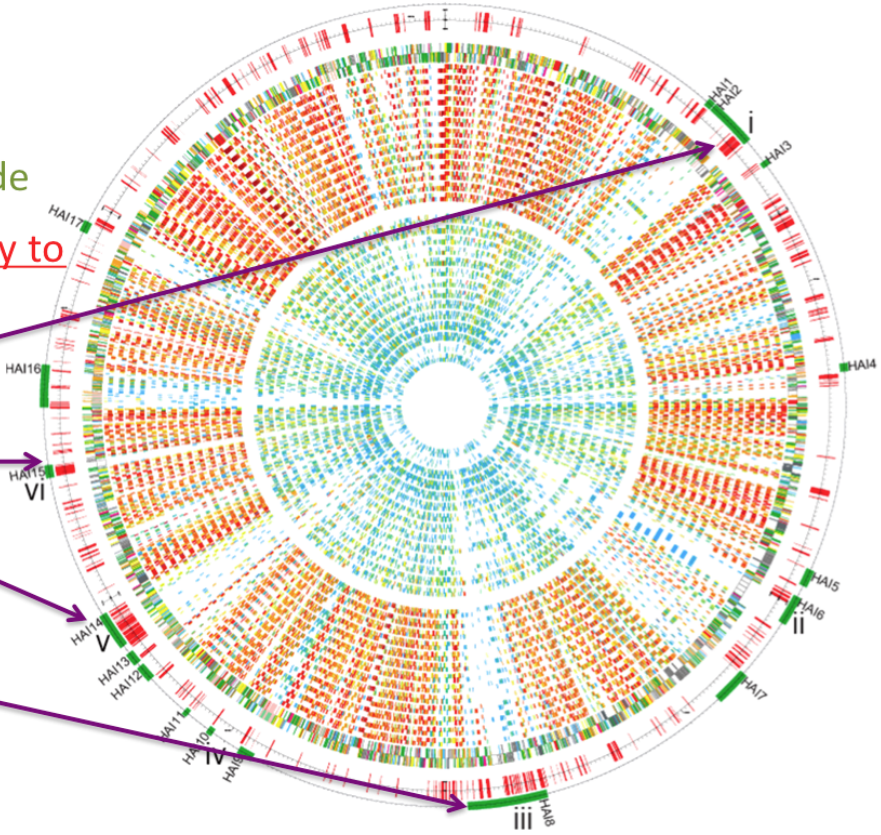
# Big data...


LET'S SOLVE THIS PROBLEM BY USING THE BIG DATA NONE OF US HAVE THE SLIGHTEST IDEA WHAT TO DO WITH
TOM FISH BURNE
©marketoonist.com

# GenomeDiagram [a] [b] [c]

[a] Pritchard *et al.* (2006) *Bioinformatics* doi:10.1093/bioinformatics/btk021
[b] Toth *et al.* (2006) *Ann. Rev. Phytopath.* doi:10.1146/annurev.phyto.44.070505.143444
[c] http://biopython.org

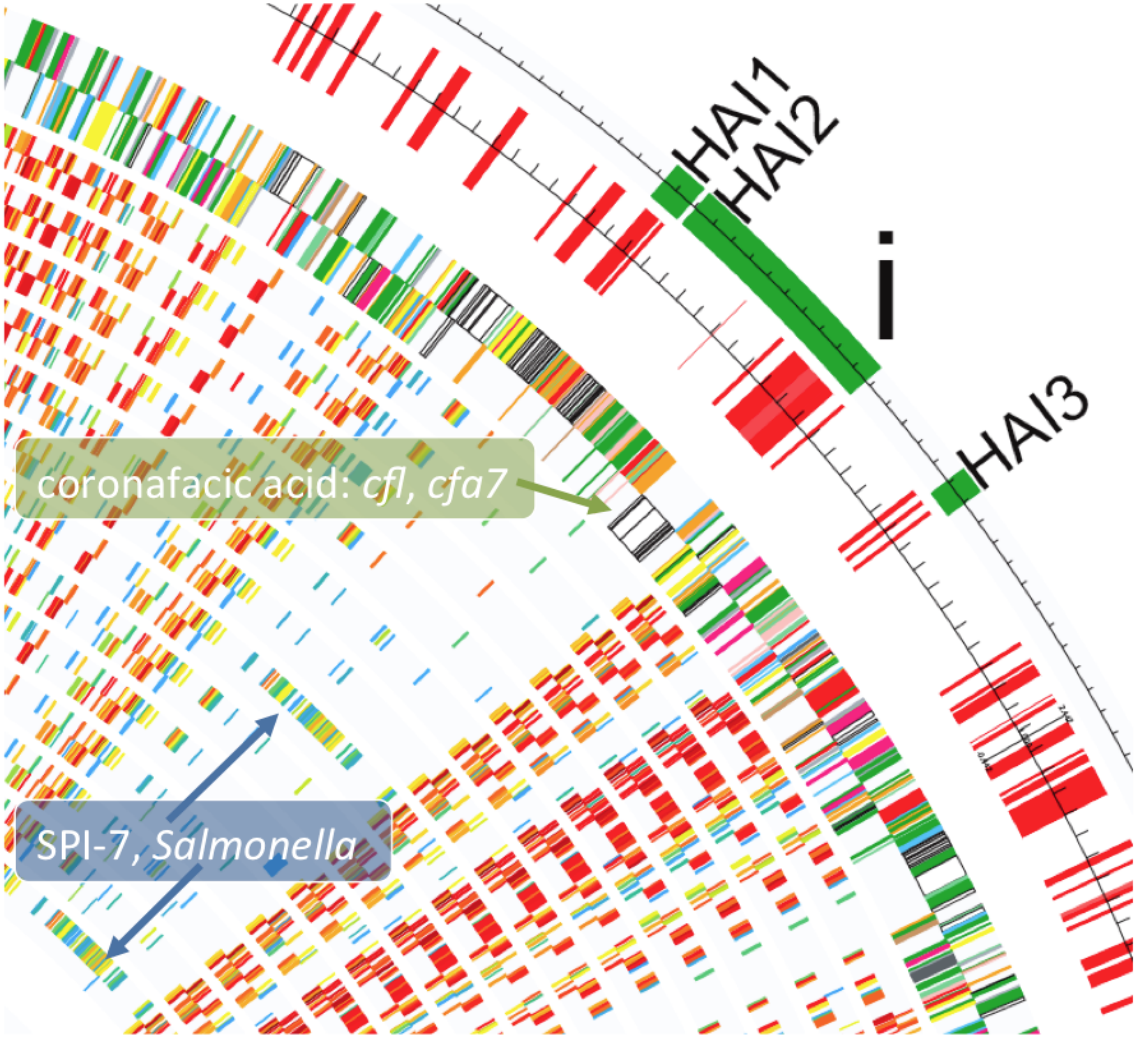
- Comparison against plant- (13) and animal-associated (14) bacteria
- Plant-associated in centre
- Animal-associated on outside
- Red marks: greater similarity to plant-associated bacteria
- **HAI2**: Phytotoxin
- **HAI15**: Adherence
- **HAI14**: Nitrogen fixation
- **HAI8**: T3SS



# Functional adaptation in Pba [a] [b]

[a] Toth *et al.* (2006) *Ann. Rev. Phytopath.* doi:10.1146/annurev.phyto.44.070505.143444

[b] http://biopython.org




Coronatine (*P. syringae*) interferes with jasmonate responses in host, as a jasmonate mimic

Coronafacic acid – *Pseudomonas syringae* phytotoxin precursor (coronatine)
- payload

SPI-7 - *Salmonella* Typhi Pathogenicity island
- delivery system

# GenomeDiagram/SciArt [a] [b] [c]

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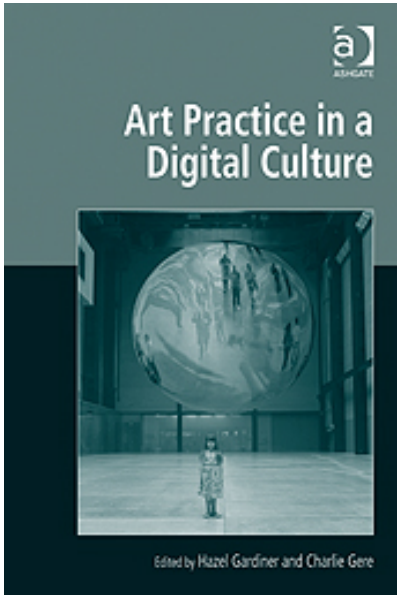
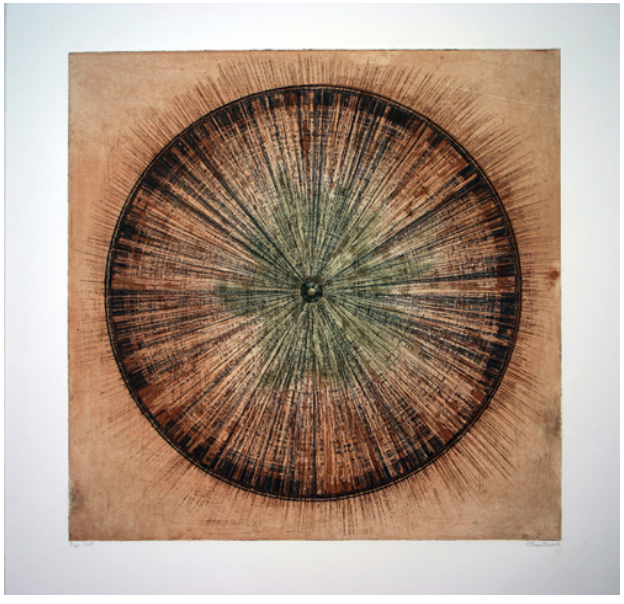
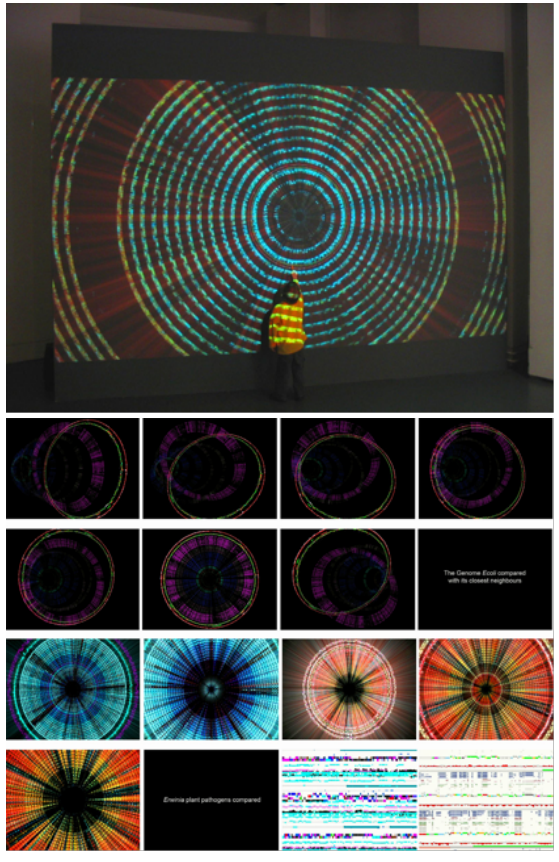
[a] Pritchard *et al.* (2006) *Bioinformatics* doi:10.1093/bioinformatics/btk021

[b] Shemilt (2009) in "Digital Visual Culture: Theory and Practice" ISBN 978-1-84150-248-9

[c] Shemilt (2010) in "Art Practice in a Digital Culture", ISBN 978-0-7546-7623-2





## Influence

Free open-source comparative genomics visualisation library

BIOPYTHON

## Impact

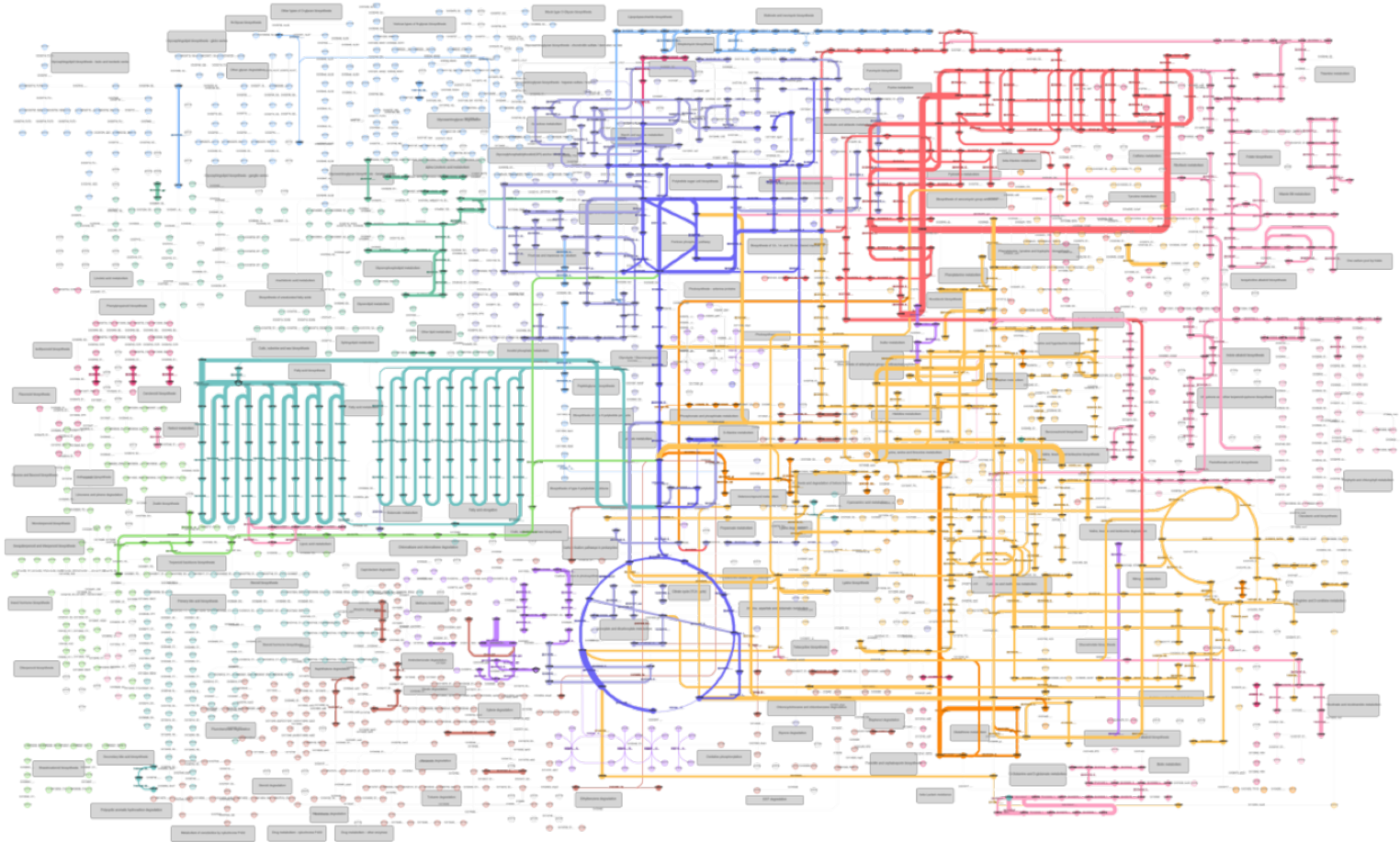
Artwork (prints, audio-visual installation) exhibited in UK and internationally

# Comparative metabolism [a] [b] [c]

[a] Biopython KGML/KEGG visualisation module

[b] https://github.com/widdowquinn/Notebooks-Bioinformatics

[c] http://biopython.org



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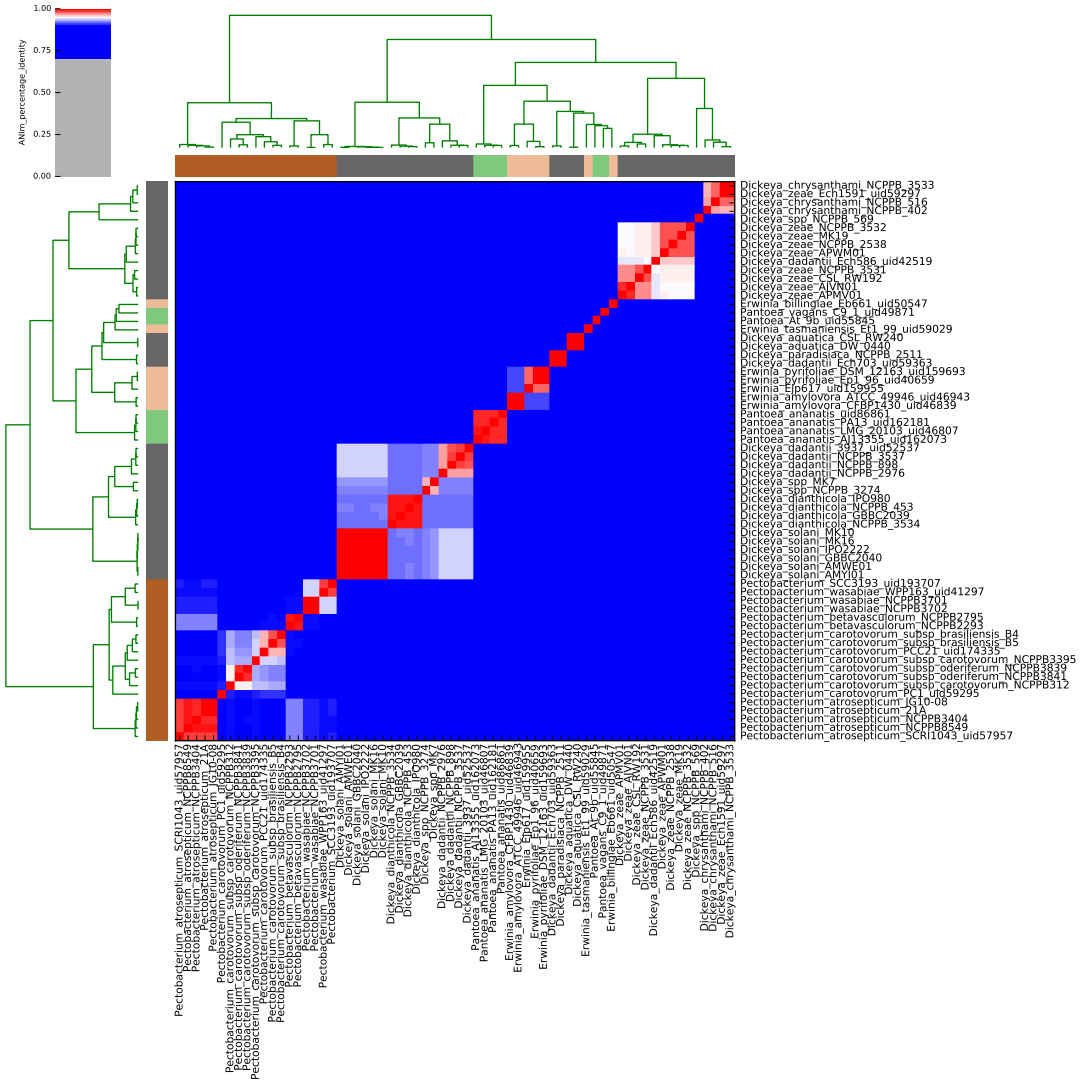
# PyANI: prokaryote classification [a] [b]

[a] http://widdowquinn.github.io/pyani/

[b] Pritchard *et al.* (2016) *Anal. Methods* doi:10.1039/C5AY02550H



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# Data visualisation is art and science

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. . .storytelling in pictorial or graphical format

- Stories to yourself (sense-making)
- Stories to others (communication)
- Cautionary tales

# Data visualisation is art and science

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. . .storytelling in pictorial or graphical format

- Stories to yourself (sense-making)
  - summarise big stories quickly
  - data exploration and mining
  - identify areas/items of importance
  - find relationships and patterns
- Stories to others (communication)

- Cautionary tales

# Data visualisation is art and science

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# Data visualisation is art and science

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  - demonstrate significance
- Cautionary tales
  - avoid distortion
  - make the reader think about the data, not the presentation
  - avoid *chartjunk* (excessive decoration)
  - aim for high data:ink ratio

# The point of data visualisation [a]

[a] https://en.wikipedia.org/wiki/Data_visualization

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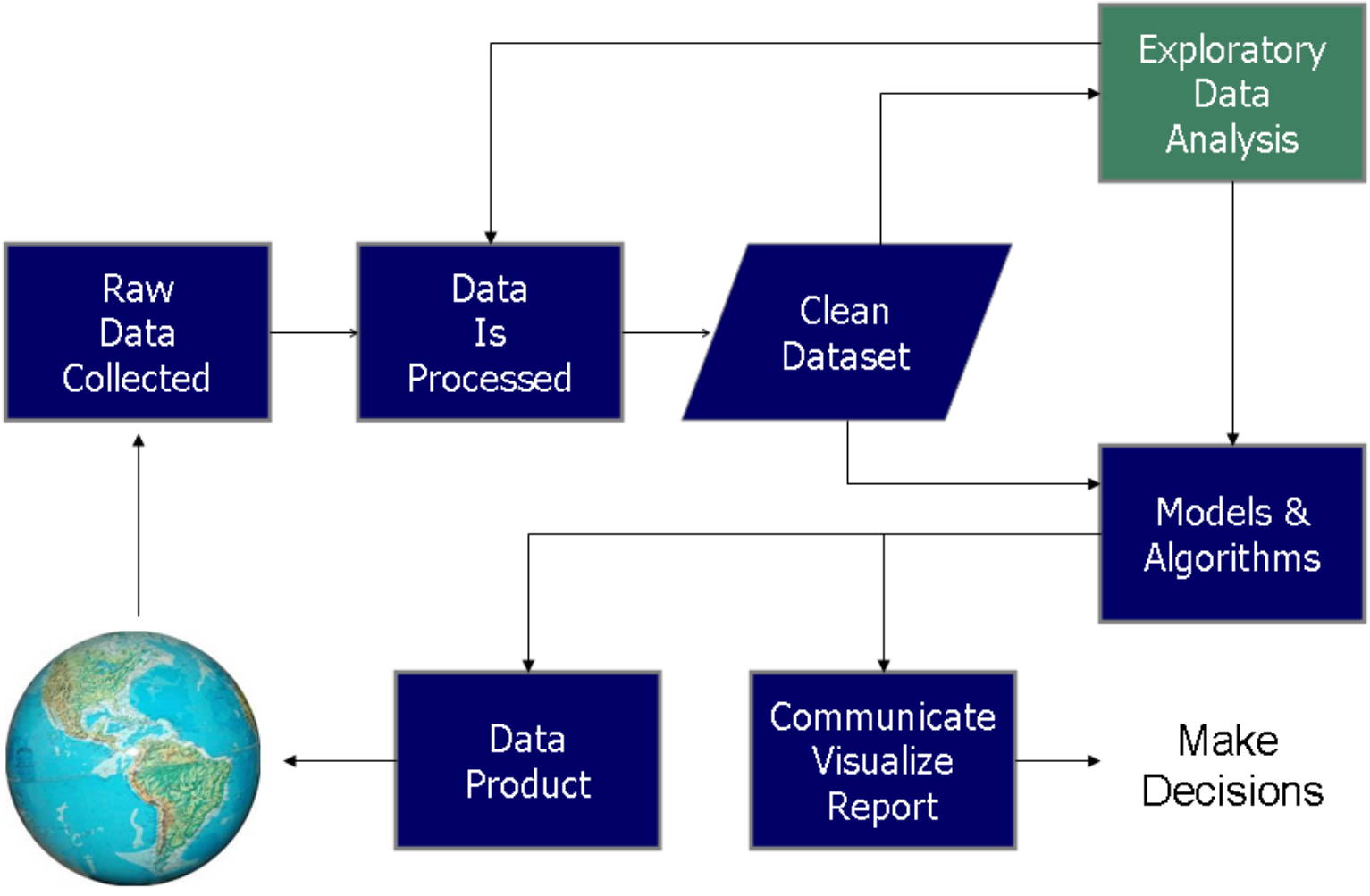
## Where does visualisation belong?



# Communicating effectively

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- Understand the data
- Know (or be receptive to) the message
- Know your audience

# Communicating effectively

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- Understand the data
  - size
  - cardinality
  - meaning
  - relationships
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The James Hutton Institute

- Understand the data
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- Know (or be receptive to) the message
  - what does pictorial representation mean?
  - match graphical relationships to data relationships
- Know your audience

# Communicating effectively

The James Hutton Institute

- Understand the data
  - size
  - cardinality
  - meaning
  - relationships
- Know (or be receptive to) the message
  - what does pictorial representation mean?
  - match graphical relationships to data relationships
- Know your audience
  - how do people process pictorial information
  - how does your audience process information
  - domain-specific representations

# A model of communication [a]

[a] Randy Olson (2009) *Don't Be Such a Scientist*

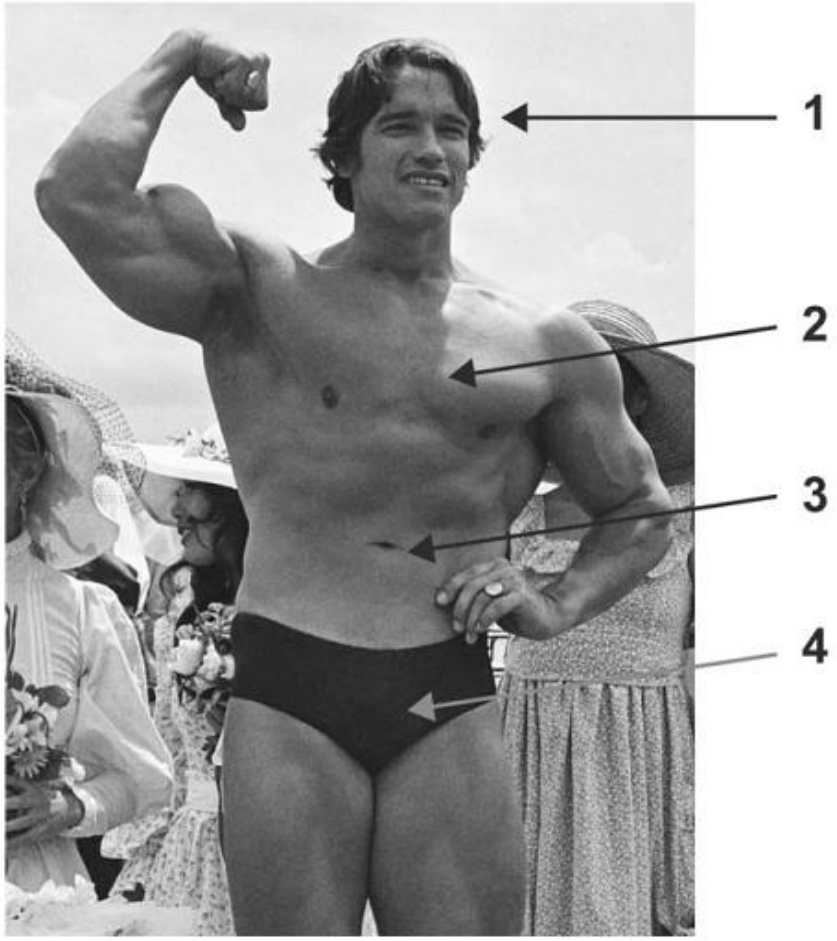


**Figure 1-1.** The four organs of mass communication. To reach the broadest audience, you need to move the process out of the *head* (1) and into the *heart* (2) with sincerity, into the *gut* (3) with humor and intuition, and, ideally, if you're sexy enough, into the *lower organs* (4) with sex appeal. Photo courtesy of © Mirkine/Sygma/Corbis.

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# Elementary Perceptual Tasks [a]

[a] Cleveland & McGill (1984) *J. Am. Stat. Ass.*

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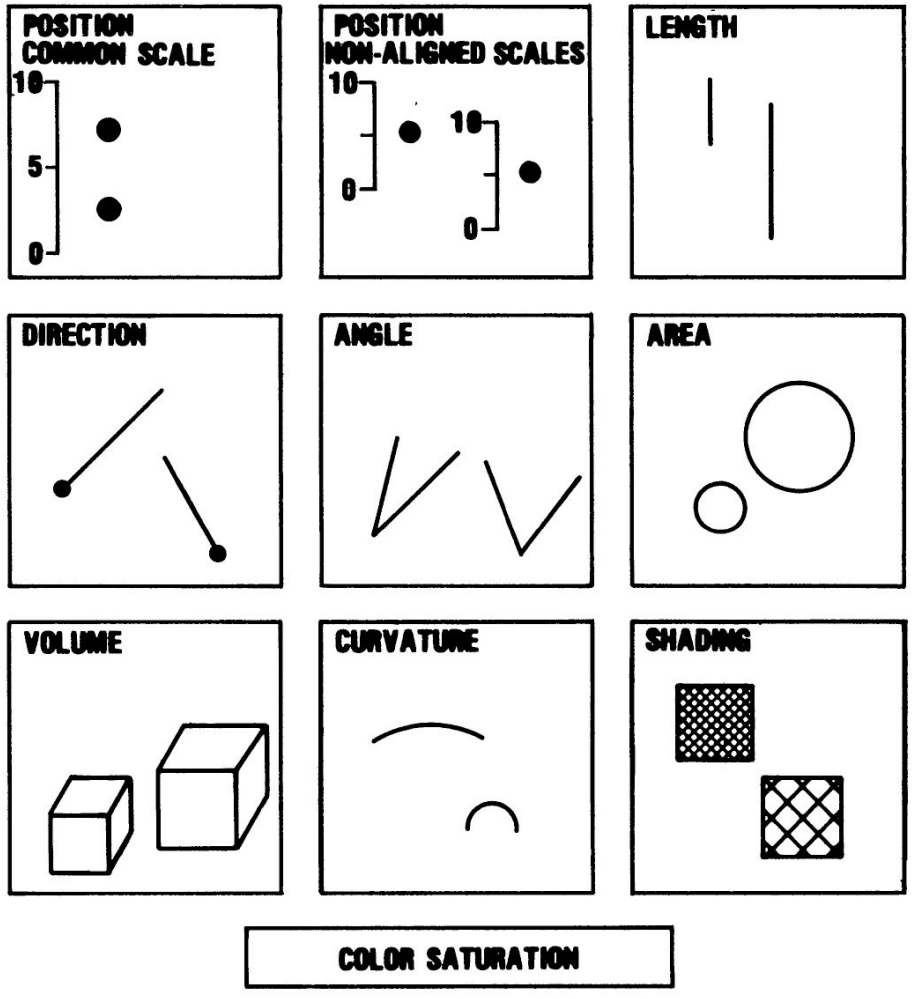
## The most basic visual tasks:

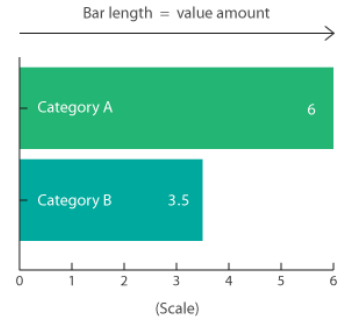


# Implementations [a]

[a] http://www.datavizcatalogue.com/

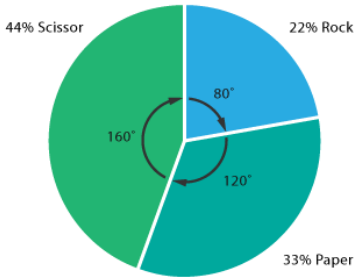
## Position: common scale

- Scatterplot
- Bar Chart



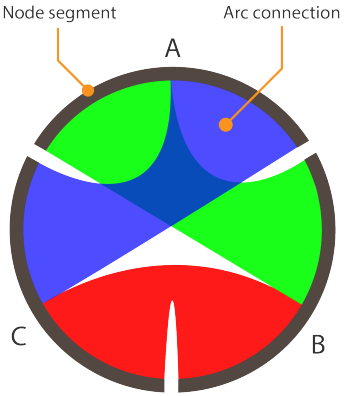

## Angle

- Pie Chart
- Do(ugh)nut Chart




## Curvature

- Arc Diagram
- Chord Diagram



# Gestalt principles [a]

[a] https://emeeks.github.io/gestaltdataviz

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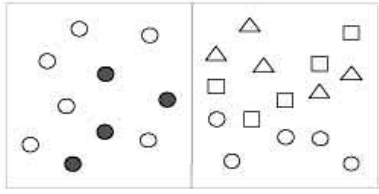
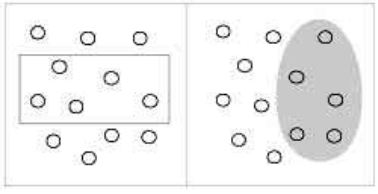
- **proximity**: close objects perceived as groups

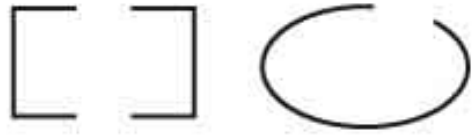
- **similarity**: similar attributes perceived as groups



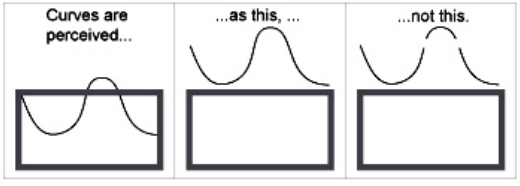
- **enclosure**: bounded objects perceived as groups



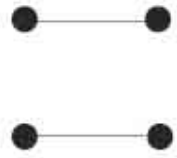
- **closure**: open objects perceived as complete



- **continuity**: aligned objects perceived as continuous




- **connection**: connected items perceived as groups



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# What works best? Experiment [a] [b]

[a] Cleveland & McGill (1984) *J. Am. Stat. Ass.*
[b] Heer & Bostock (2010) *CHI 2010*

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## Empirical measurements of interpretation

- Subjects shown graphs representing same data
- ($\log_2$) error in subjects' accuracy compared by graph type

## Judgement types

- 1-3: Position on a common scale (bar chart, stacked bar chart)
- 4-5: Length encoding (stacked bar chart)
- 6: Angle (pie chart)
- 7-9: Area (bubble chart, aligned rectangles, treemap)

# What works best? Result [a] [b]

[a] Cleveland & McGill (1984) *J. Am. Stat. Ass.*
[b] Heer & Bostock (2010) *CHI 2010*

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- We have inherent biases that can distort information recovered
- Position > Angle ≈ Length > Area
- Accuracy plateaus as charts increase in size
- Gridlines improve accuracy
- Aspect ratios affect area judgements (squares worst)

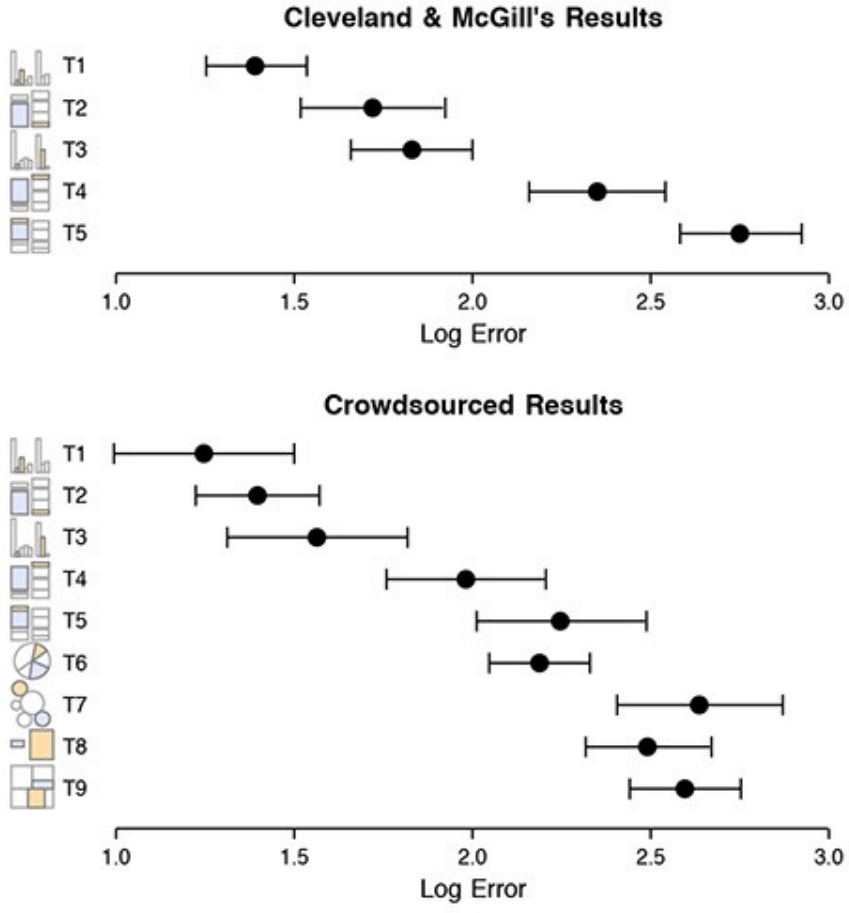


Figure 4: Proportional judgment results (Exp. 1A & B). Top: Cleveland & McGill's [7] lab study. Bottom: MTurk studies. Error bars indicate 95% confidence intervals.

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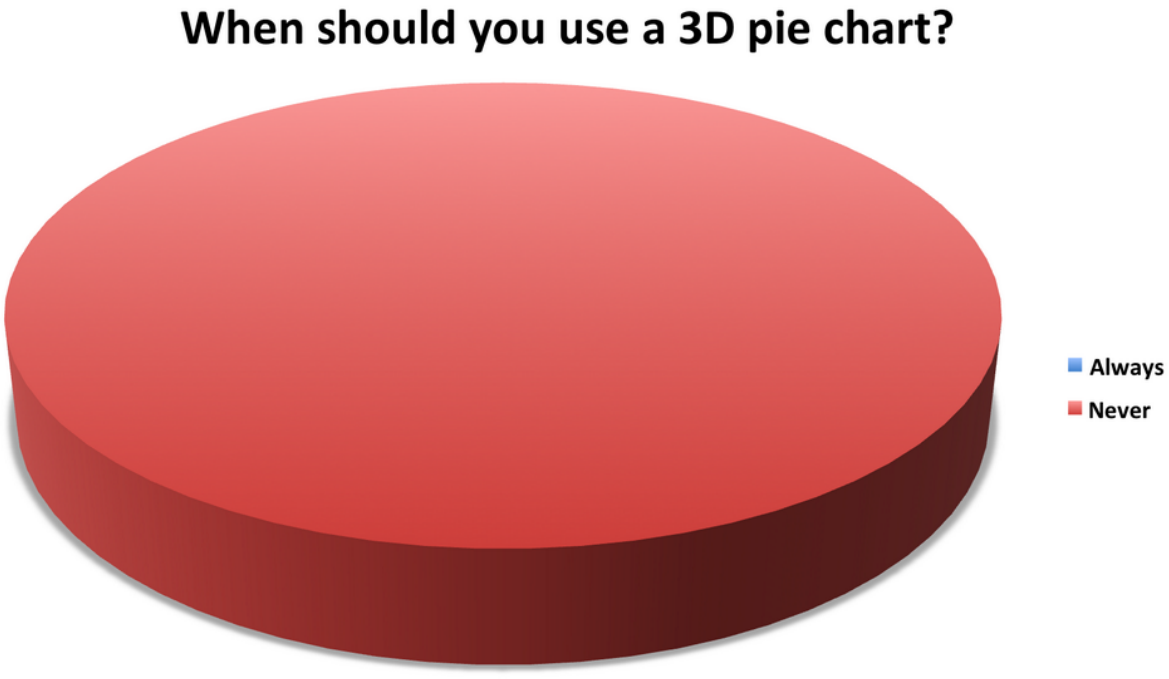
# People hate pie charts

http://www.storytellingwithdata.com/blog/2011/07/death-to-pie-charts

**especially Edward Tufte**

A table is nearly always better than a dumb pie chart; the only worse design than a pie chart is several of them[...] pie charts should never be used. - *"The Visual Display of Quantitative Information"*



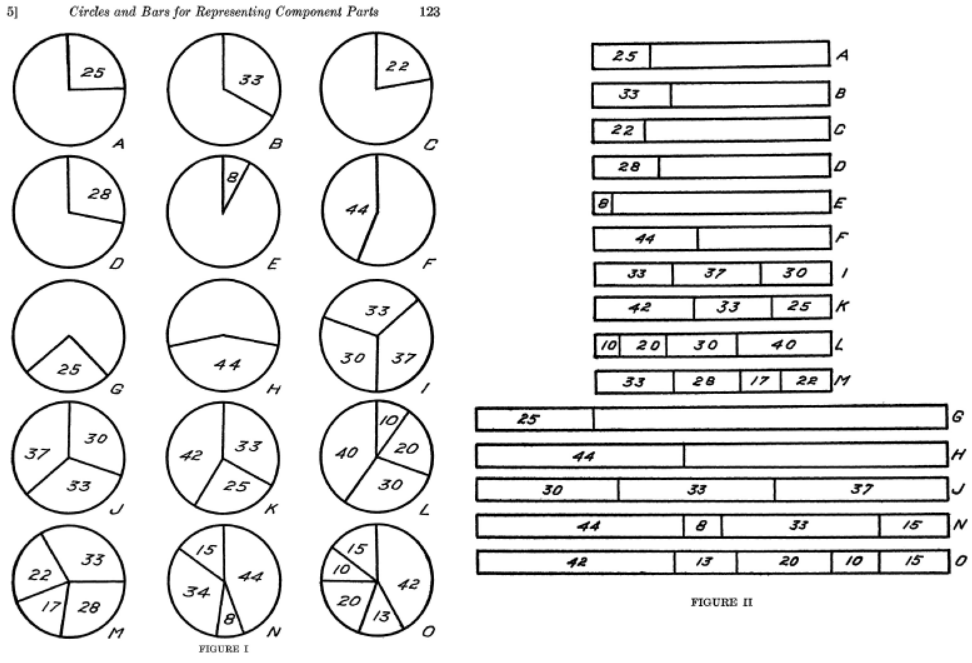

# "E pur si muove..." [a] [b]

[a] Eells (1926) *J Am. Stat. Ass.*

[b] Simkin & Hastie (1987) *J Am. Stat. Ass.*

## For proportions of a whole:

- Pie charts read as accurately as bar charts
- As number of components in the chart increases, bars are less efficient than pie charts



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# Bar charts are bad...mmmkay?

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There is an ongoing backlash against bar charts

(and I'm not picking on Nick, he just tweets a lot...)



But are they really that bad?

# Interpretation of bars and lines [a]

[a] Zacks & Tversky (1999) *Mem. Cognit.*

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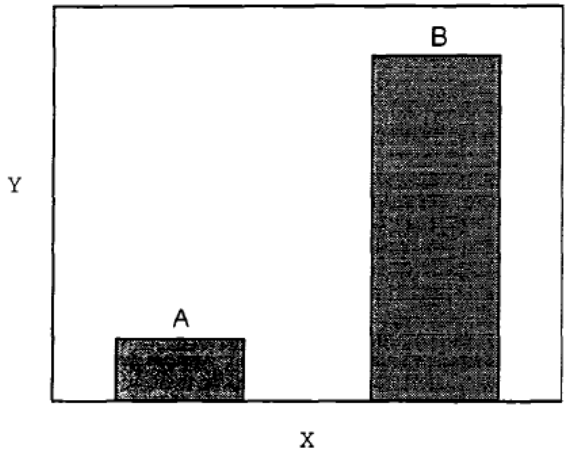
## People interpret bars and lines differently

Experiment 1: In absence of context (arbitrary $X$, $Y$)

- **bars**: discrete comparison (24:0)
- **lines**: trend assessment (0:35)



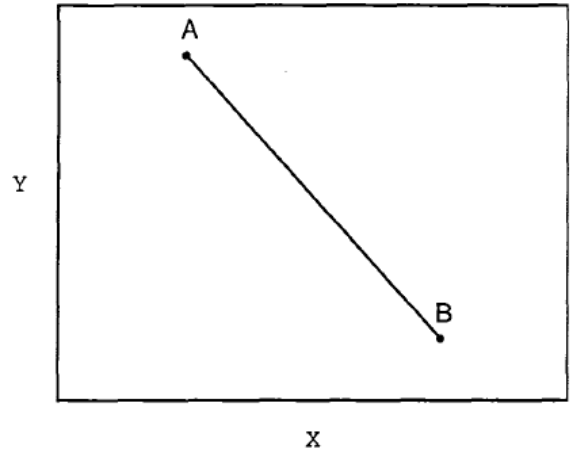




**Figure 1:** Examples of the bar and line graph stimuli used in Experiment 1.

# Interpretation of bars and lines [a]

[a] Zacks & Tversky (1999) *Mem. Cognit.*

## People interpret bars and lines differently

Experiment 2: With context (discrete or continuous data)

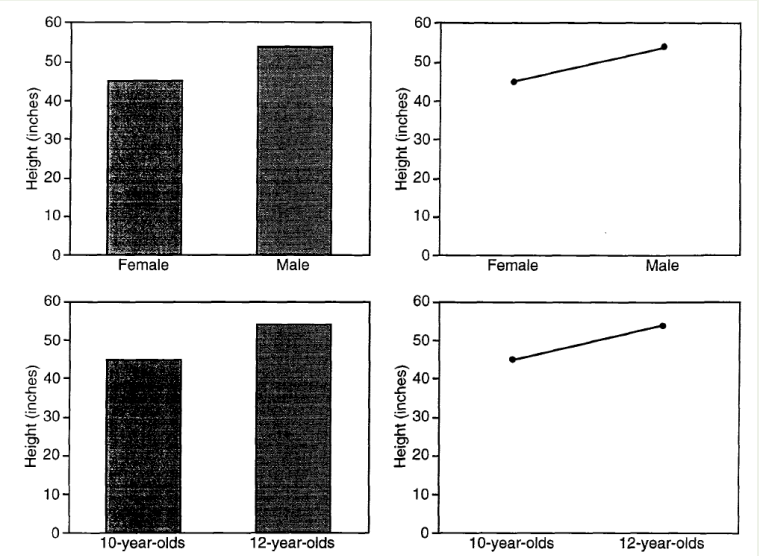



**Figure 2:** Examples of the bar and line graph stimuli, and the continuous and discrete conceptual domains used in Experiment 2.

| | Gender (discrete domain) | | Age (continuous domain) | |
|---|---|---|---|---|
| | Bar graph | Line graph | Bar graph | Line graph |
| Discrete comparison | 28 | 22 | 28 | 9 |
| Trend assessment | 0 | 3 | 2 | 14 |

Table 2: Frequency of data characterization responses as a function of graph type (bar graph or line graph) and conceptual domain (gender or age).

# Bars vs. lines

- People naturally interpret bar charts as categorical data
- People naturally interpret line graphs as trends
- Using bars for trend data or lines for categorical data can mislead the reader

# Bar charts can mislead [a]

[a] Weissgerber *et al.* (2015) *PLoS Biol.* doi:10.1371/journal.pbio.1002128

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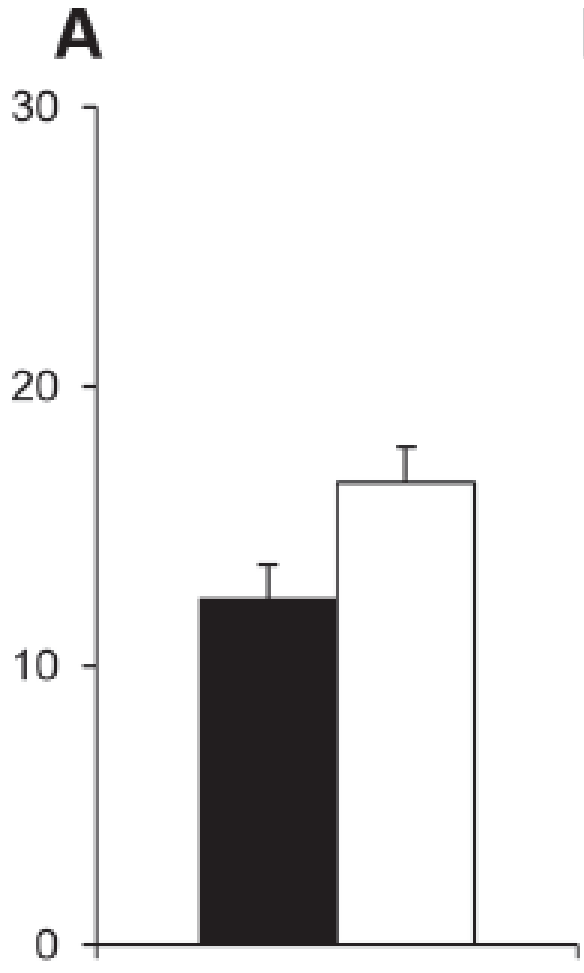
- Do these bars differ in value?



# Bar charts can mislead [a]

[a] Weissgerber *et al.* (2015) *PLoS Biol.* doi:10.1371/journal.pbio.1002128

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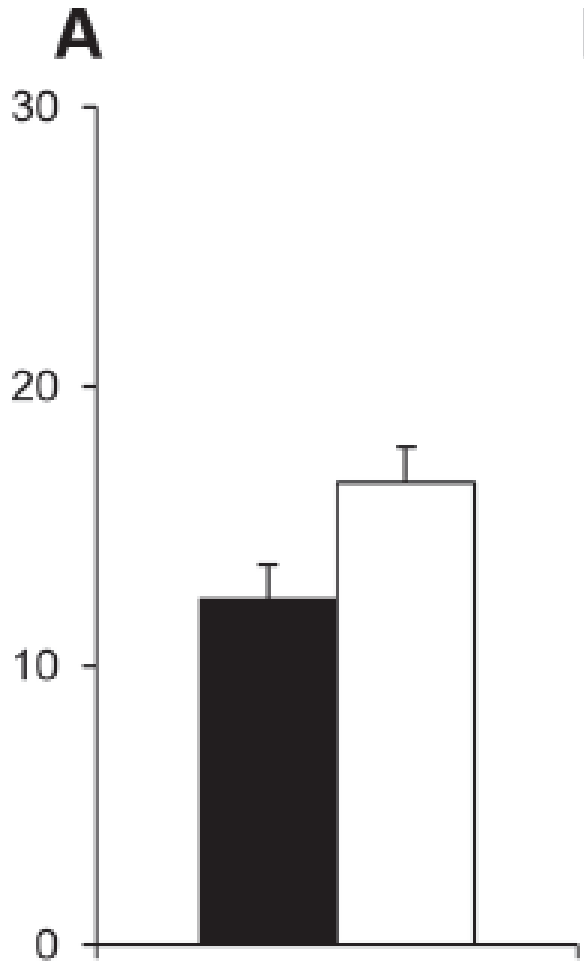
- Do these bars differ in value?
- Bar charts represent data as a single point: lossy compression.
- Could different datasets give the same bar chart?



# Bars are lossy compression [a]

[a] Weissgerber *et al.* (2015) *PLoS Biol.* doi:10.1371/journal.pbio.1002128

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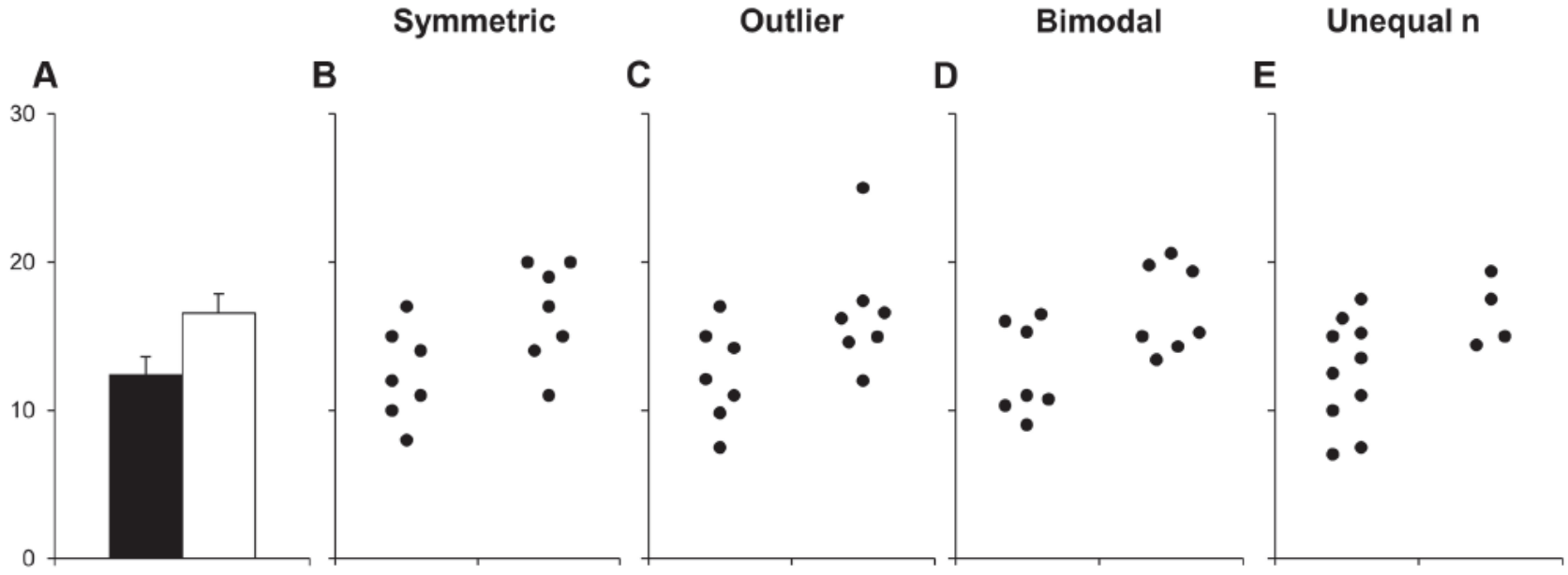
## Bars hide detail:

- Number of data points
- Variance of data points
- Distribution of data points (outliers, etc.)



# Bars may mislead on statistics [a]

[a] Weissgerber *et al.* (2015) *PLoS Biol.* doi:10.1371/journal.pbio.1002128

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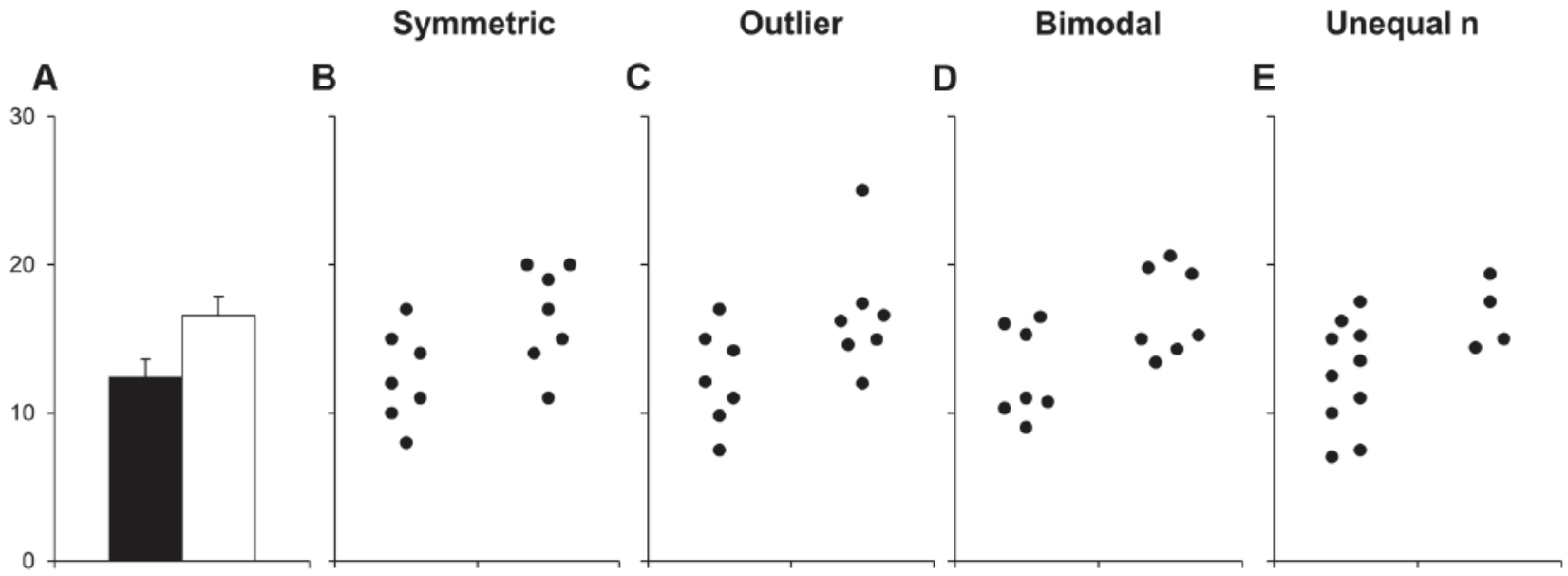
## Bars may imply incorrect test statistics:

Overlaps, outliers, covariates, sample sizes masked




| Test | | | | |
|---|---|---|---|---|
| | p value | | | |
| T-test: Equal var. | 0.035 | 0.050 | 0.026 | 0.063 |
| T-test: Unequal var. | 0.035 | 0.050 | 0.026 | 0.035 |
| Wilcoxon | 0.054 | 0.073 | 0.128 | 0.103 |

# Bars for paired data [a]

[a] Weissgerber *et al.* (2015) *PLoS Biol.* doi:10.1371/journal.pbio.1002128

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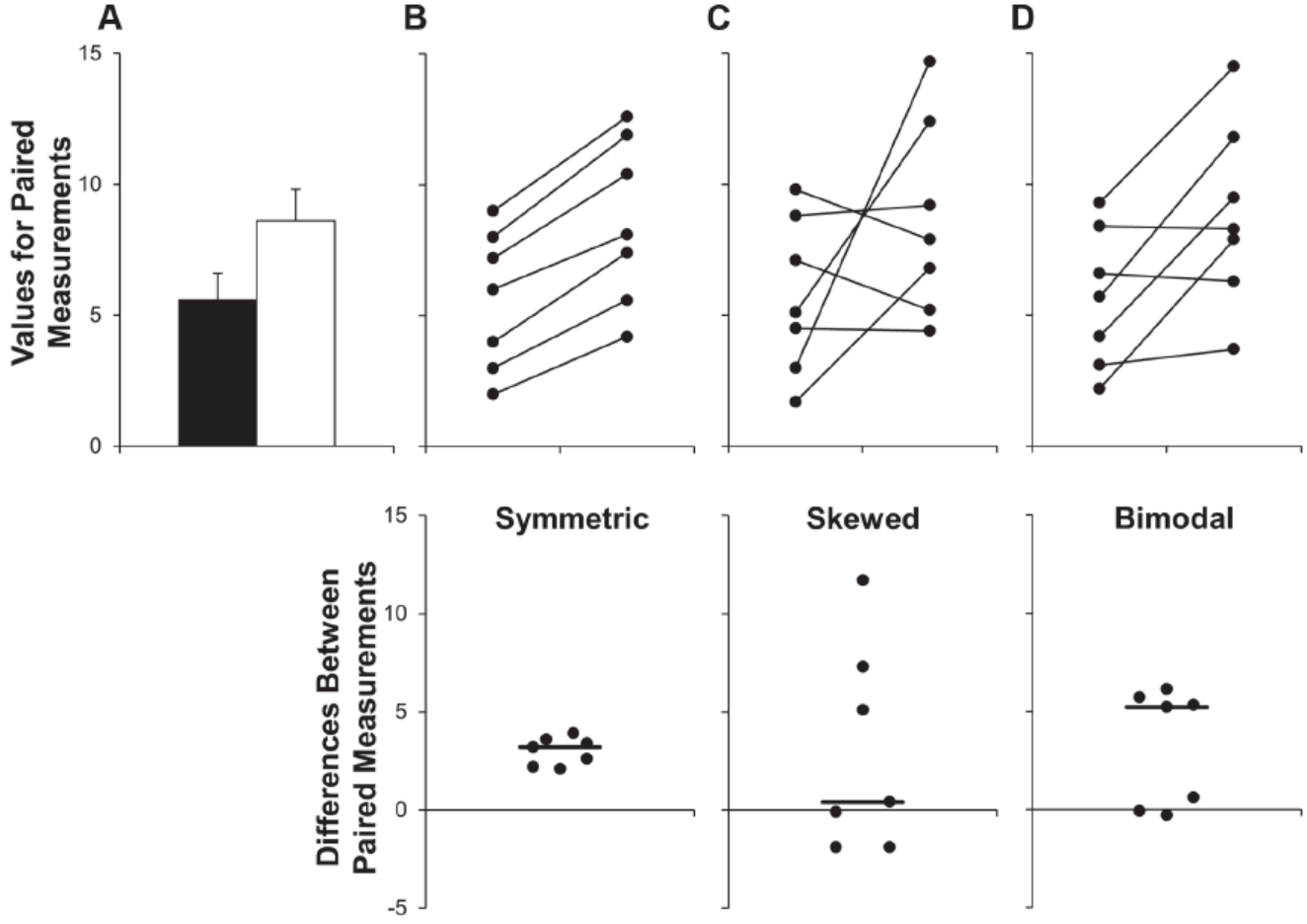
## Bars imply independence of data:



# Better than bar charts?

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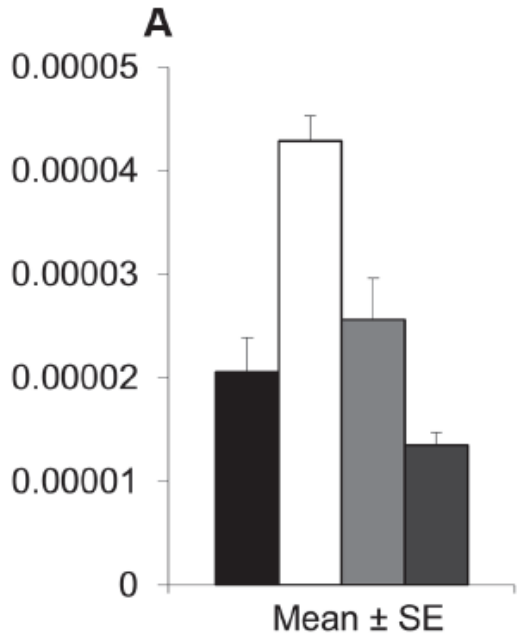
Bar chart with SE bars suggests group 2 is highest



# Better than bar charts?

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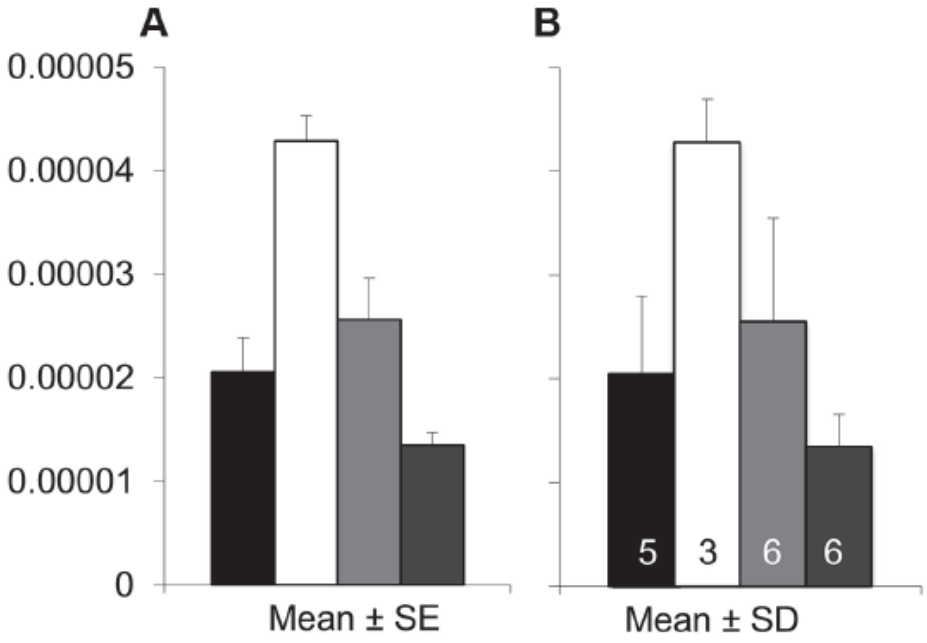
Bar chart with SD bars suggests there is overlap



# Better than bar charts?

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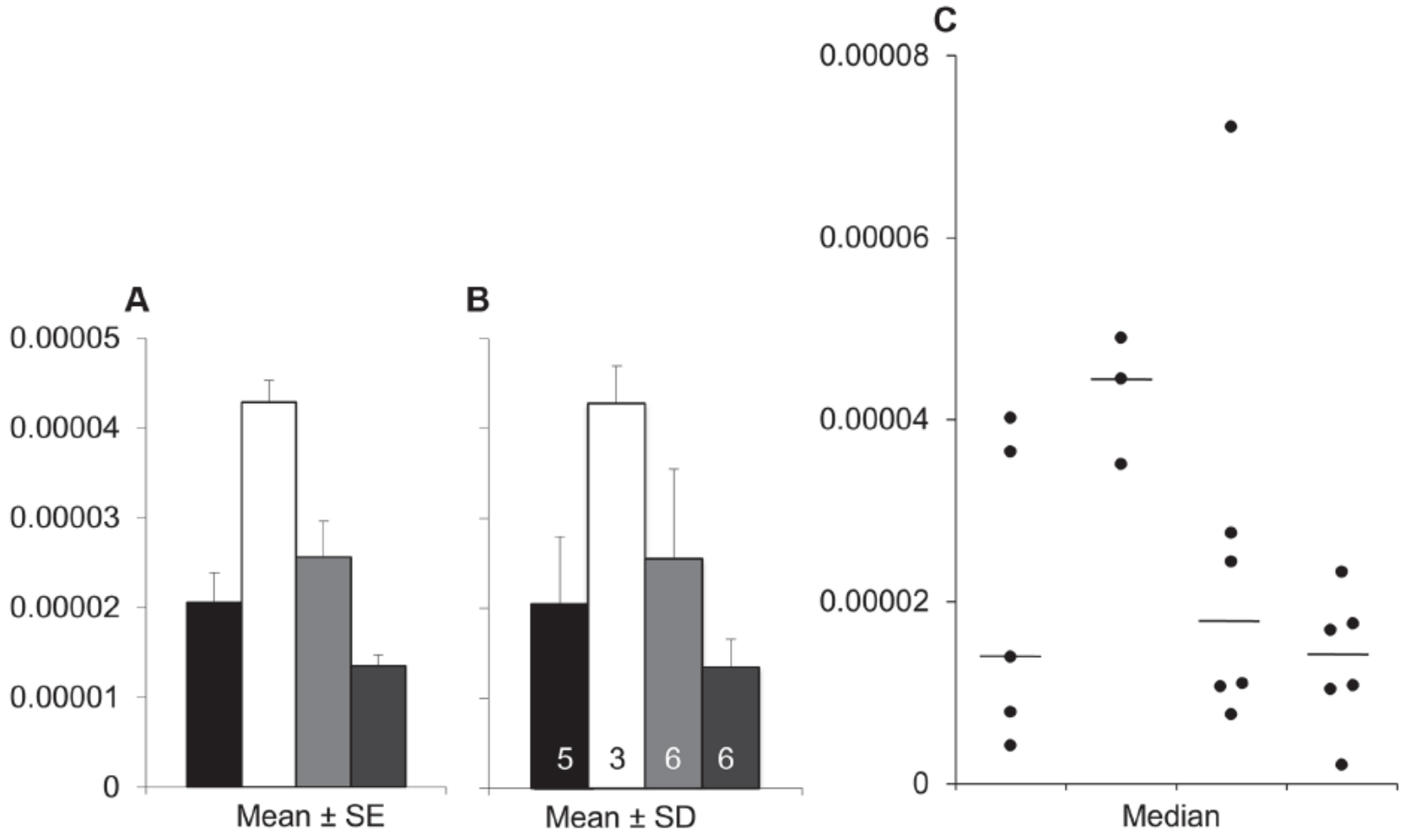
Univariate scatterplots show sample sizes, outliers, variance



# Any chart can mislead

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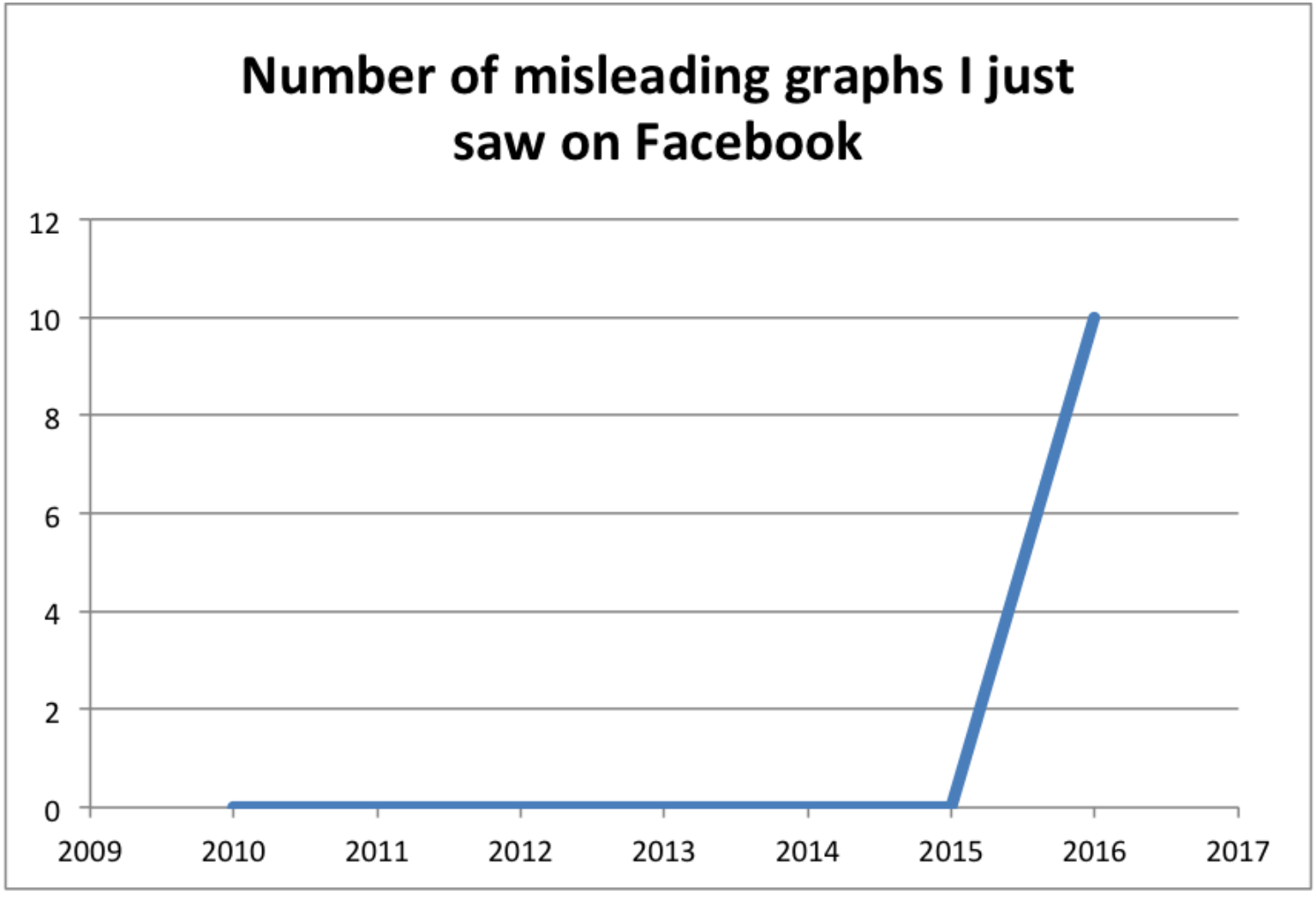
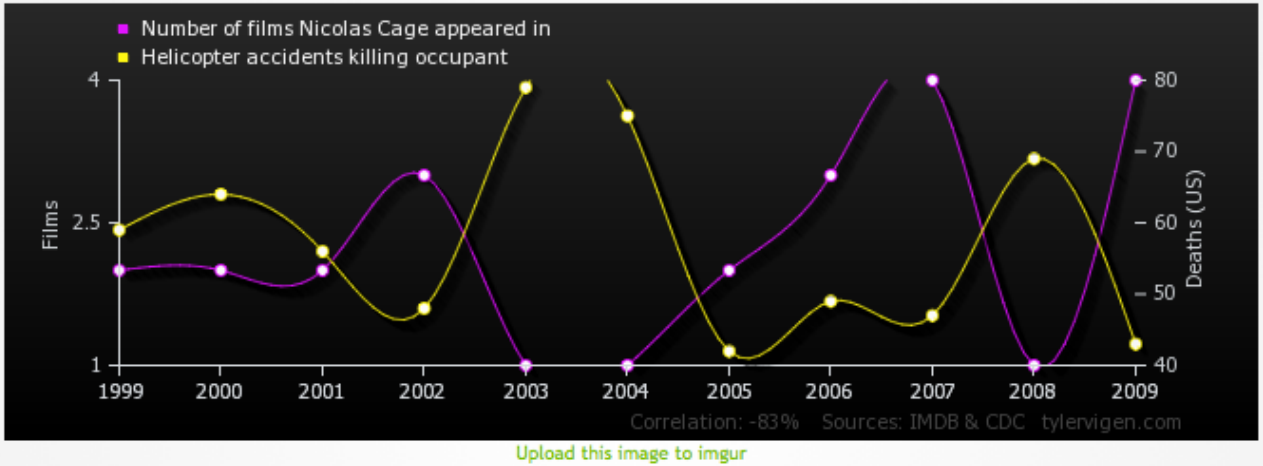


# Any chart can mislead [a]

[a] Spurious Correlations, tylervigen.com

## Number of films Nicolas Cage appeared in
inversely correlates with
## Helicopter accidents killing occupant




Upload this image to imgur

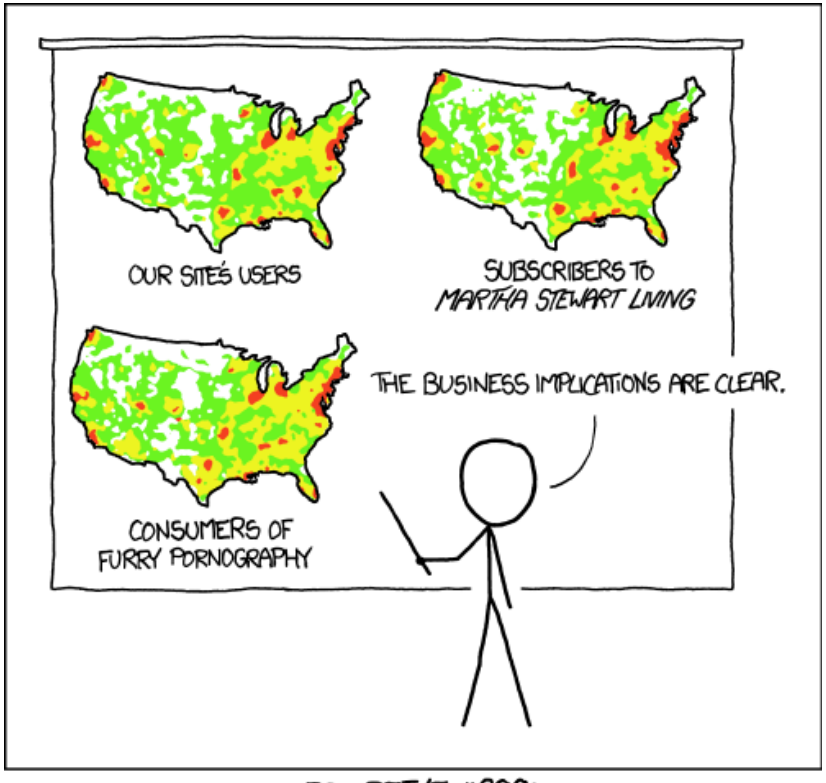
| | 1999 | 2000 | 2001 | 2002 | 2003 | 2004 | 2005 | 2006 | 2007 | 2008 | 2009 |
|---|---|---|---|---|---|---|---|---|---|---|---|
| *Number of films Nicolas Cage appeared in Films (IMDB)* | 2 | 2 | 2 | 3 | 1 | 1 | 2 | 3 | 4 | 1 | 4 |
| *Helicopter accidents killing occupant Deaths (US) (CDC)* | 59 | 64 | 56 | 48 | 79 | 75 | 42 | 49 | 47 | 69 | 43 |

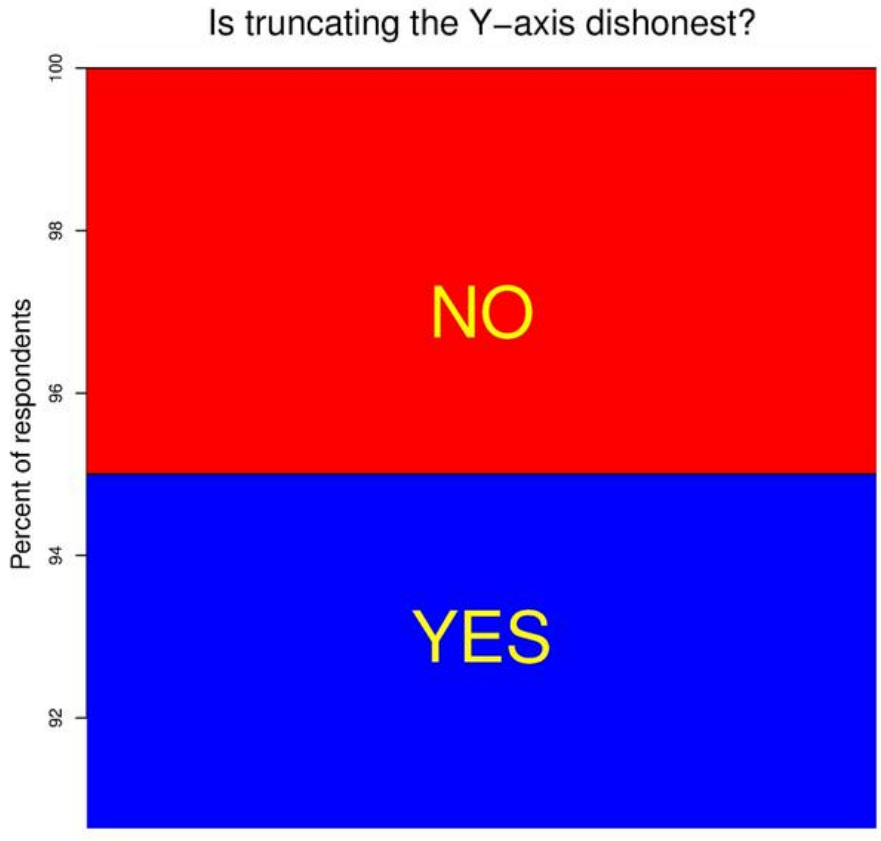
**Correlation: -0.827811**

Permalink - View all correlations - Discover a new correlation

# Any chart can mislead [a]

[a] https://xkcd.com/1138/



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# Scatterplots [a]

[a] http://www.datavizcatalogue.com/

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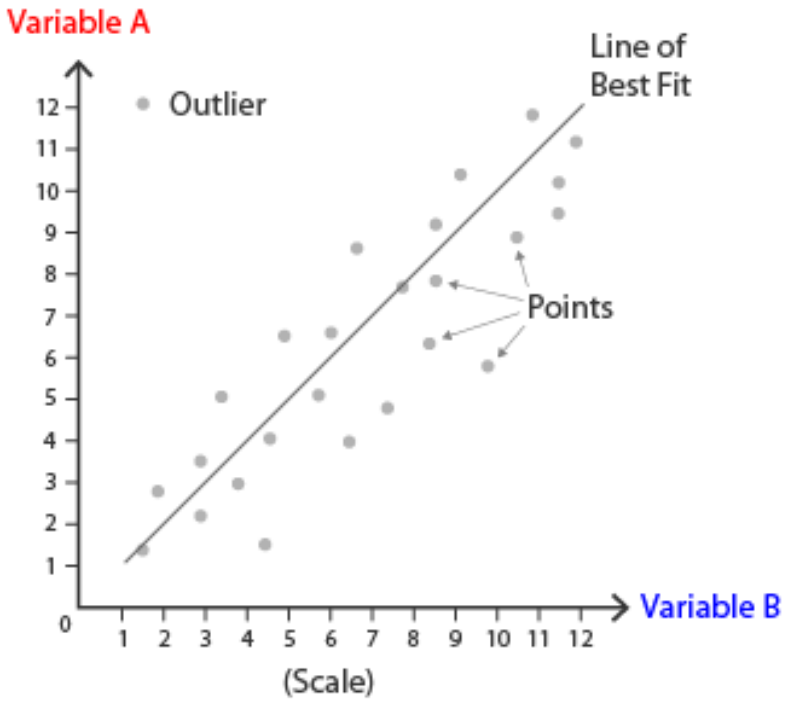
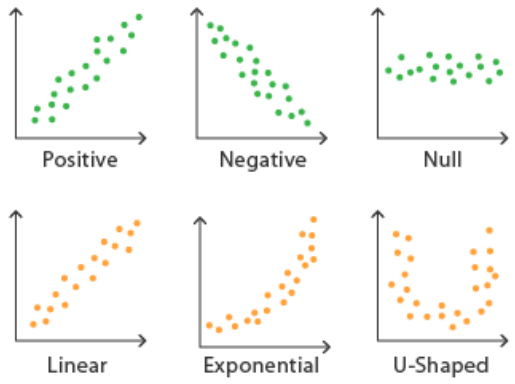
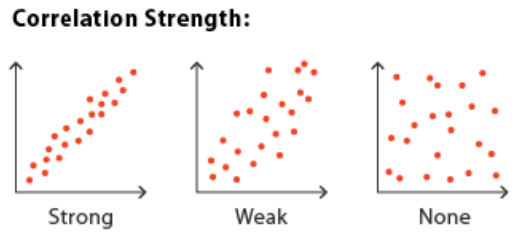
## Scatterplots should be awesome:

- Positions on common scale (lowest error representation)
- Show all data: outliers, sample sizes, trends, etc.



# Framing affects interpretation [a]

[a] Cleveland *et al.* (1982) *Science* doi:10.1126/science.216.4550.1138

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## Point cloud size affects interpretation of correlation (more diffuse interpreted as lower correlation coefficient)

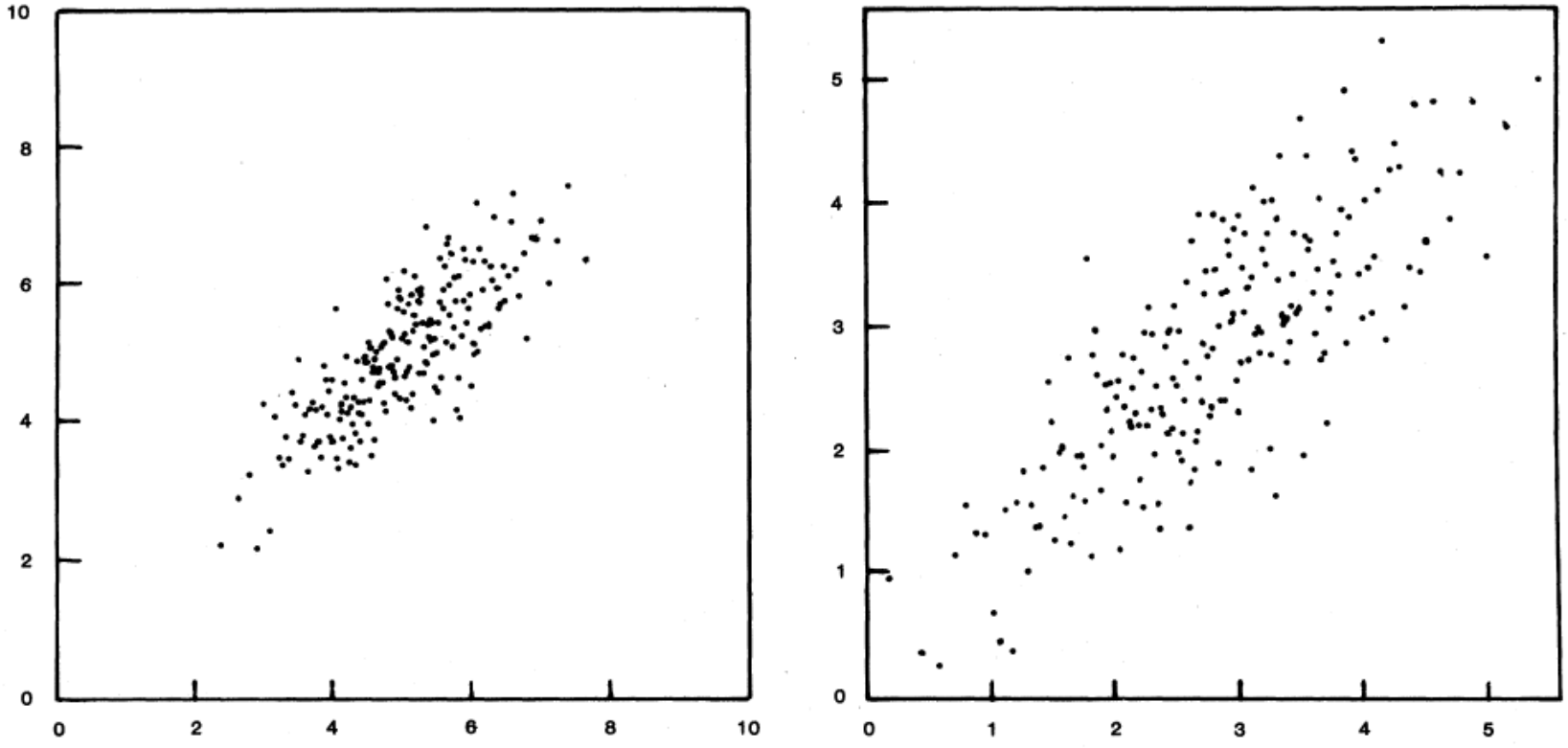


Fig. 1. Reductions of two scatterplots used in the three types of experiments. The left panel is point-cloud size 2 and the right panel is point-cloud size 4. In both panels $w(r) = .4$ and $r = .8$.

# Interpreting correlation is difficult [a]

[a] Fisher *et al.* (2014) *PeerJ* doi:10.7717/peerj.589

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## People don't judge significance well

- 47.4% of significant relationships correctly classified
- 74.6% of non-significant relationships correctly classified

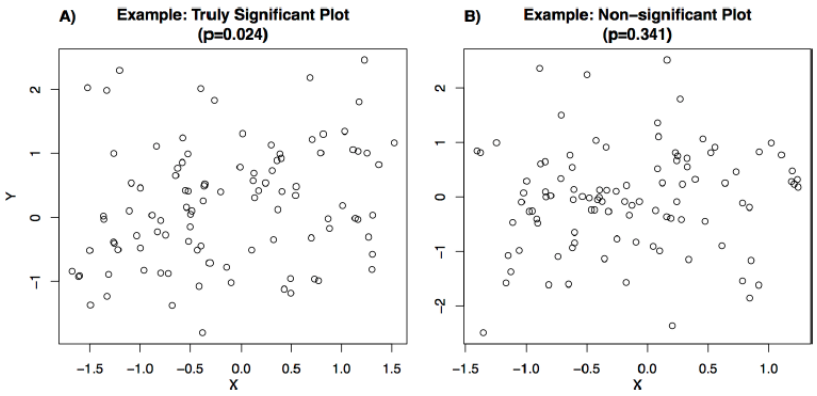
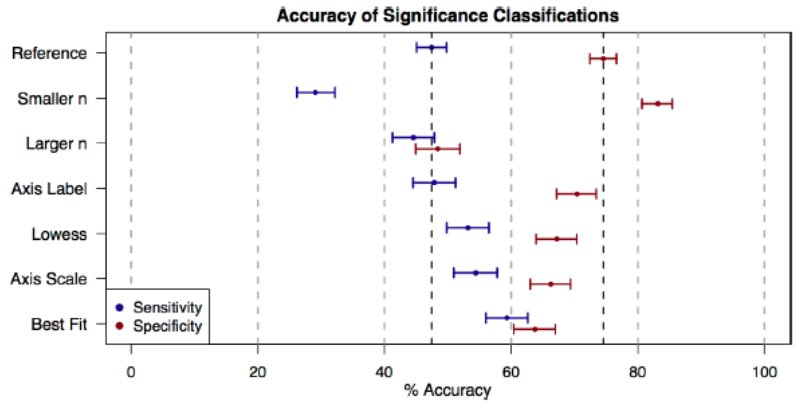



Figure 1 Examples of plots shown to users.



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# Latency affects usage

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Increasing latency to 0.5s:

- decreases user activity
- decreases dataset coverage
- reduces rate of hypothesis generation
- changes data exploration strategy
- reduces future interaction with other graphics

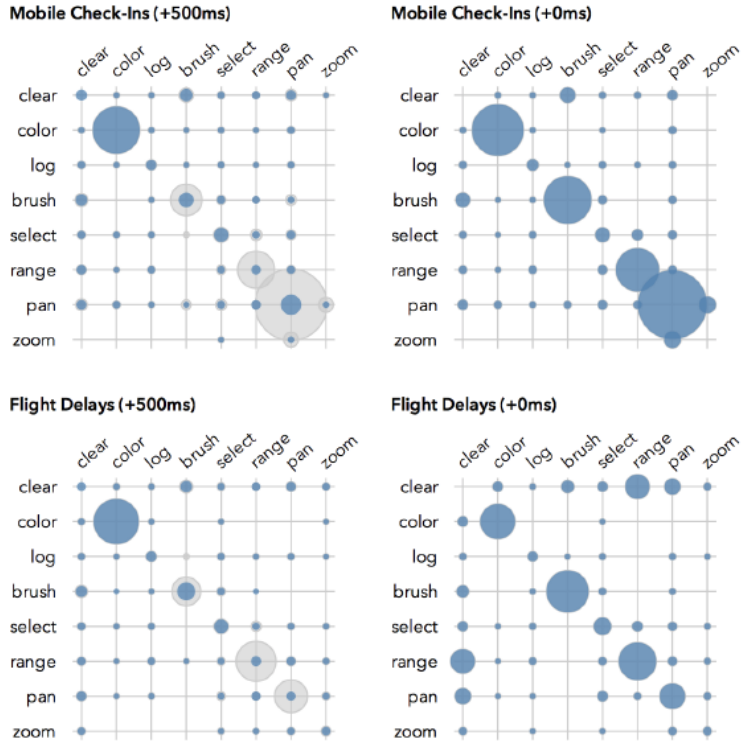


Fig. 4. Transitions between application events by analysis scenario and latency condition. Circular area represents the number of transitions between pairs of event types. Gray circles represent transitions between triggered events; blue circles between processed events. Rows represent source nodes and columns represent target nodes.

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# Python libraries

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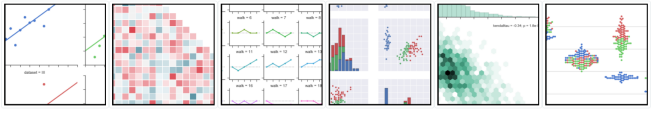
- Matplotlib http://matplotlib.org/

matplotlib

- Seaborn https://stanford.edu/ mwaskom/software/seaborn/

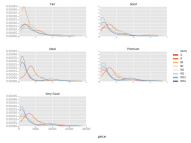
Seaborn: statistical data visualization



- ggplot for Python http://yhat.github.io/ggplot/

ggplot

A package for plotting in Python.



- Bokeh http://bokeh.pydata.org/

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# Exercise choices [a]

[a] https://github.com/widdowquinn/Teaching-Data-Visualisation

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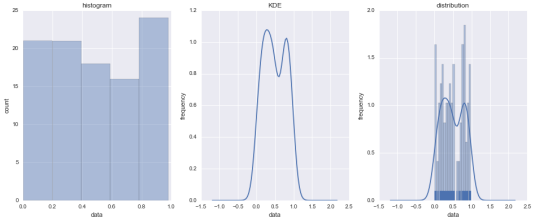
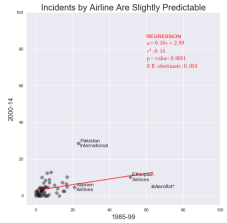
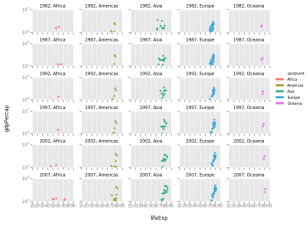
- One-variable, continuous data



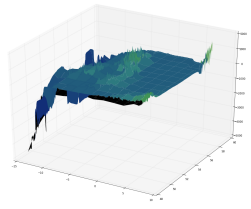

- Two-variable, continuous x, y data



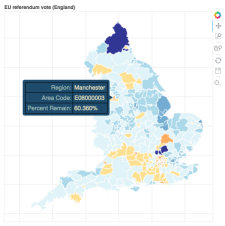

- Grammar of Graphics



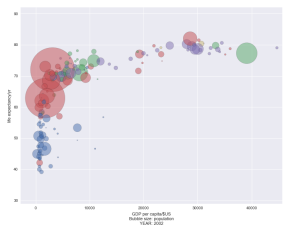
- Arrays, colormaps, surface plots



- Interactive map with bokeh




- Making movies



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# Let's get started [a]

[a] https://xkcd.com/1654/

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INSTALL.SH

```
#!/bin/bash

pip install "$1" &
easy_install "$1" &
brew install "$1" &
npm install "$1" &
yum install "$1" & dnf install "$1" &
docker run "$1" &
pkg install "$1" &
apt-get install "$1" &
sudo apt-get install "$1" &
steamcmd +app_update "$1" validate &
git clone https://github.com/"$1"/"$1" &
cd "$1";./configure;make;make install &
curl "$1" | bash &
```

*Cutting corners to meet arbitrary management deadlines*

*Essential*

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