THE UNIVERSITY of EDINBURGH
informatics

Applied Machine Learning (AML)

Class Starting at 4:10pm

Oisin Mac Aodha • Siddharth N.

Applied Machine Learning

Week 5: Representing Data and Exploratory Data Analysis

This slides will be made available on the project website after the class.
This session will be recorded.

Overview

1) Outline your tasks this for week
2) Discussion of Week 4’s topics

Week 5: Your tasks for this week

1) Attend and complete Lab 2 - solutions will be online later this week
2) Watch videos for week 5 - **Optimisation** and **Generalisation**
3) Ask questions on Piazza if stuck
4) Continue working on the coursework
5) Start Tutorial 2 which takes places next week - link in week 6

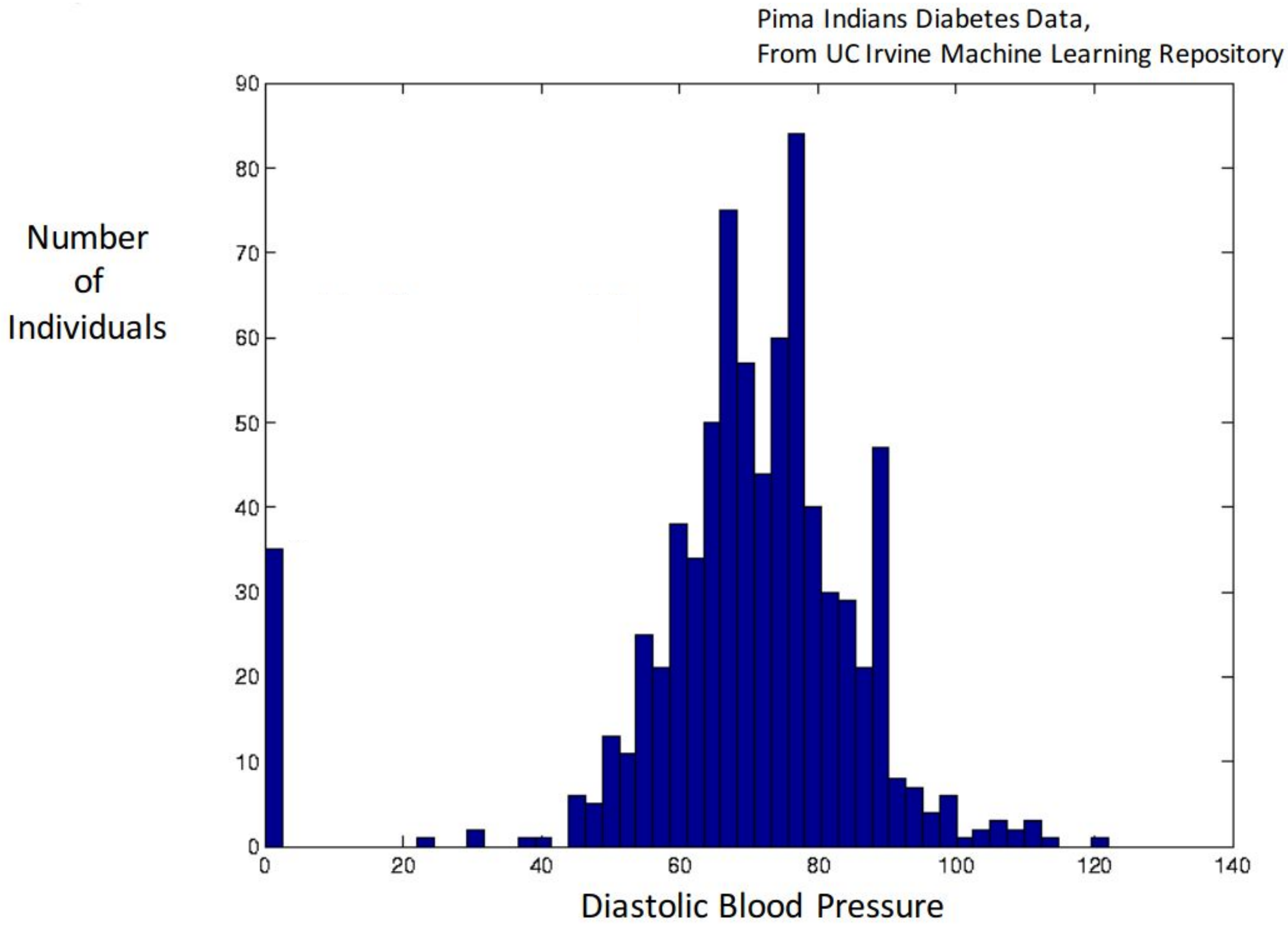
Reality of Applied Machine Learning

- Majority of time is not spent designing new ML algorithms
- It will be spent:
    - understanding the input data
    - defining the ML task
    - cleaning the data
    - designing features/attributes
    - visualising the data
    - comparing models (evaluating performance)
    - repeat

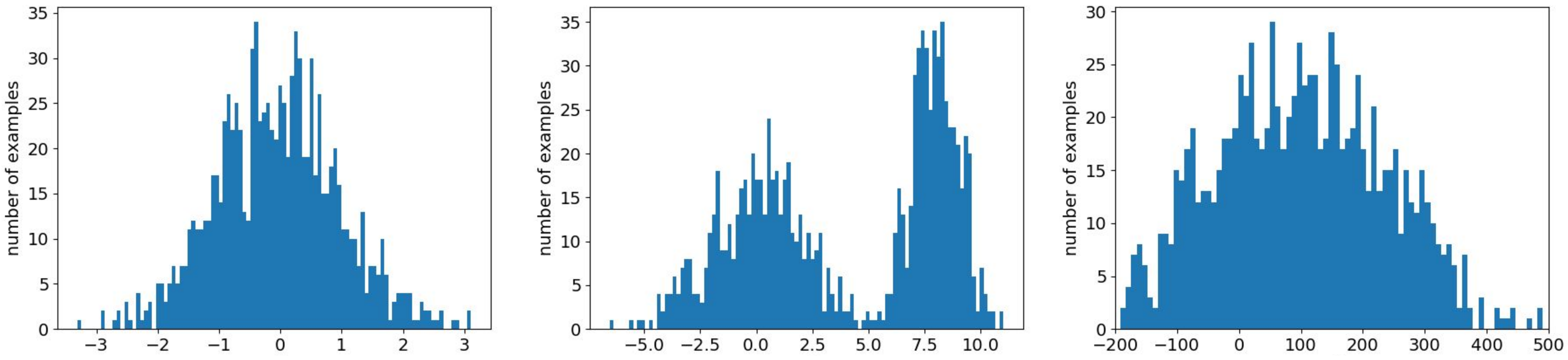
Visualisation

1) Crucial part of exploratory data analysis

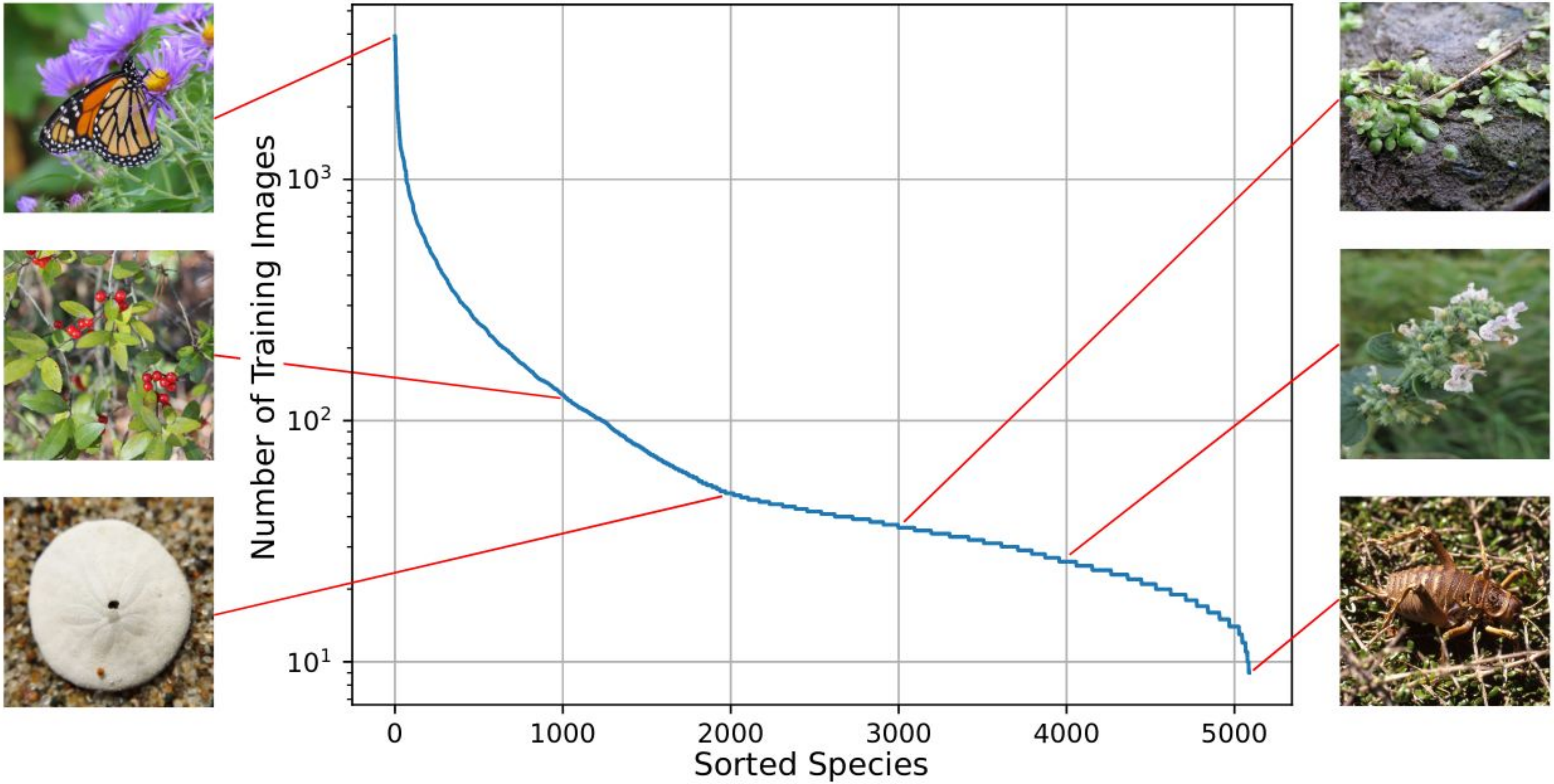
    Identify problems/anomalies in your data



Slide Credit Padhraic Smyth


number of examples
number of examples
number of examples
−3 −2 −1 0 1 2 3
−5.0 −2.5 0.0 2.5 5.0 7.5 10.0
−200 −100 0 100 200 300 400 500

x_1 x_2 x_3



https://arxiv.org/abs/1707.06642

Higher Dimensions are Challenging

Visualization is essential but not scalable as the number of dimensions increase

Scatter plot matrix

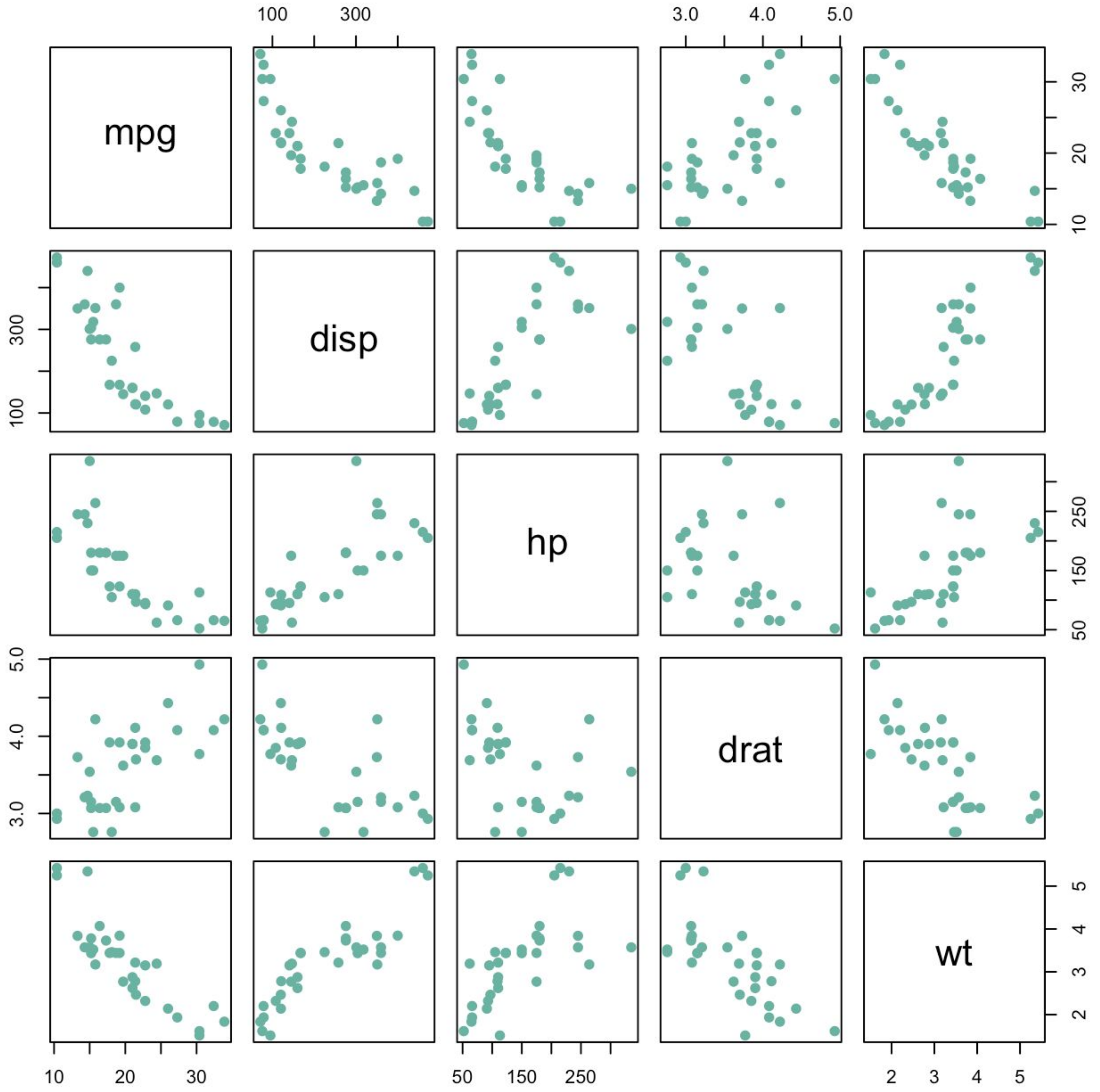


Image credit https://www.r-graph-gallery.com/98-basic-scatterplot-matrix.html

Visualisation

1) Crucial part of exploratory data analysis

    Identify problems/anomalies in your data

1) Visualisation to present results

    Convey message / summarise results

Common Visualization Mistakes

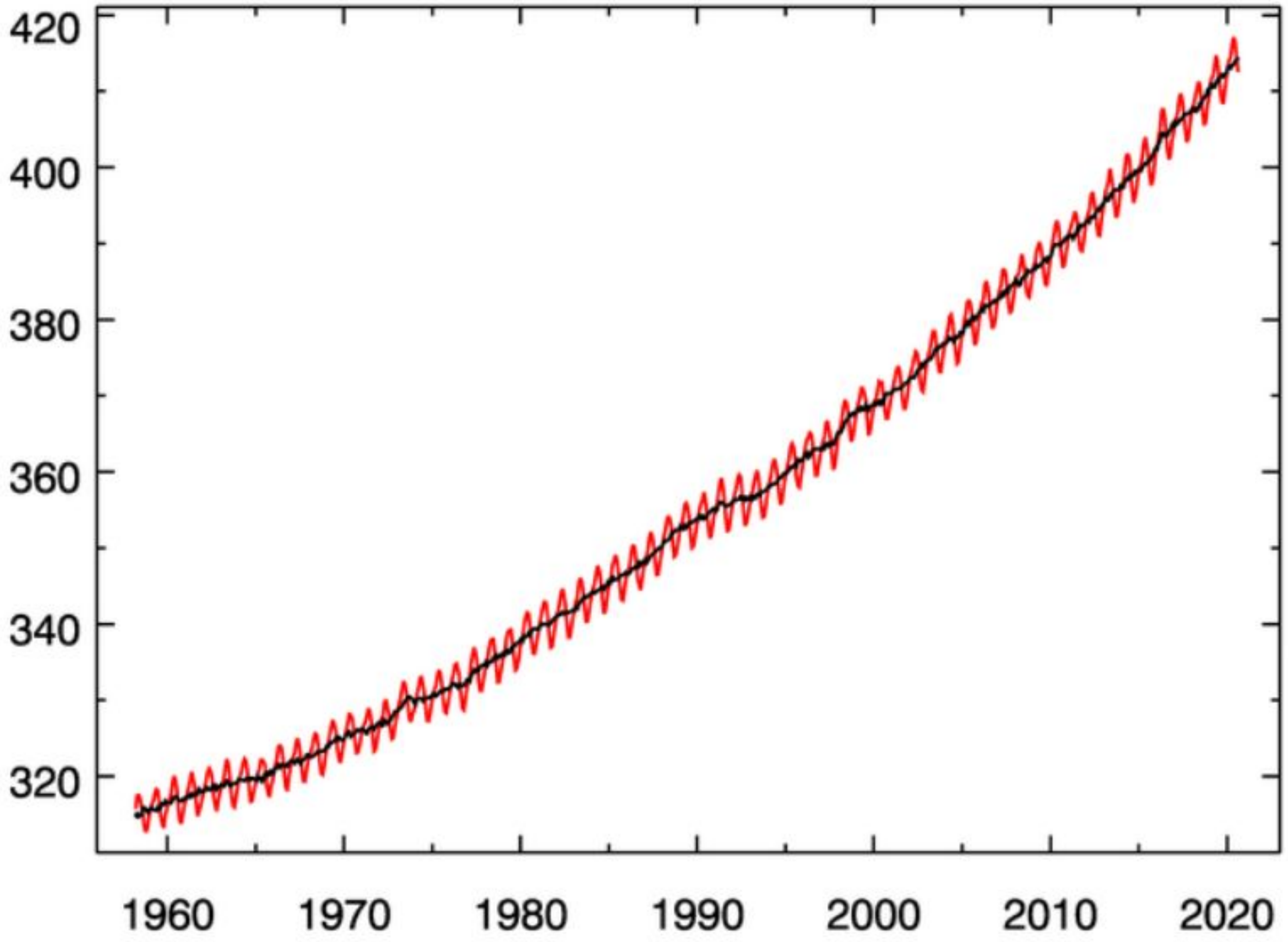
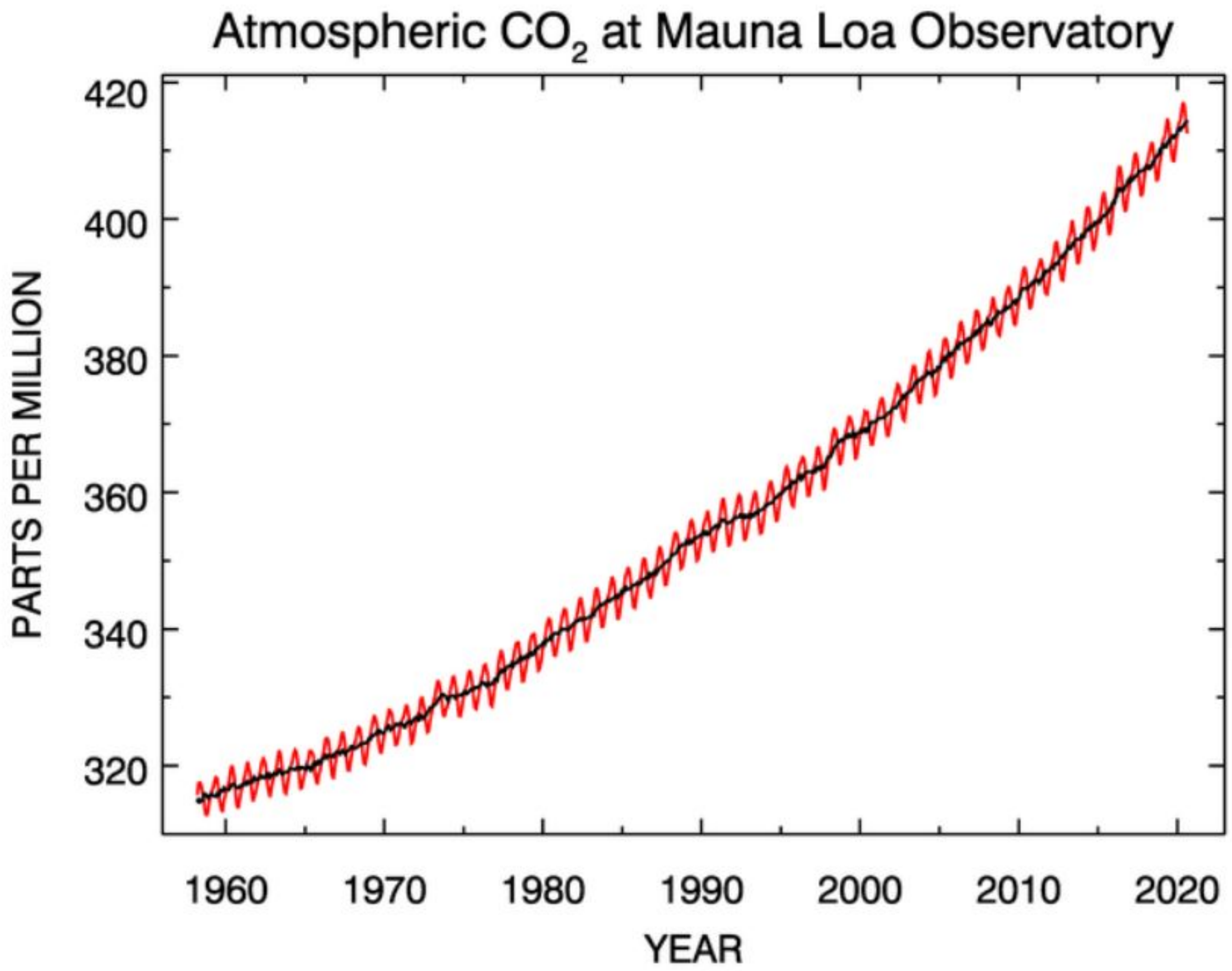


Image credit https://www.esrl.noaa.gov/gmd/ccgg/trends/mlo.html

Common Visualization Mistakes

Label your axes!



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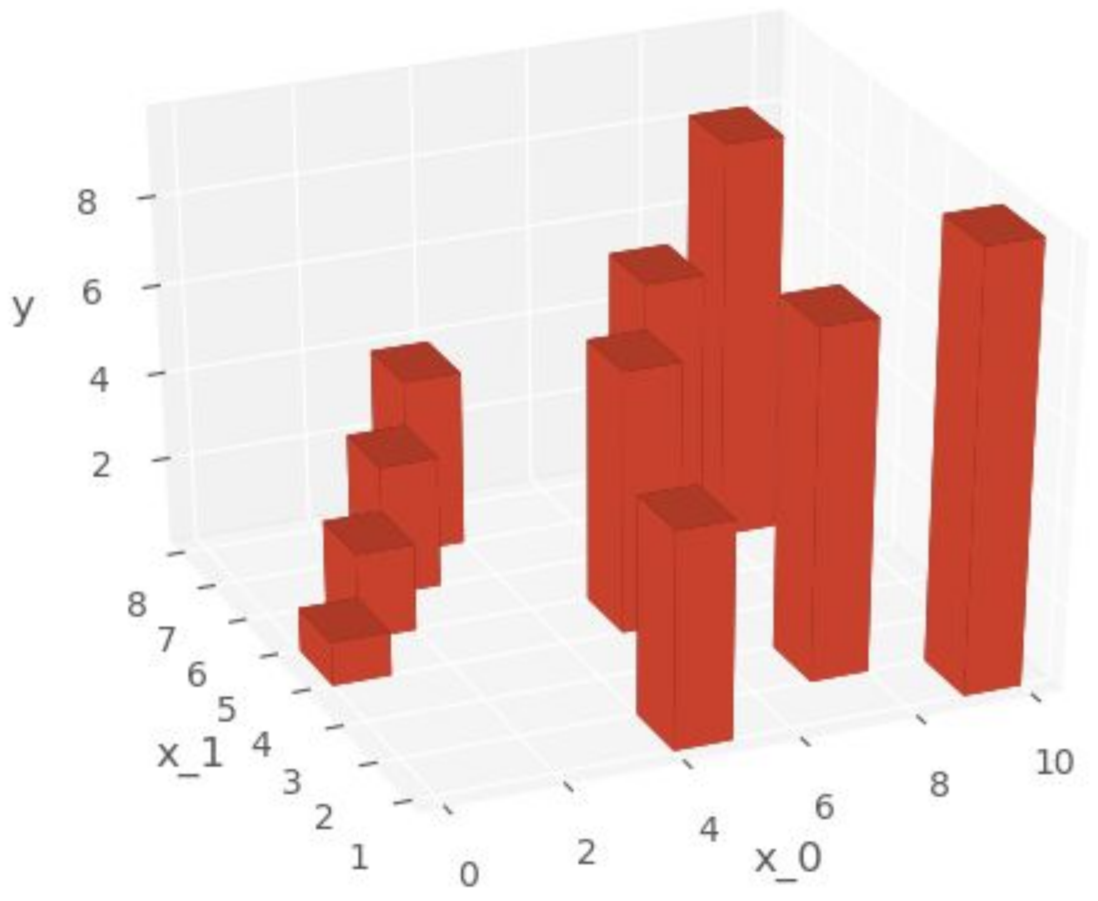
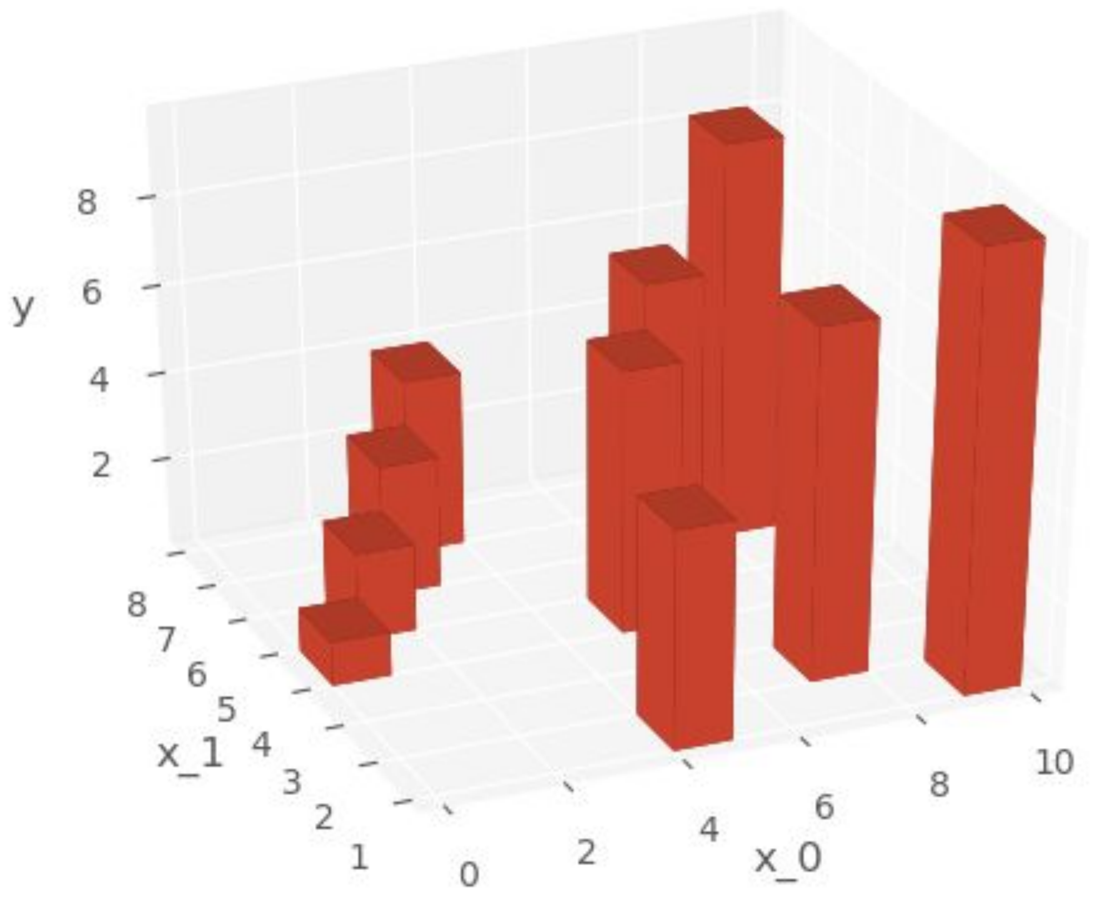
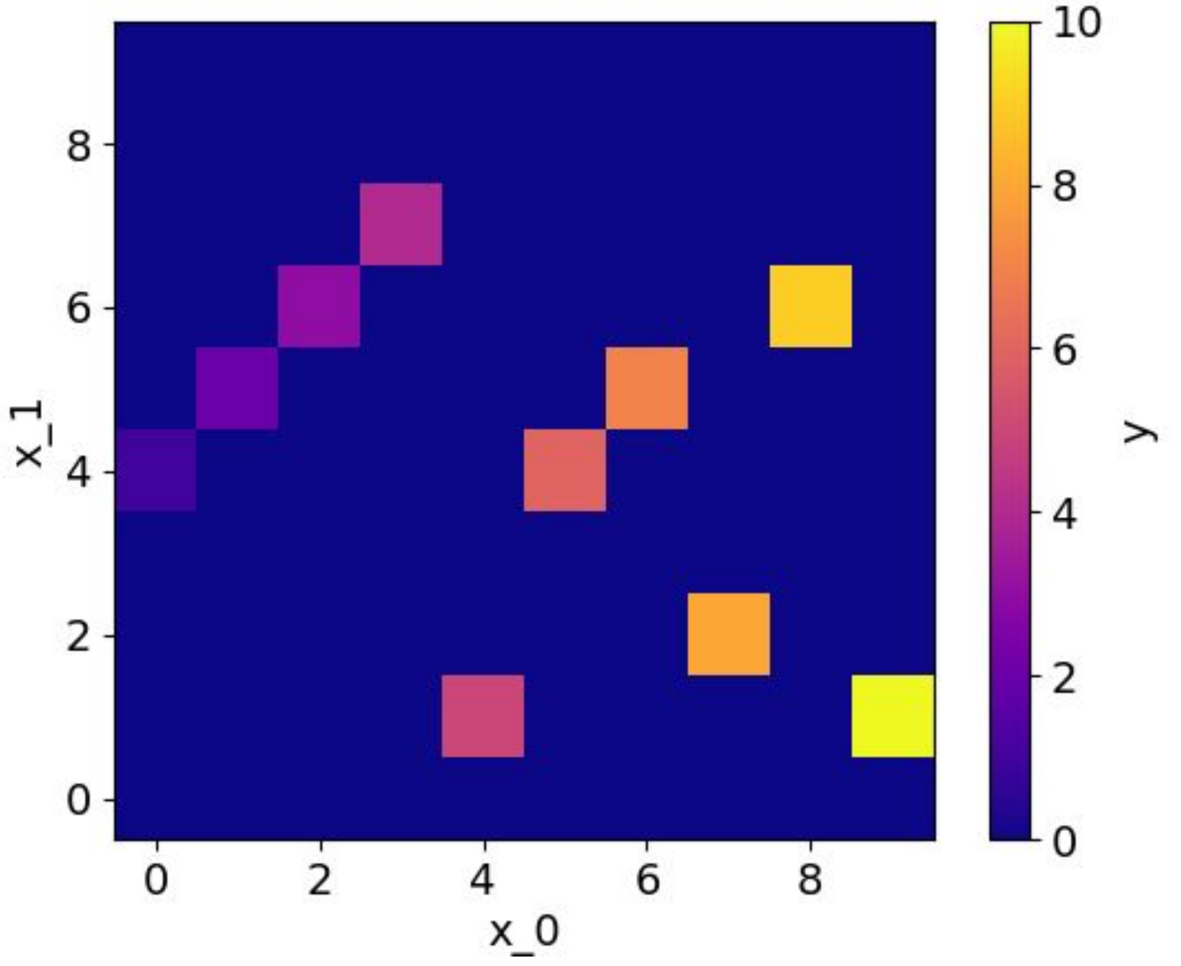
Common Visualization Mistakes



Common Visualization Mistakes

Don’t overcomplicate things e.g. 3D is rarely a good idea - use colour





Common Visualization Mistakes

Keep it “clean”

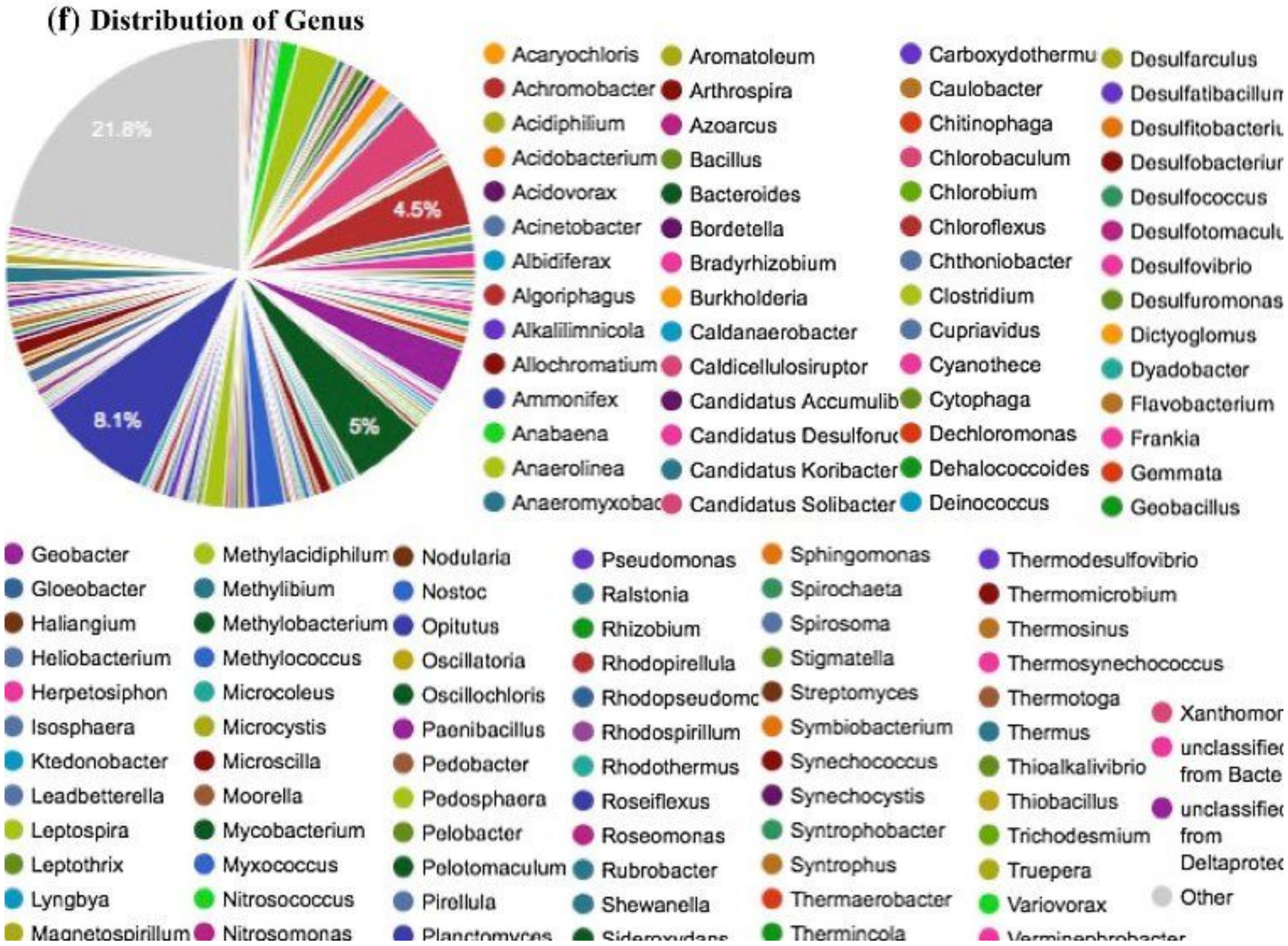
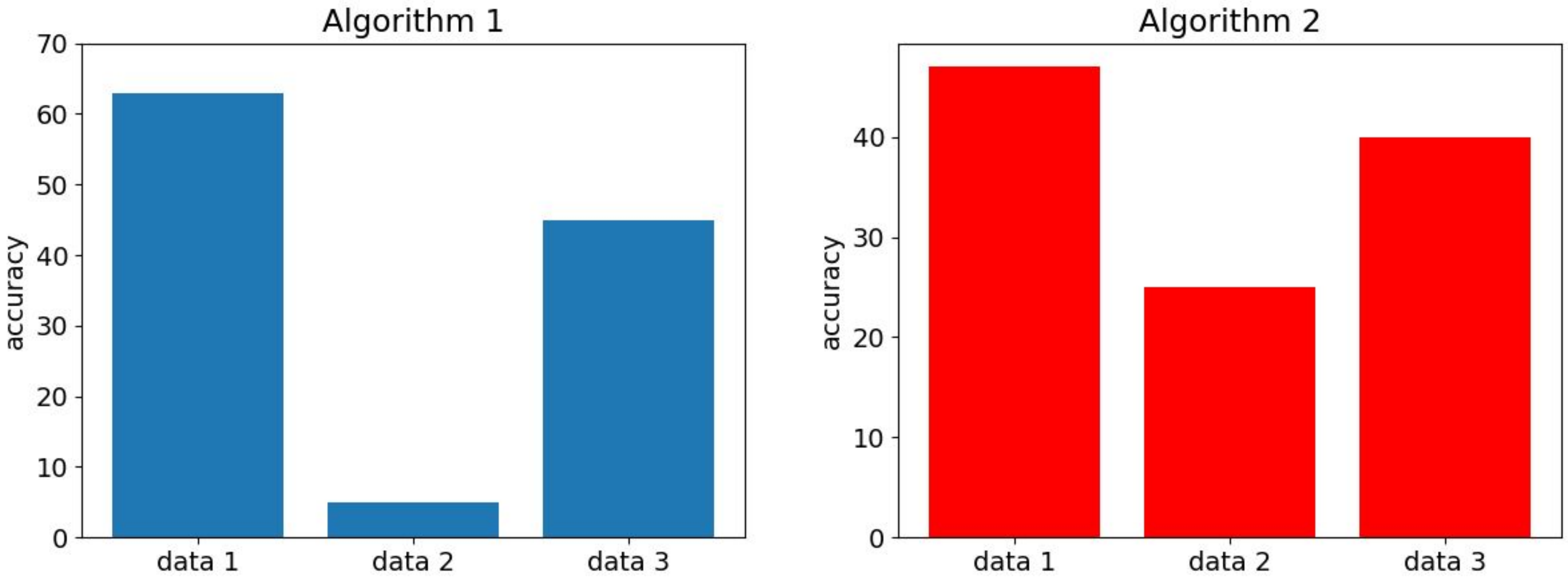


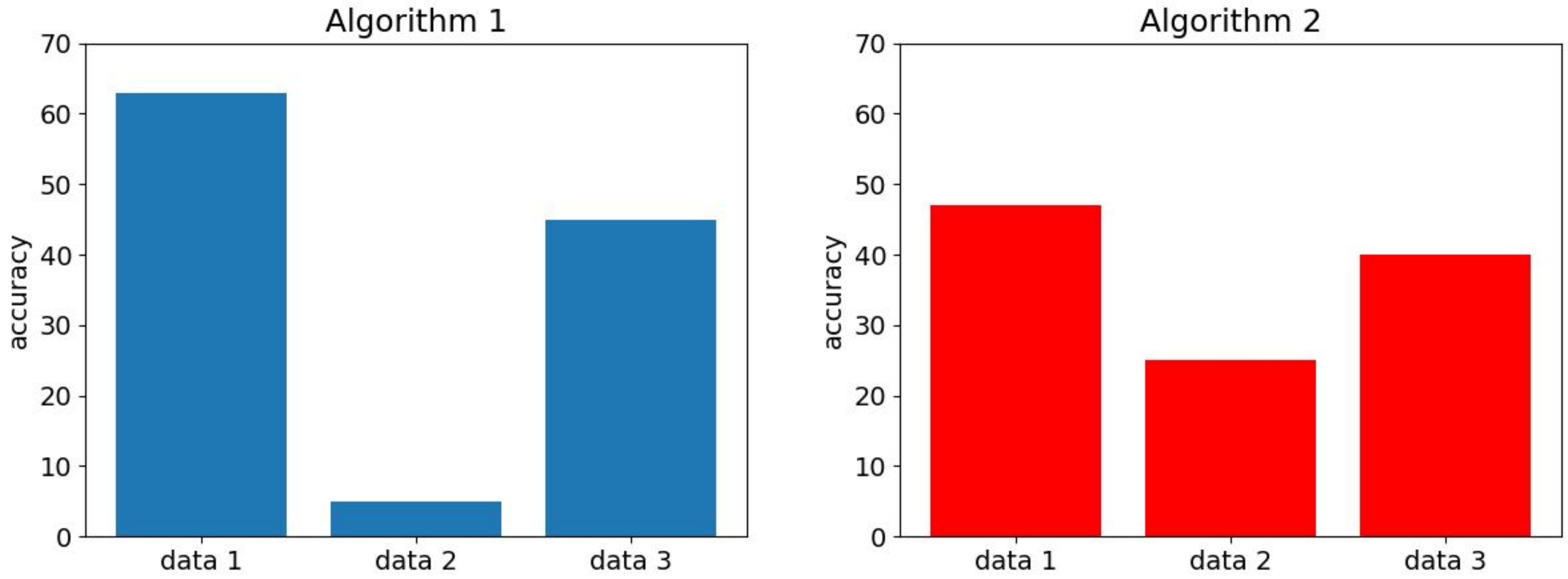
Image credit https://www.kdnuggets.com/2017/10/5-common-mistakes-bad-data-visualization.html

Common Visualization Mistakes



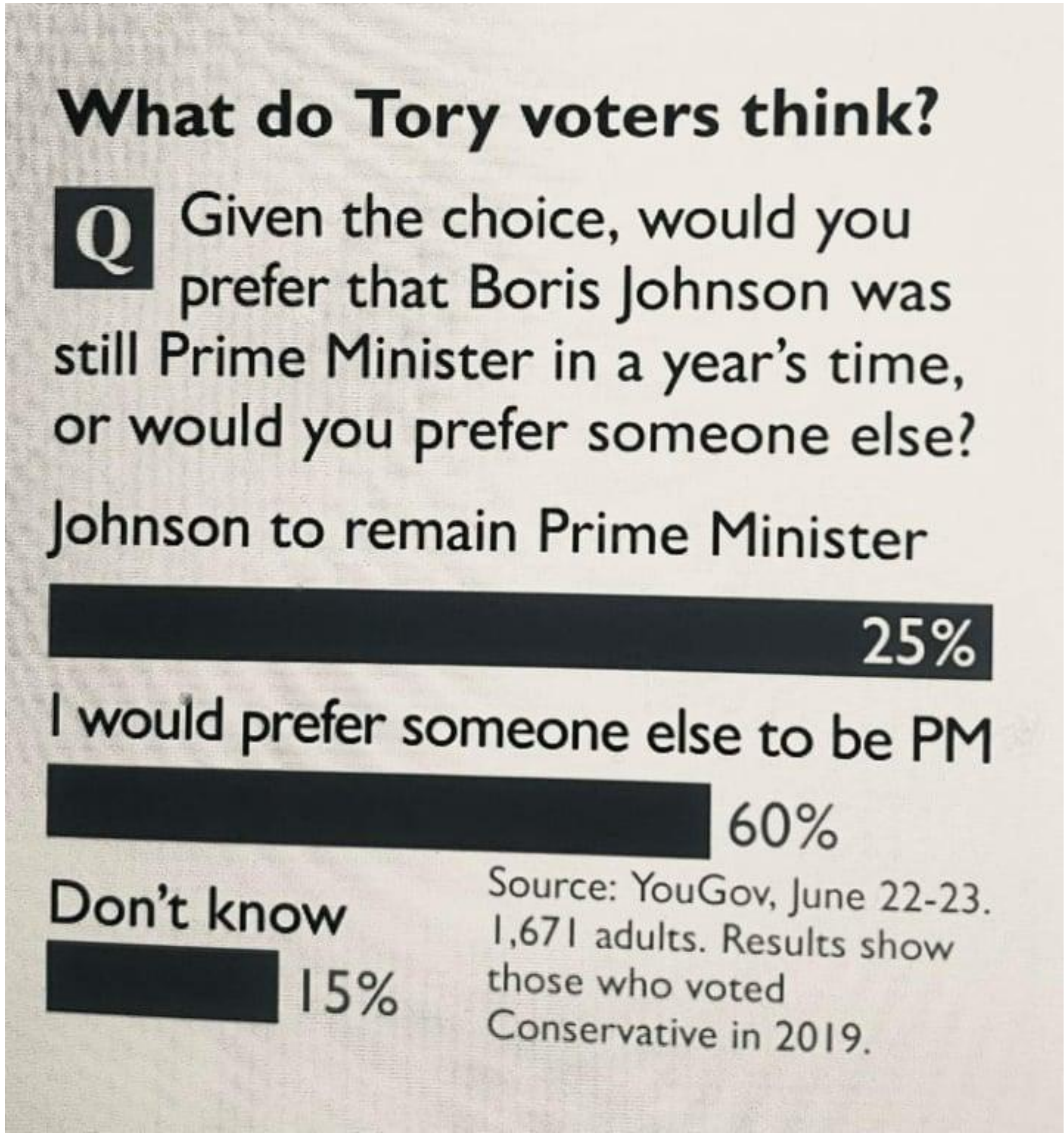
Common Visualization Mistakes

Don’t mislead



Common Visualization Mistakes

Don't mislead



Extra Resources

GOV.UK:
https://www.gov.uk/government/publications/a-bite-sized-guide-to-visualising-data-a-dstl-biscuit-book

EU Publication Office:

https://data.europa.eu/apps/data-visualisation-guide/

Additional Links

Chartjunk - “decorations in a graphic that have no purpose”

https://www.edwardtufte.com/bboard/q-and-a-fetch-msg?msg_id=00040Z

Examples of bad plots used in media

https://junkcharts.typepad.com

Plots to avoid

https://genomicsclass.github.io/book/pages/plots_to_avoid.html

Classifying New Data - Ham Likelihood

- Given an *new* email we would like to be able to classify it
- For example, given the test email: "review us now"
- $\boldsymbol{x}_t = [0, 1, 0, 1, 0, 0]^\intercal$

- Class priors:
  $p(\text{spam}) = 4/6 \quad p(\text{ham}) = 2/6$
- Per-class likelihoods:

$p(x_d\|\text{spam})$	$p(x_d\|\text{ham})$	x_d
2/4	0/2	password
1/4	2/2	review
3/4	1/2	send
3/4	1/2	us
3/4	1/2	your
1/4	1/2	account

$$
\begin{aligned}
p(\boldsymbol{x}_t|\text{ham}) &= p(0,1,0,1,0,0|\text{ham}) \\
&= (1-\frac{0}{2})(\frac{2}{2})(1-\frac{1}{2})(\frac{1}{2})(1-\frac{1}{2})(1-\frac{1}{2}) = 0.0625
\end{aligned}
$$

PCA: Maximising Variance

Recall Xv projects X onto v

$$\begin{aligned}\mathrm{Var}[X\boldsymbol{v}] &= \frac{1}{N}(X\boldsymbol{v})^\top(X\boldsymbol{v}) \\ &= \frac{1}{N}\boldsymbol{v}^\top X^\top X\boldsymbol{v} \\ &= \boldsymbol{v}^\top \frac{X^\top X}{N}\boldsymbol{v} \\ &= \boldsymbol{v}^\top S\boldsymbol{v}\end{aligned}$$

$max\ \boldsymbol{v}^\top S\boldsymbol{v}$, s.t. $\boldsymbol{v}^\top\boldsymbol{v} = 1$

solved using *Lagrange multipliers* as

$$max\ \underbrace{\boldsymbol{v}^\top S\boldsymbol{v} - \lambda\left(\boldsymbol{v}^\top\boldsymbol{v} - 1\right)}_{\mathcal{L}}$$

computing derivative w.r.t v and setting $= 0$

$$\frac{d\mathcal{L}}{d\boldsymbol{v}} = 2S\boldsymbol{v} - 2\lambda\boldsymbol{v} = 0$$

$$S\boldsymbol{v} = \lambda\boldsymbol{v} \quad \square$$

$v \longrightarrow$ direction of max variance

$$S\boldsymbol{v} = \lambda\boldsymbol{v}$$

left multiply by $\boldsymbol{v}^\top$

$$\begin{aligned}\boldsymbol{v}^\top S\boldsymbol{v} &= \boldsymbol{v}^\top\lambda\boldsymbol{v} \\ &= \lambda\boldsymbol{v}^\top\boldsymbol{v} \\ &= \lambda \quad \square\end{aligned}$$

$\lambda \longrightarrow$ max variance

PCA: Finding Principal Components

More generally, solve for $SV = \Lambda V$ using Eigen decomposition

$$V = [\boldsymbol{v}_1, \ldots, \boldsymbol{v}_D], \ \Lambda = \begin{bmatrix} \lambda_1 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \lambda_D \end{bmatrix} \quad \boldsymbol{v}_i \in \mathbb{R}^D, \ V \in \mathbb{R}^{D\times D}, \ \Lambda^{D\times D}$$

Eigenvalues

Solve $|S - \lambda I| = 0$

$$\begin{vmatrix} 2.0 - \lambda & 0.8 \\ 0.8 & 0.6 - \lambda \end{vmatrix} = 0$$

$$\lambda^2 - 2.6\lambda + 0.56 = 0$$

$$\implies \{\lambda_1, \lambda_2\} = \{2.36, 0.23\}$$

Eigenvectors

Find i^{th} eigenvector by solving $S\boldsymbol{v}_i = \lambda_i \boldsymbol{v}_i$

$$\begin{bmatrix} 2.0 & 0.8 \\ 0.8 & 0.6 \end{bmatrix} \begin{bmatrix} v_{1,1} \\ v_{1,2} \end{bmatrix} = 2.36 \begin{bmatrix} v_{1,1} \\ v_{1,2} \end{bmatrix} \implies \boldsymbol{v}_1 = \begin{bmatrix} 2.2 \\ 1 \end{bmatrix}$$

$$\begin{bmatrix} 2.0 & 0.8 \\ 0.8 & 0.6 \end{bmatrix} \begin{bmatrix} v_{2,1} \\ v_{2,2} \end{bmatrix} = 0.23 \begin{bmatrix} v_{2,1} \\ v_{2,2} \end{bmatrix} \implies \boldsymbol{v}_2 = \begin{bmatrix} -0.41 \\ 0.91 \end{bmatrix}$$

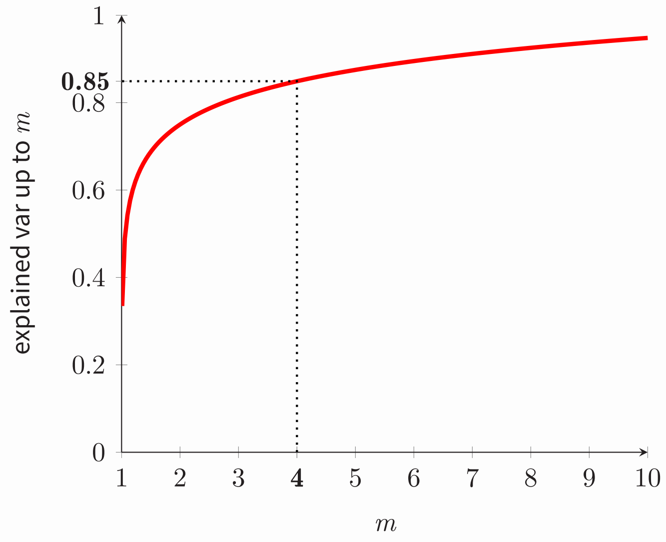
PCA: Picking number of dimensions

Given: eigenvectors $V = [\boldsymbol{v}_1, \ldots, \boldsymbol{v}_D]$; **Require:** $M \ll D$

Known: eigenvalue λ_i = variance along $\boldsymbol{v}_i$

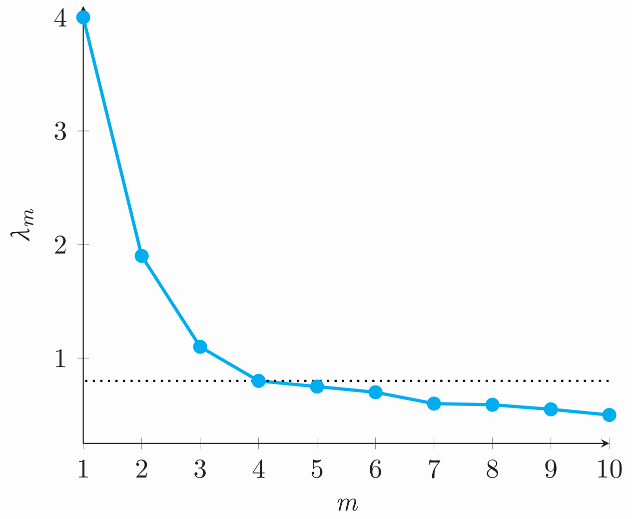
Explained variance

- sort eigenvectors s.t. $\lambda_1 \geq \ldots \geq \lambda_D$
- choose top M eigenvectors that explain "most" variance (typically 85%, 90%, or 95%)



Elbow plot

- plot eigenvalues in descending order $\lambda_1 \geq \ldots \geq \lambda_D$
- choose point at which curve "bends" most (i.e. elbow)



PCA: Dimensionality Reduction

Let $V_M = [\boldsymbol{v}_1, \ldots, \boldsymbol{v}_M] \in \mathbb{R}^{D\times M}$ denote the *truncated* eigenvector matrix for $M \ll D$

Reduction

Dimensionality reduction on data $\boldsymbol{x}_i$

$$\boldsymbol{e}_i^\top = \boldsymbol{x}_i^\top V_M \quad \in \mathbb{R}^M$$

More generally, projected data E

$$\begin{aligned} E &= \left[\boldsymbol{e}_1^\top, \ldots, \boldsymbol{e}_N^\top\right] \\ &= \left[\boldsymbol{x}_1^\top V_M, \ldots, \boldsymbol{x}_N^\top V_M\right] \\ &= X V_M \quad \in \mathbb{R}^{N\times M} \end{aligned}$$

Reconstruction

Recover data $\hat{\boldsymbol{x}}_i$ from $\boldsymbol{e}_i$ using $V_M^\top$

$$\hat{\boldsymbol{x}}_i^\top = \boldsymbol{e}_i^\top V_M^\top = \left(\boldsymbol{x}_i^\top V_M\right) V_M^\top \quad \in \mathbb{R}^D$$

More generally, reconstructed data $\hat{X}$

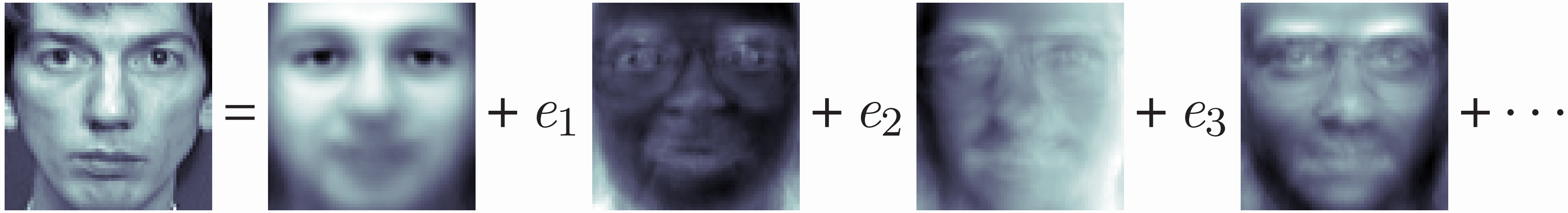
$$\begin{aligned} \hat{X} &= \left[\hat{\boldsymbol{x}}_1^\top, \ldots, \hat{\boldsymbol{x}}_N^\top\right] \\ &= X V_M V_M^\top \quad \in \mathbb{R}^{N\times D} \end{aligned}$$

$V_M V_M^\top \in \mathbb{R}^{D\times D}$ is the data *projection* matrix

PCA Example 2: Eigenfaces

Projection

Projecting face $\boldsymbol{x}_i$ onto $\boldsymbol{e}_i = [e_{i1}, \ldots, e_{iM}]$



Reconstruction

Reconstructing face $\hat{\boldsymbol{x}}_i$ using M components

$M = 10$ $\quad$ $M = 30$ $\quad$ $M = 50$ $\quad$ $M = 70$ $\quad$ $M = 90$

$(90 \ll 4096!)$

The MovieFlix Corporation wants to improve the algorithm it uses to recommend new movies to its customers. It has decidede to release a portion of its data to the public in the hope that researchers will be able to find patterns in users' preferences for the different movies. The data is represented as a matrix X where rows $i = 1, \ldots, n$ correspond to customers, and columns $j = 1, \ldots, c$ correspond to movies, and X_{ij} is a numeric value that reflects the degree to which customer i enjoyed movie j. Assume the data is complete; i.e., we know the rating of every user for every movie.

MovieFlix decides to carry out PCA on X treating each row (i.e. each customer) as a data vector. How will this help them understand the patterns in the preference data?

PCA relationship between X and X^T

Instead of thinking about the data as rows of customer responses, we can think of a movie as the response it elicits from N customers.

PCA relationship between X and X^T

Instead of thinking about the data as rows of customer responses, we can think of a movie as the response it elicits from N customers.

recall $Sv = \lambda v$

$\left(\frac{1}{N}X^T X\right) v = \lambda v \quad \left(\because S = \frac{1}{N}X^T X\right)$

pre-multiply by X

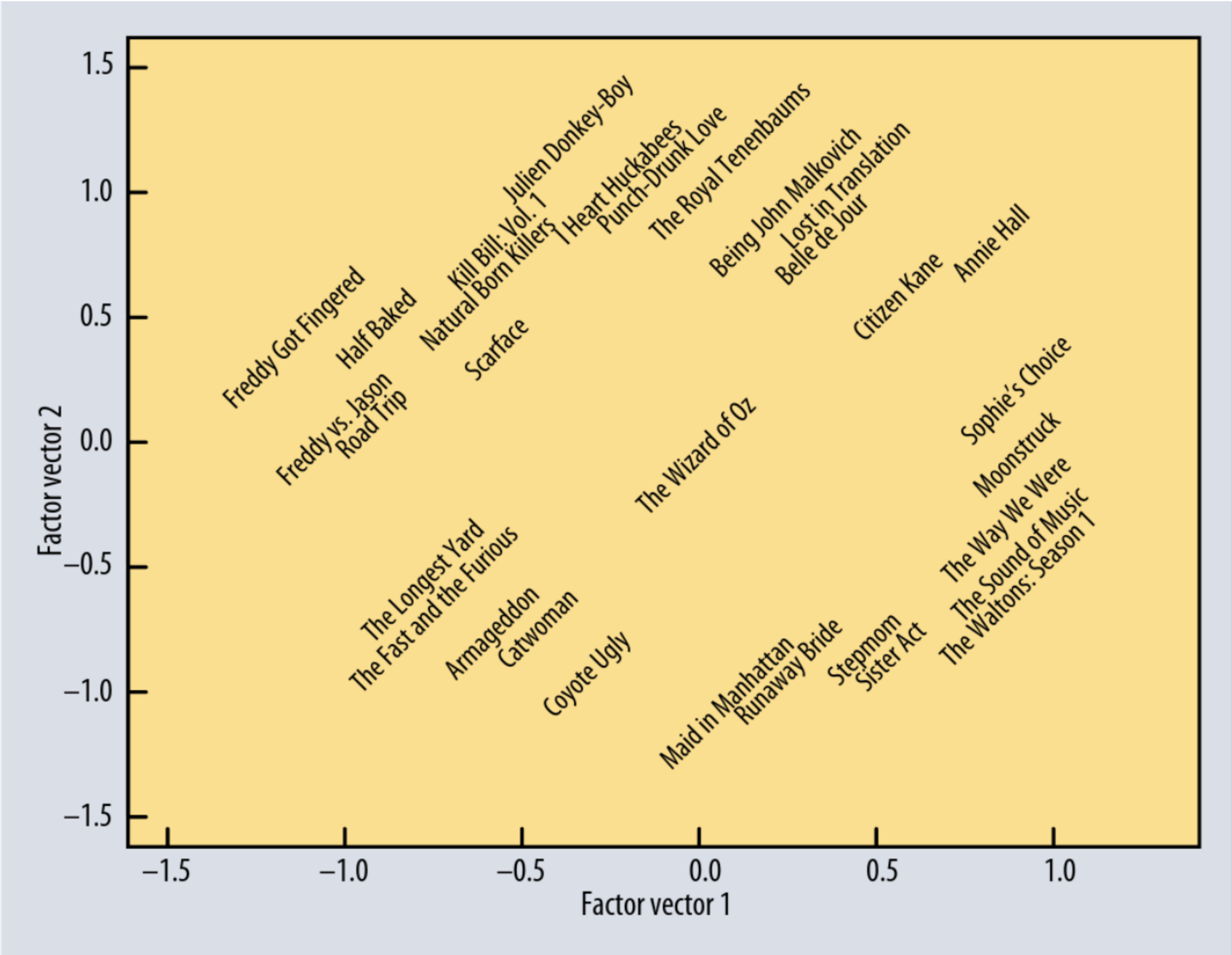
$\left(\frac{1}{N}XX^T\right)(Xv) = \lambda(Xv) \Rightarrow S'v' = \lambda v'$

$S' = \frac{1}{N}(X^T)^T X^T = \frac{1}{N}XX^T$

v' new PC direction

same eigenvalues!

In the famous Netflix challenge, as similar low-rank idea can be used as in PCA, but almost all of the entries in X are missing—not every person has seen every film!



credit: Yehuda Koren, Robert Bell, & Chris Volinsky, Matrix Factorization Techniques for Recommender Systems