CS 260: Foundations of Data Science

Prof. Thao Nguyen

Fall 2025

HAVERFORD COLLEGE

Materials by Sara Mathieson

Admin

- **Final project check-ins** during lab

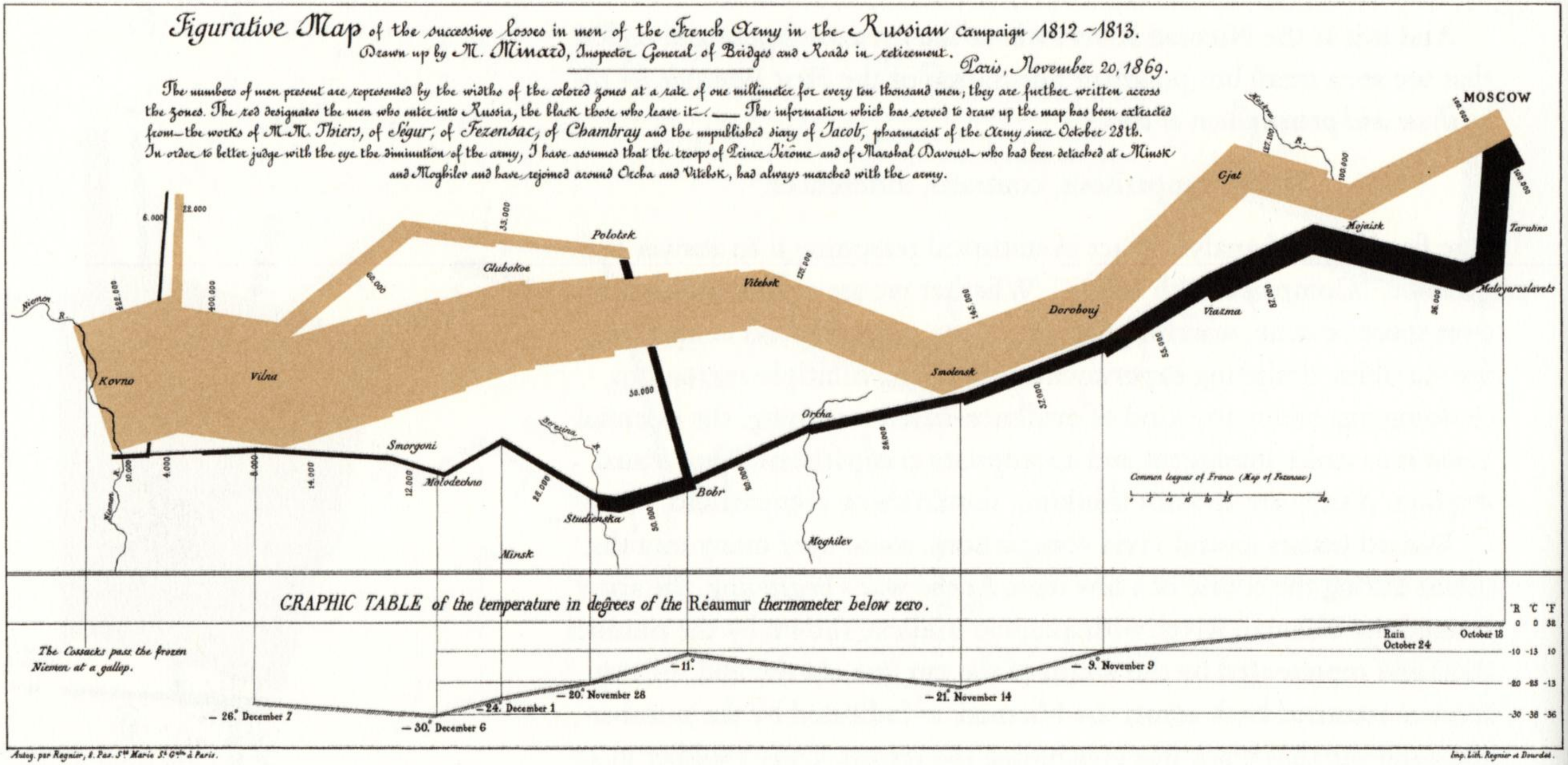
Outline for today

- Revisit data visualization
- Real-world data science exercise
- Begin: clustering

Outline for today

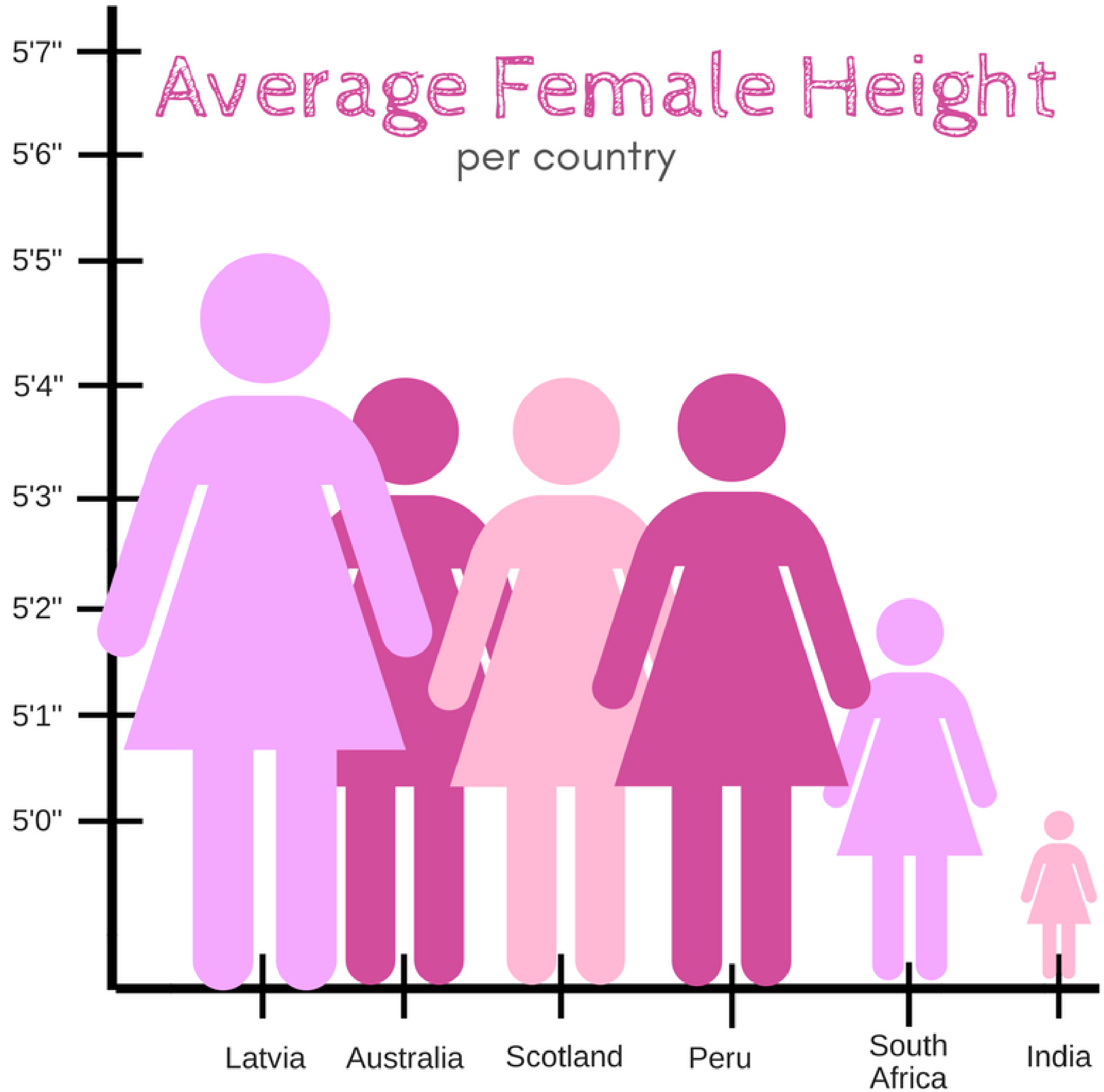
- Revisit data visualization
- Real-world data science exercise
- Begin: clustering

Visualization can illuminate…

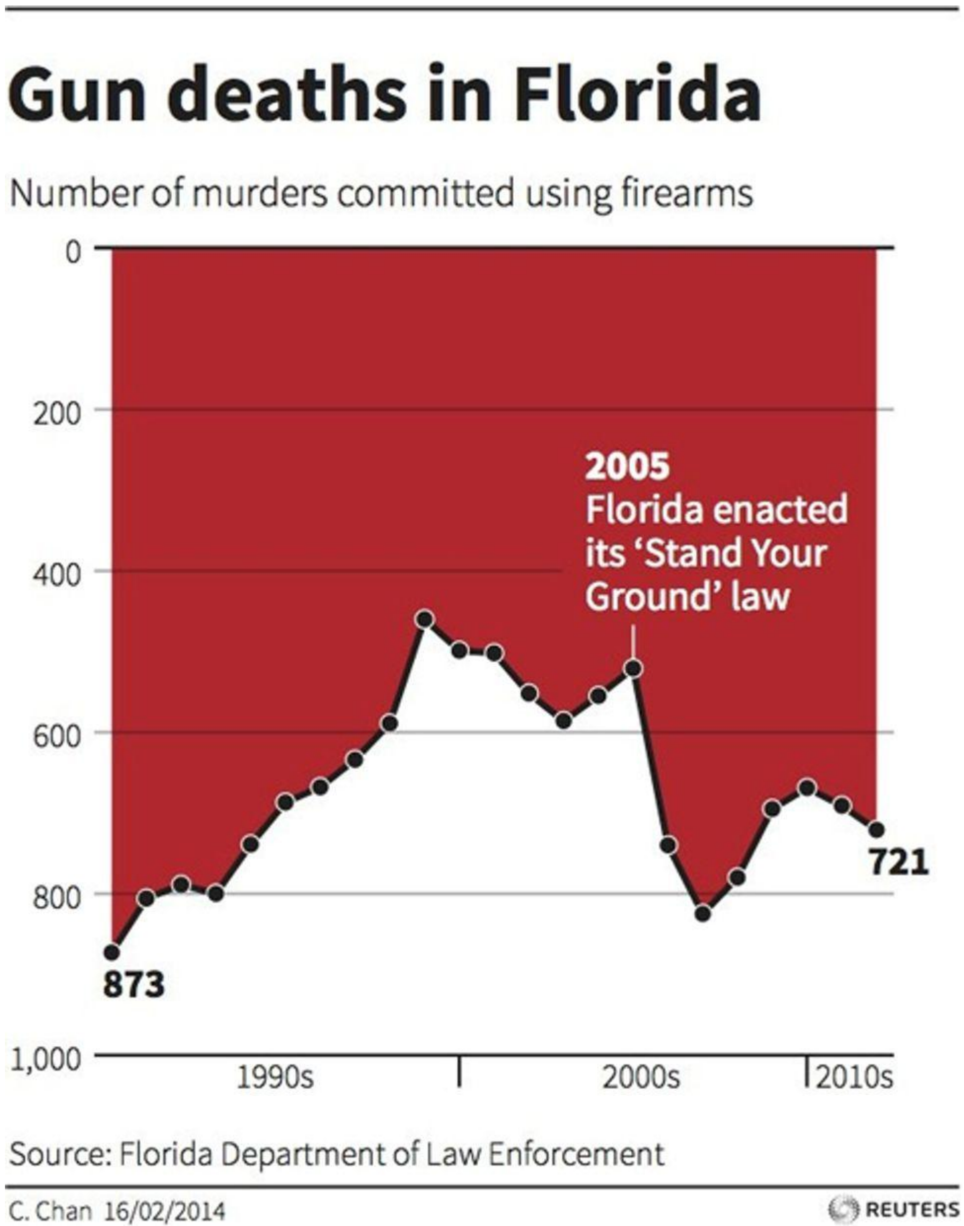


Size of Napoleon’s army on the advance (in tan) and retreat (in black) from Moscow in 1812

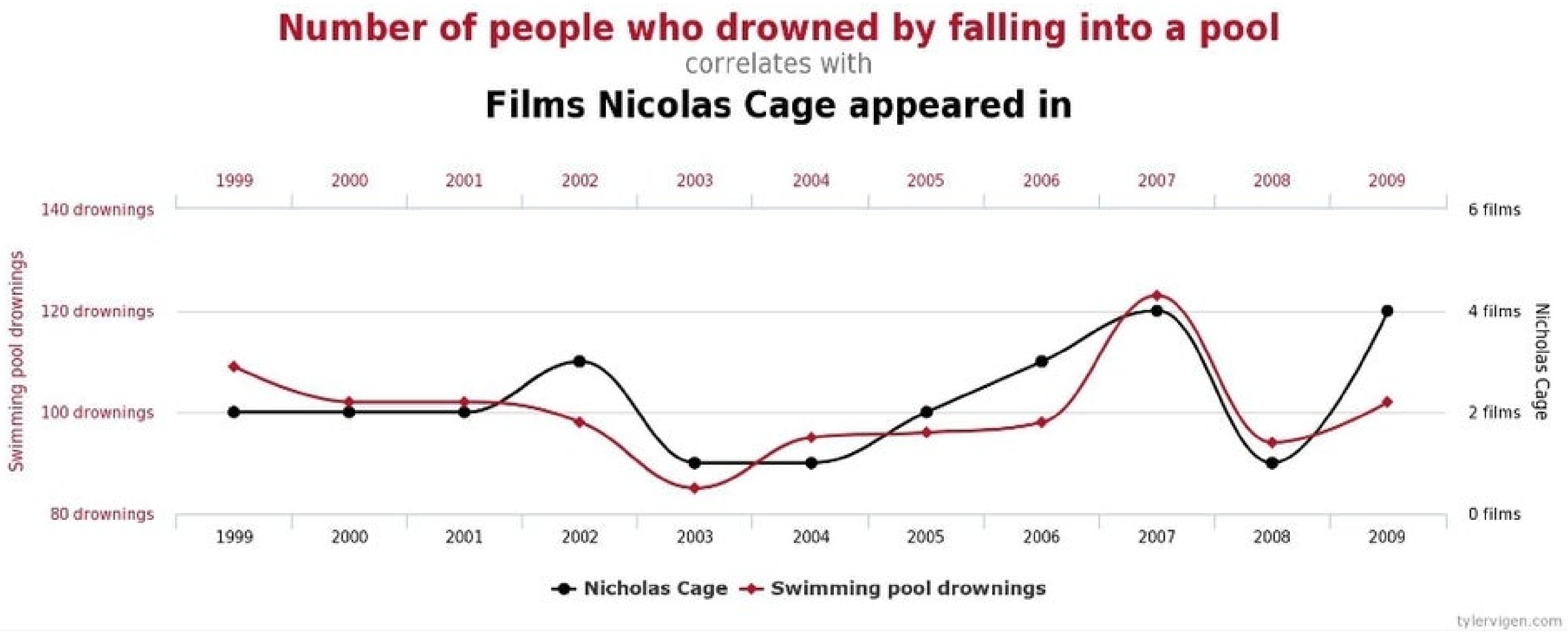
… but also mislead



… but also mislead



… but also mislead



Visualizing amounts

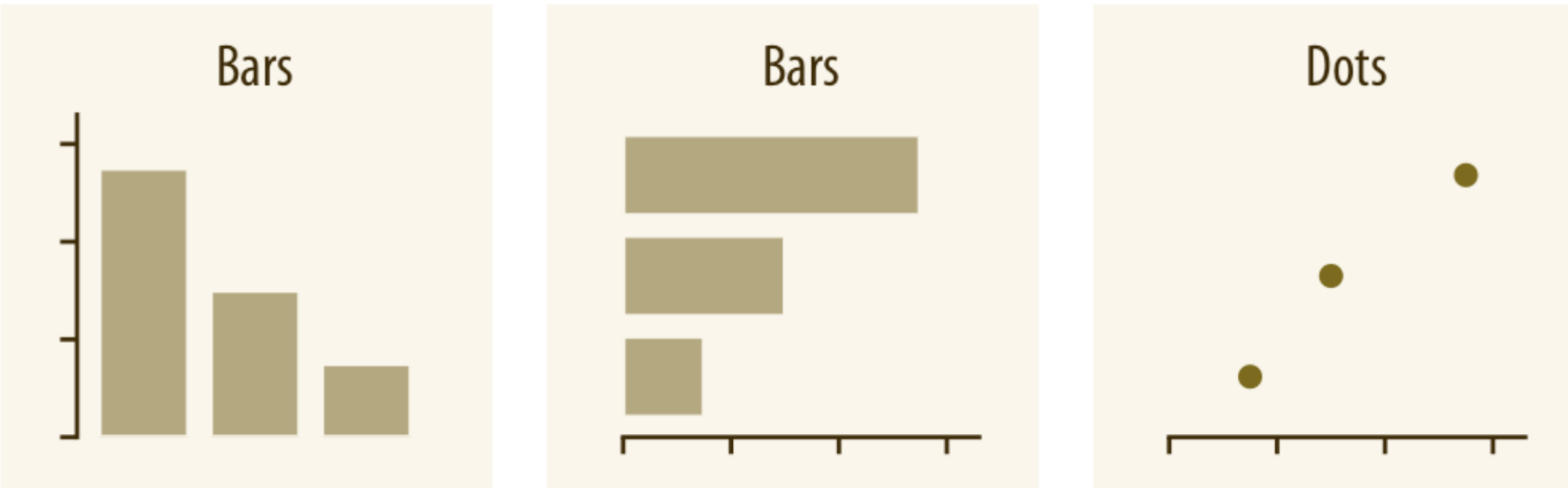


Figure from “Fundamentals of Data Visualization” by Claus Wilke

Visualizing amounts

Figure from “Fundamentals of Data Visualization” by Claus Wilke

Visualizing distributions

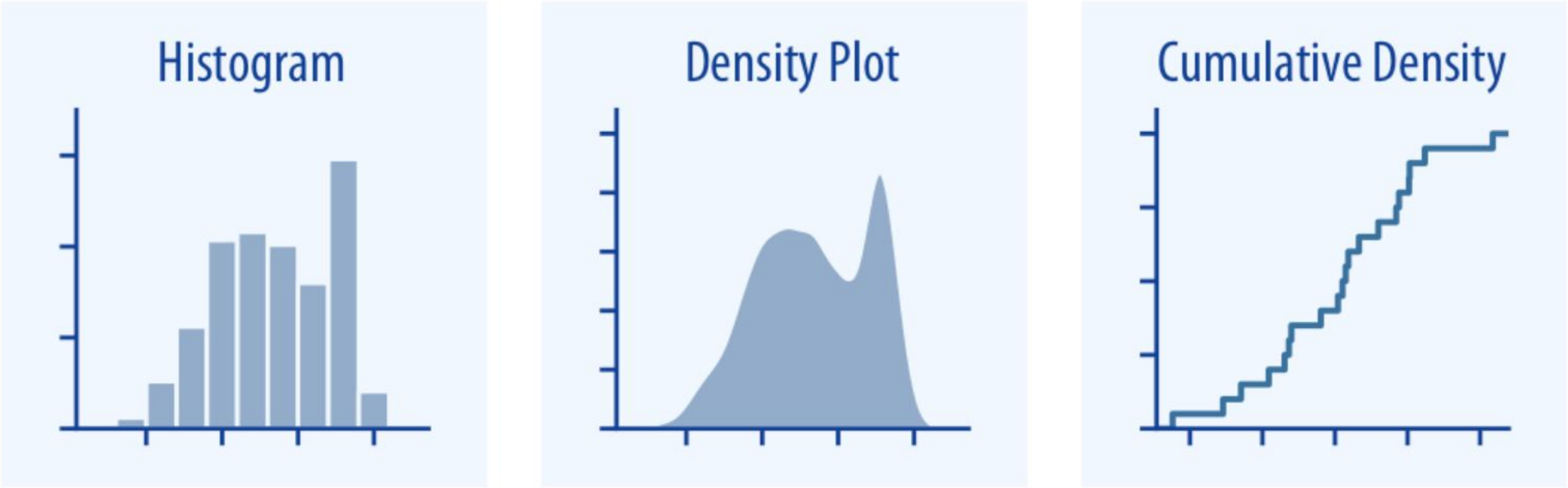


Figure from "Fundamentals of Data Visualization" by Claus Wilke

Visualizing distributions

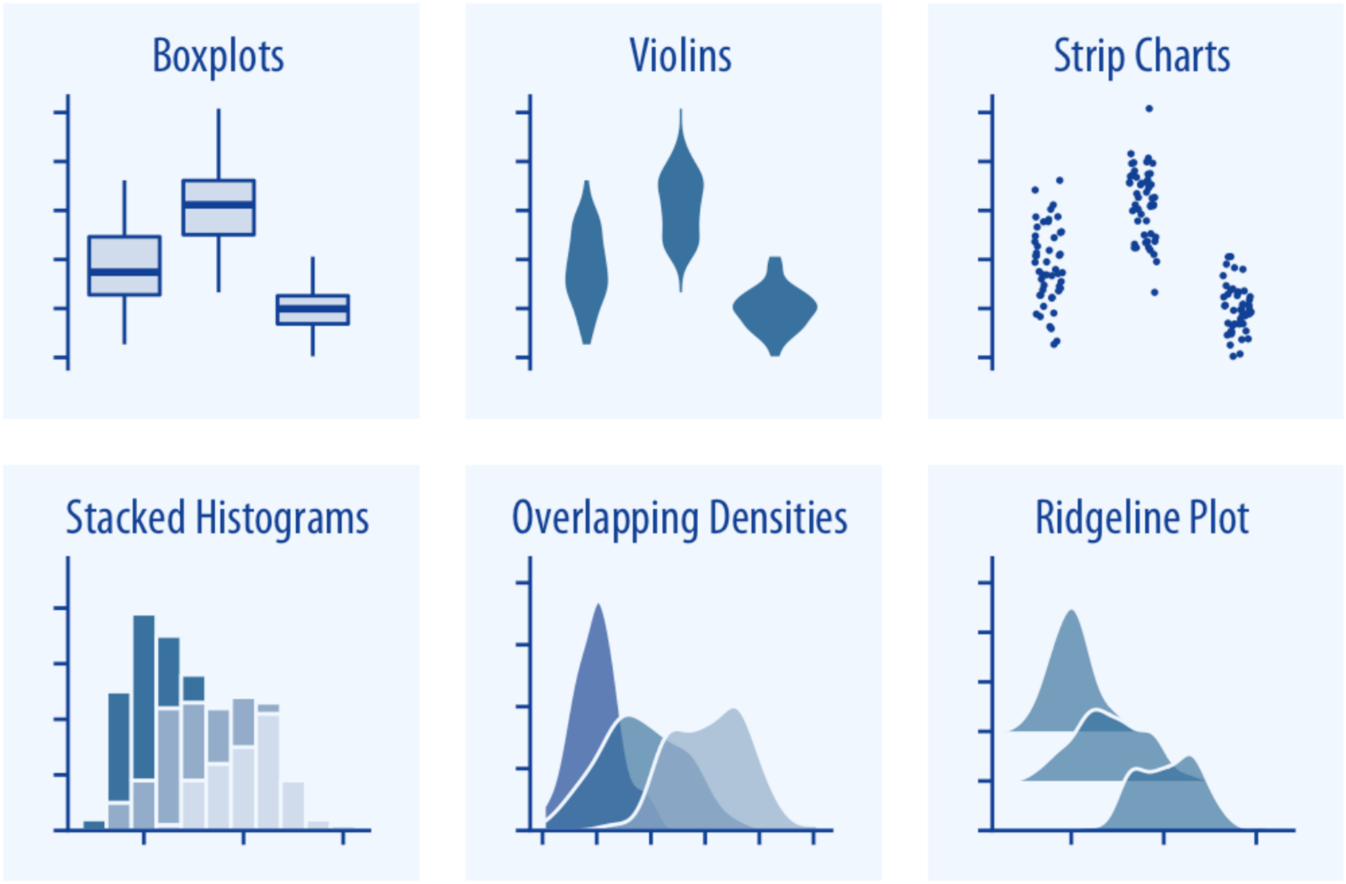
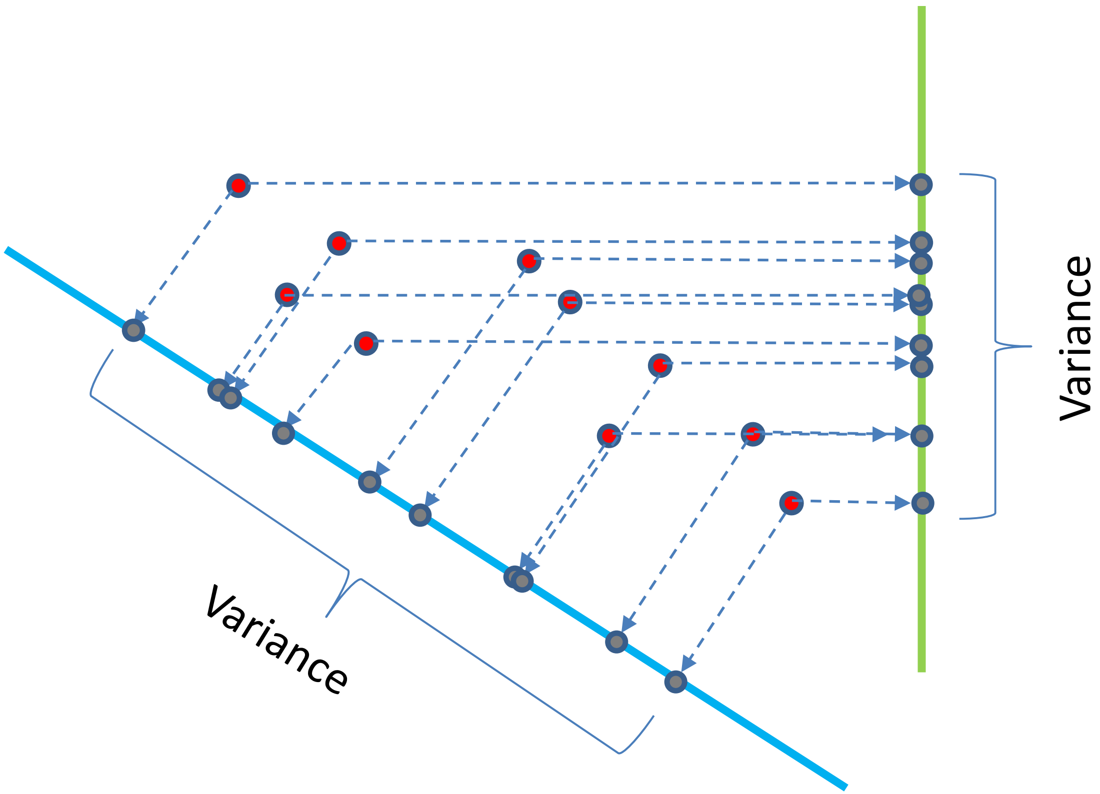


Figure from “Fundamentals of Data Visualization” by Claus Wilke

Alternative to PCA

Reducing dimensions

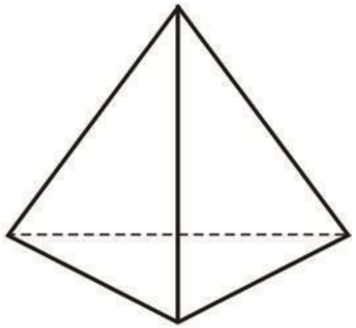
- How?
  - Project the points from high-dimensions to low dimensions



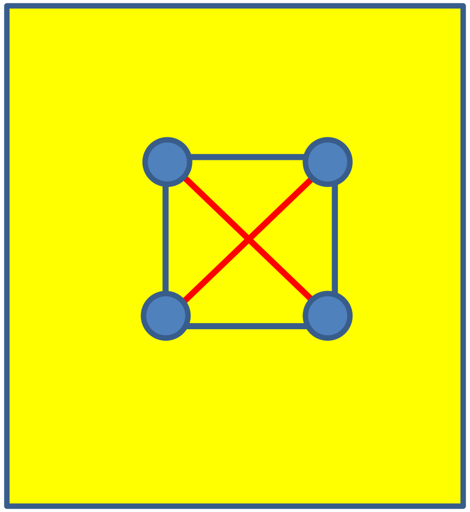
Prefer the blue line because more spread of the original data is represented→ Principal Component Analysis (**PCA**)

Reducing dimensions

- How?
  - Project the points from high-dimensions to low dimensions
  - Reconstruct high dimensional relationships in low dimensions



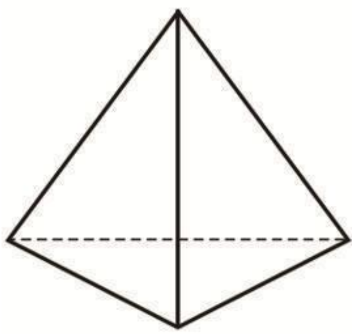
Tetrahedron with length 1 sides.
All pairwise distances between the four points = 1



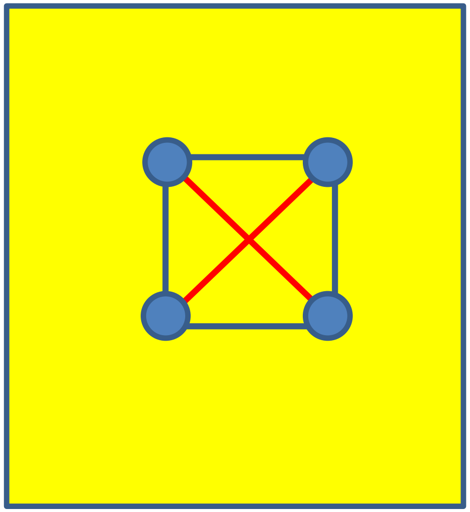
Try to arrange four points in 2D such that pairwise distances are as close as possible to the original pairwise distances

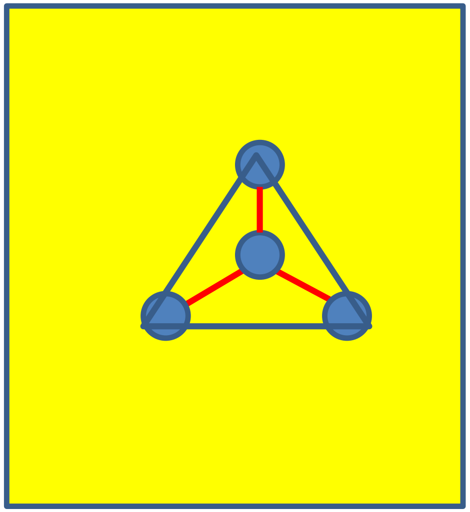
Reducing dimensions

- How?
  - Project the points from high-dimensions to low dimensions
  - Reconstruct high dimensional relationships in low dimensions



Tetrahedron with length 1 sides.
All pairwise distances between the four points = 1



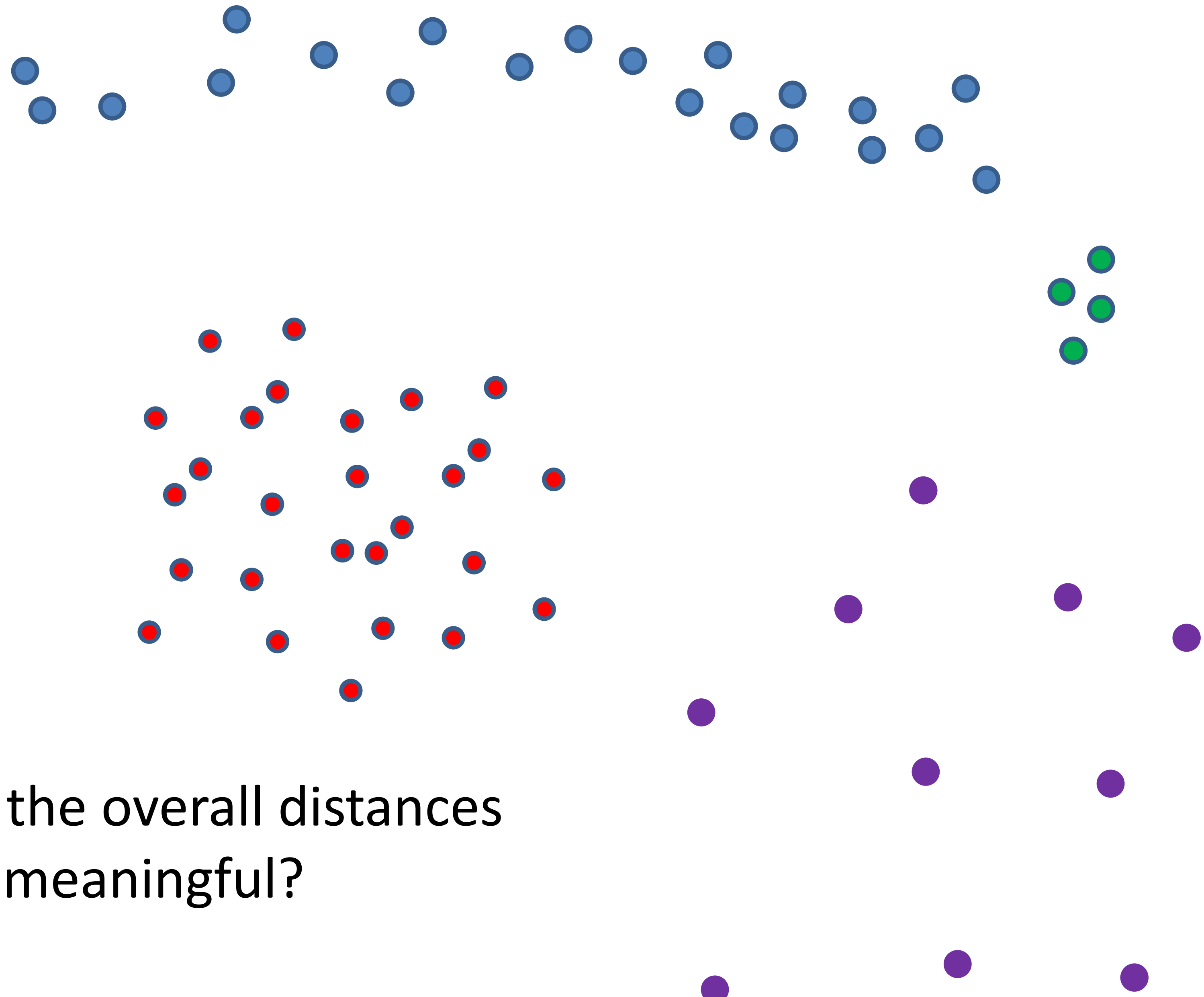


A lot of the time we want to create <u>clusters.</u>

Distances in the original data may not be meaningful

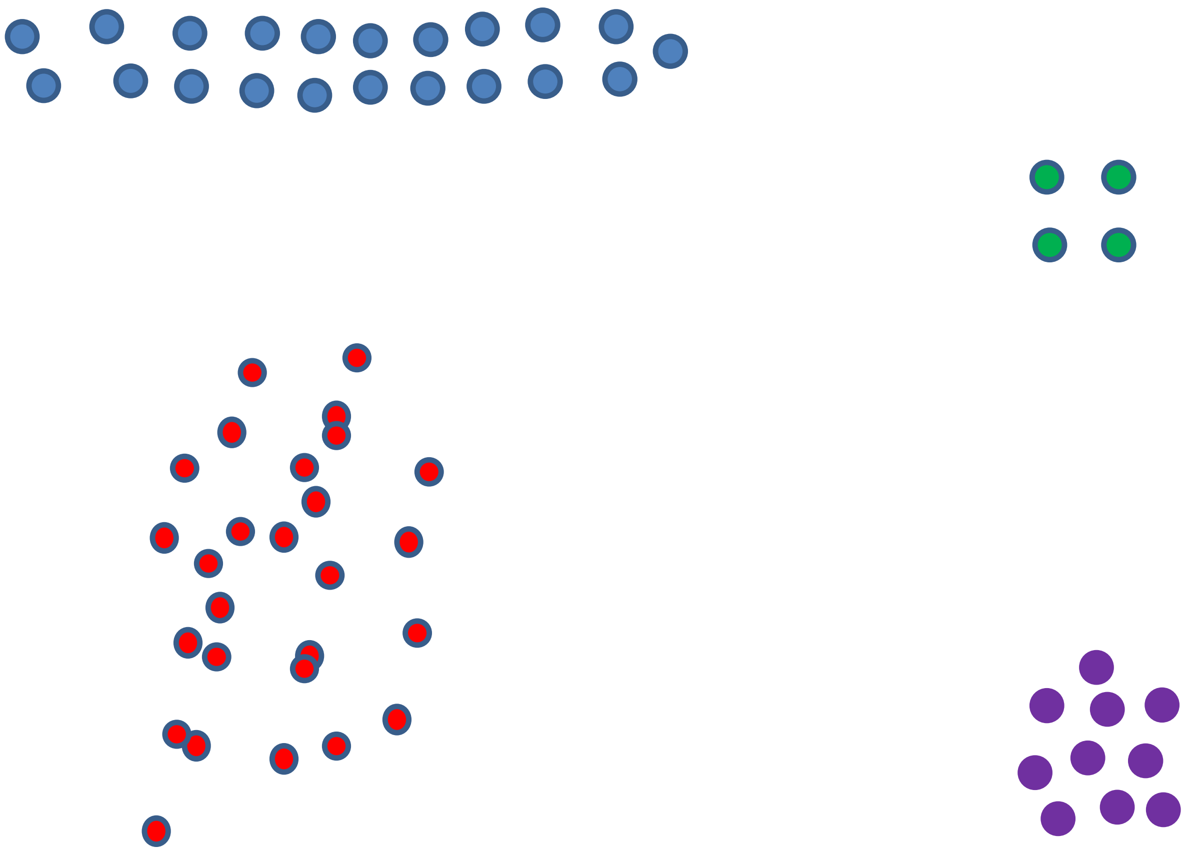
So we want some kind of <u>embedding</u> that preserves clustering

Linear projection (e.g. PCA) is only one type of embedding



What if the overall distances
are not meaningful?

Focus on your neighbors

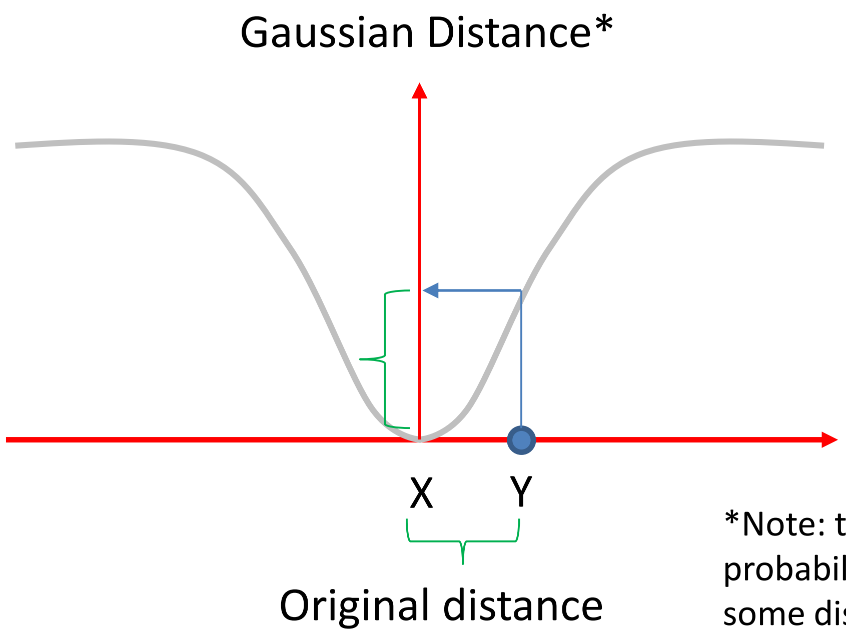


What if the overall distances are not meaningful?

Focus on your neighbors

t-SNE (t-distributed Stochastic Neighborhood Embedding)

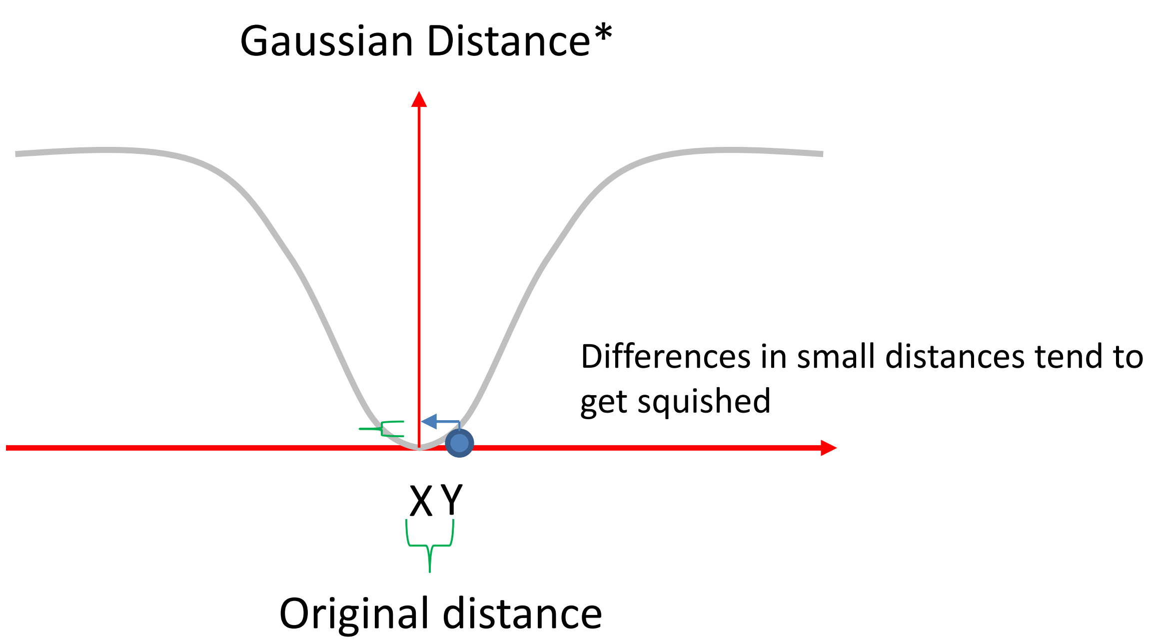
- Define distances between a point X to a point Y by a Gaussian function centered at X



*Note: the actual algorithm uses notions of probability (i.e., probability of finding Y at some distance from X). I use notion of distance as a proxy

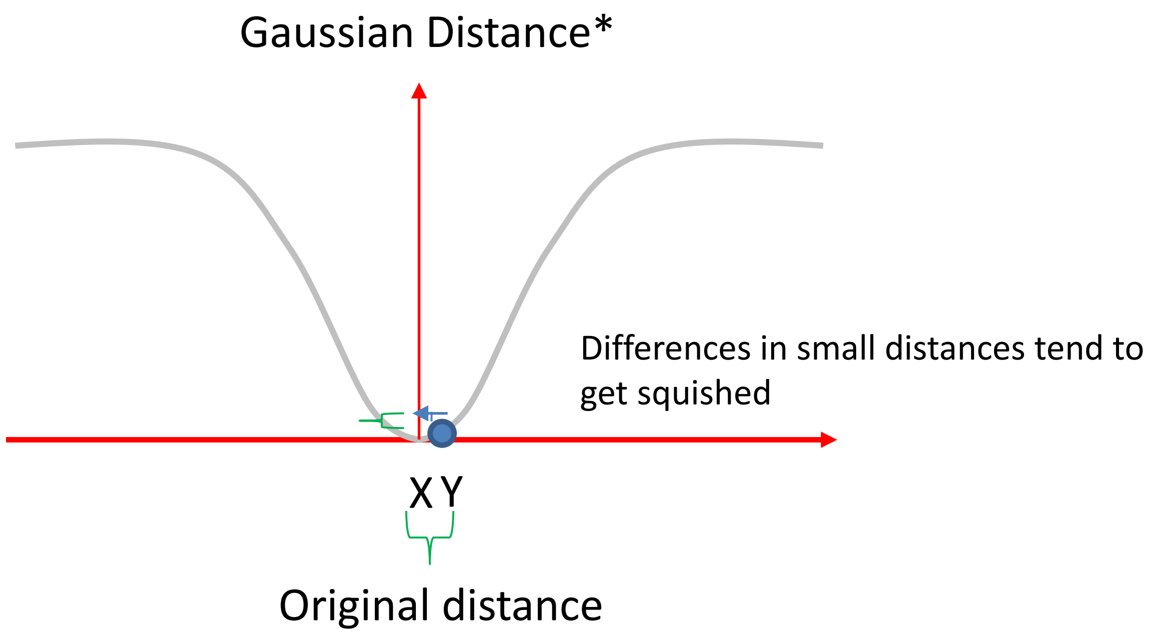
t-SNE (t-distributed Stochastic Neighborhood Embedding)

- Define distances between a point X to a point Y by a Gaussian function centered at X



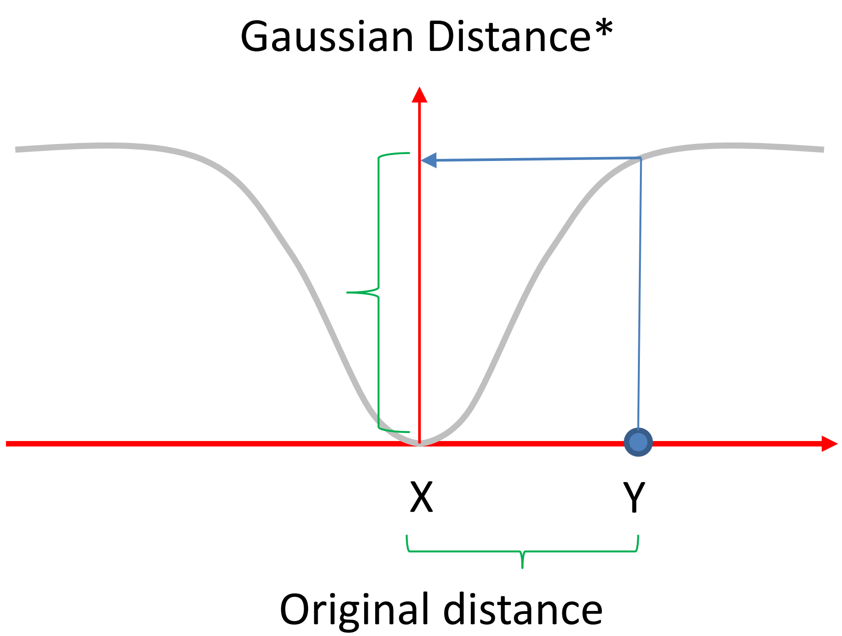
t-SNE (t-distributed Stochastic Neighborhood Embedding)

- Define distances between a point X to a point Y by a Gaussian function centered at X



t-SNE (t-distributed Stochastic Neighborhood Embedding)

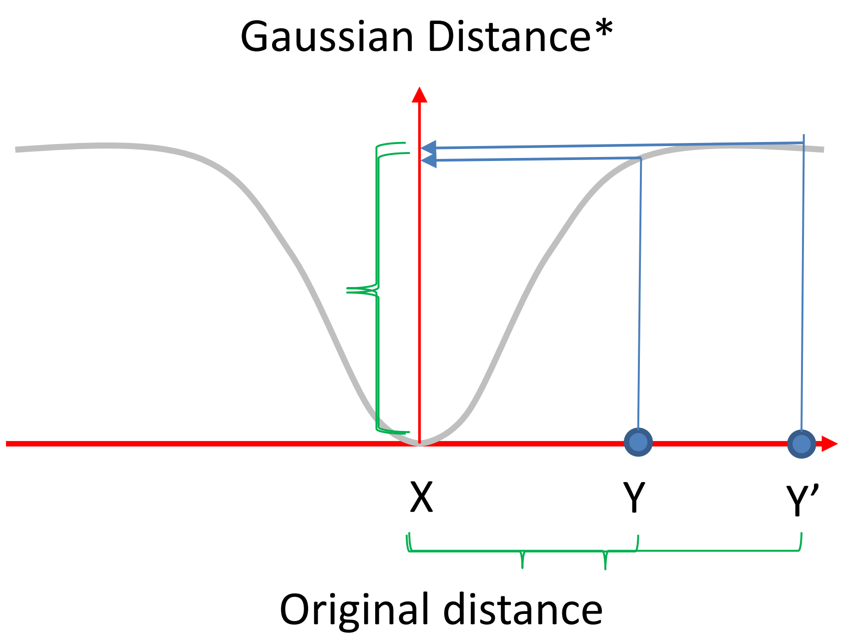
- Define distances between a point X to a point Y by a Gaussian function centered at X



Difference in large distances tend to get REALLY squished

t-SNE (t-distributed Stochastic Neighborhood Embedding)

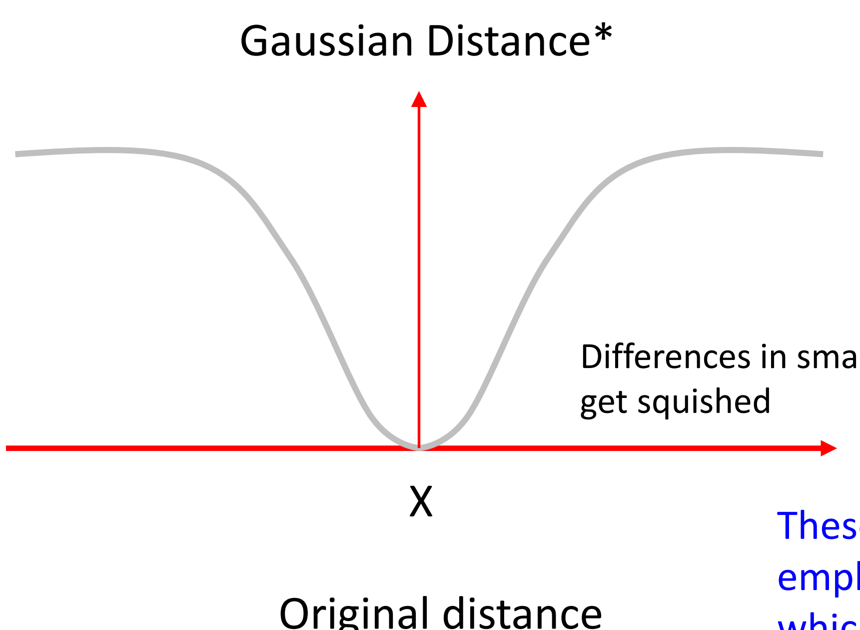
- Define distances between a point X to a point Y by a Gaussian function centered at X



Difference in large distances tend to get REALLY squished

t-SNE (t-distributed Stochastic Neighborhood Embedding)

- Define distances between a point X to a point Y by a Gaussian function centered at X

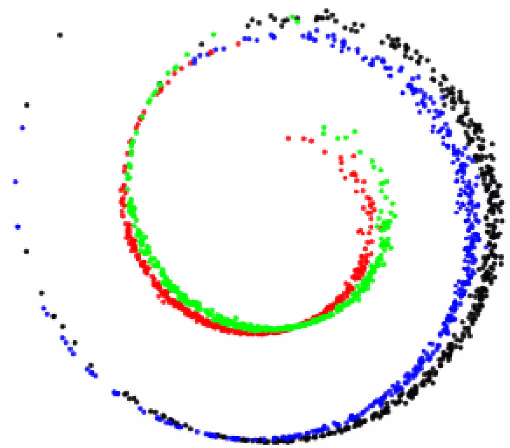


Difference in large distances tend to get REALLY squished

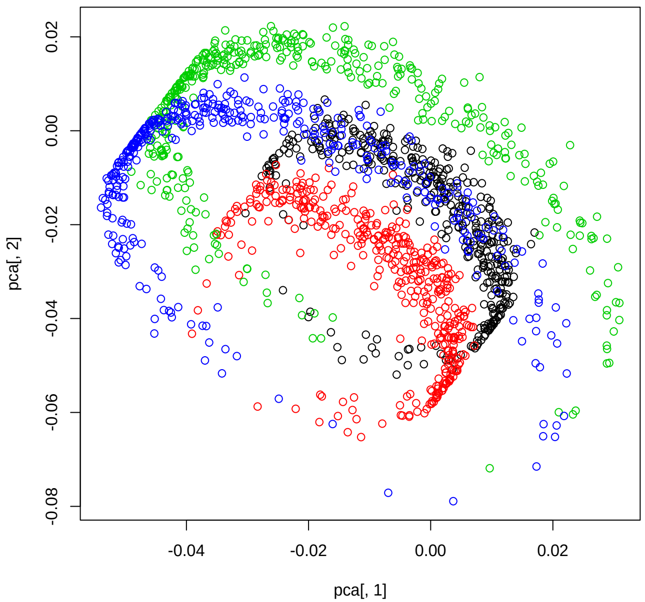
Differences in small distances tend to get squished

These two in combination tend to emphasize intermediate distances which emphasizes clusters

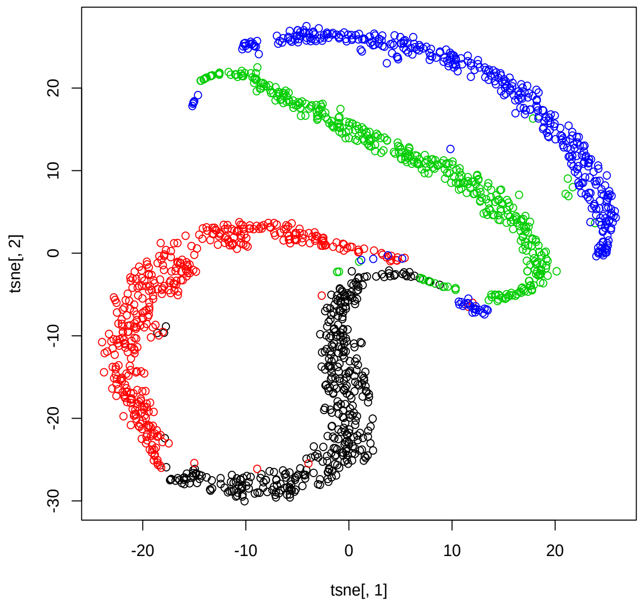
Original data



PCA

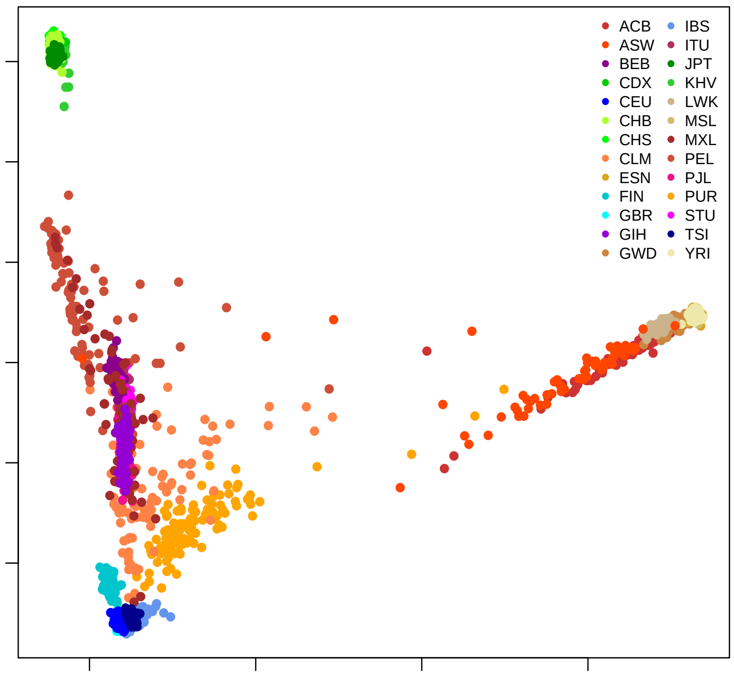


t-SNE

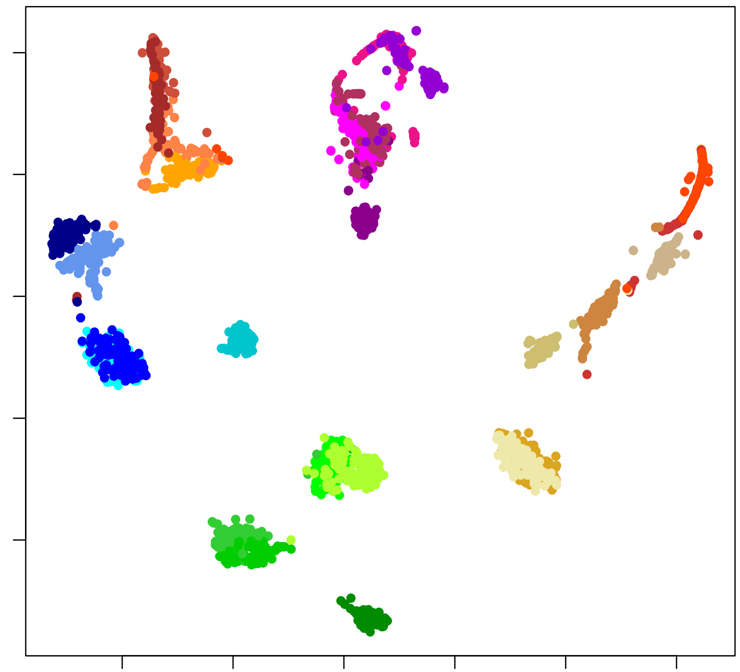


"swissroll data" **Dinoj Surendran**

PCA

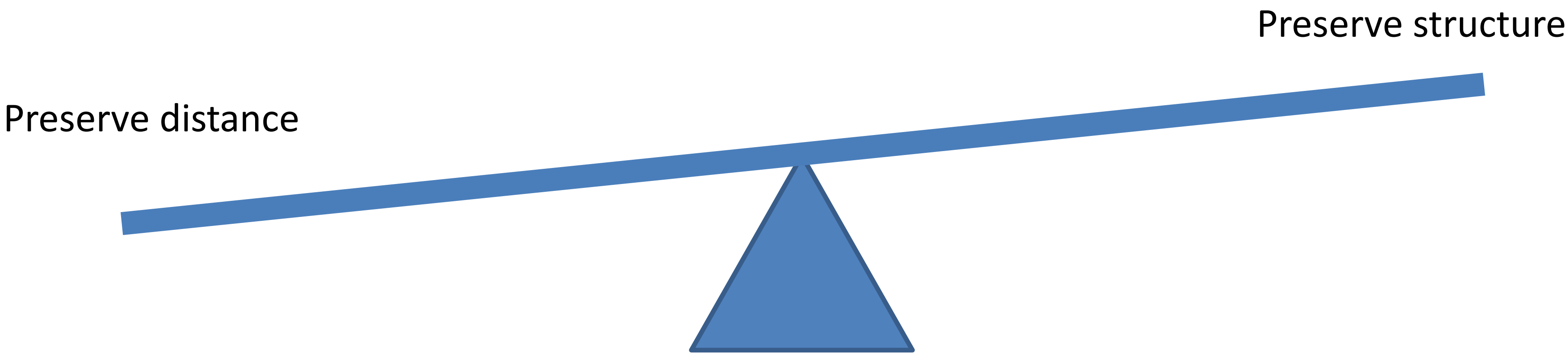


t-SNE



CHB	Han Chinese in Beijing, China
JPT	Japanese in Tokyo, Japan
CHS	Southern Han Chinese
CDX	Chinese Dai in Xishuangbanna, China
KHV	Kinh in Ho Chi Minh City, Vietnam
CEU	Utah Residents (CEPH) with Northern and Western European Ancestry
TSI	Toscani in Italia
FIN	Finnish in Finland
GBR	British in England and Scotland
IBS	Iberian Population in Spain
YRI	Yoruba in Ibadan, Nigeria
LWK	Luhya in Webuye, Kenya
GWD	Gambian in Western Divisions in the Gambia

MSL	Mende in Sierra Leone
ESN	Esan in Nigeria
ASW	Americans of African Ancestry in SW USA
ACB	African Caribbeans in Barbados
MXL	Mexican Ancestry from Los Angeles USA
PUR	Puerto Ricans from Puerto Rico
CLM	Colombians from Medellin, Colombia
PEL	Peruvians from Lima, Peru
GIH	Gujarati Indian from Houston, Texas
PJL	Punjabi from Lahore, Pakistan
BEB	Bengali from Bangladesh
STU	Sri Lankan Tamil from the UK
ITU	Indian Telugu from the UK



How to visualize data always depends on the data, and the question

There is rarely if ever a single correct approach

Outline for today

- Revisit data visualization
- Real-world data science exercise
- Begin: clustering

Discussion: admissions at Haverford

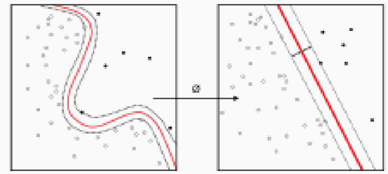
- Haverford has suddenly started receiving 10x more applications than usual
- You are tasked with creating an algorithm to determine whether or not an applicant should be admitted
- Questions:
  - How would you encode features?
  - How would you use past admission data to train?
  - What loss function are you trying to optimize?

Outline for today

- Revisit data visualization
- Real-world data science exercise
- Begin: clustering

Supervised Learning:
makes use of examples where we know the underlying "truth" (label/output)

Machine learning and data mining



Problems [show]

Supervised learning [hide]
(**classification** · **regression**)

Decision trees · Ensembles (Bagging, Boosting, Random forest) · *k*-NN · Linear regression · Naive Bayes · Neural networks · Logistic regression · Perceptron · Relevance vector machine (RVM) · Support vector machine (SVM)

Clustering [hide]

BIRCH · **Hierarchical** · *k*-means · Expectation-maximization (EM) · DBSCAN · OPTICS · Mean-shift

Dimensionality reduction [hide]

Factor analysis · CCA · ICA · LDA · NMF · PCA · t-SNE

Structured prediction [hide]

Graphical models (Bayes net, CRF, HMM)

Anomaly detection [hide]

k-NN · Local outlier factor

Neural nets [hide]

Autoencoder · Deep learning · Multilayer perceptron · RNN · Restricted Boltzmann machine · SOM · Convolutional neural network

Reinforcement Learning [hide]

Q-Learning · SARSA · Temporal Difference (TD)

Theory [show]

Machine learning venues [show]

Machine learning portal

V · T · E

Unsupervised Learning:
Learn underlying structure or features without labeled training data

Image: wikipedia

Unsupervised learning: 3 main areas

1) Clustering: group data points into clusters based on features only
2) Dimensionality reduction: remove feature correlation, compress data, visualize data
3) Structured prediction: model latent variables (example: Hidden Markov Models)

Unsupervised learning examples from biology: clustering

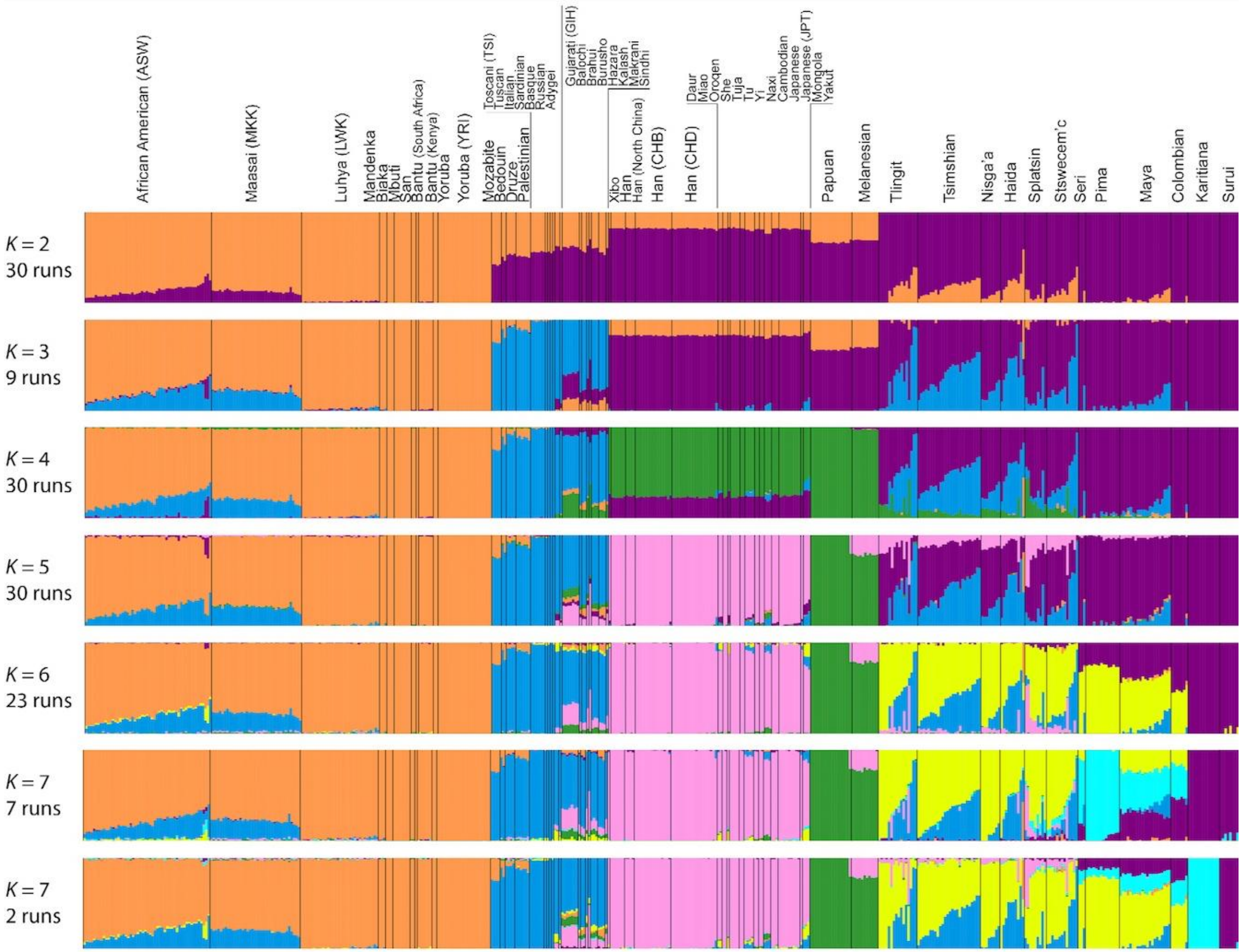
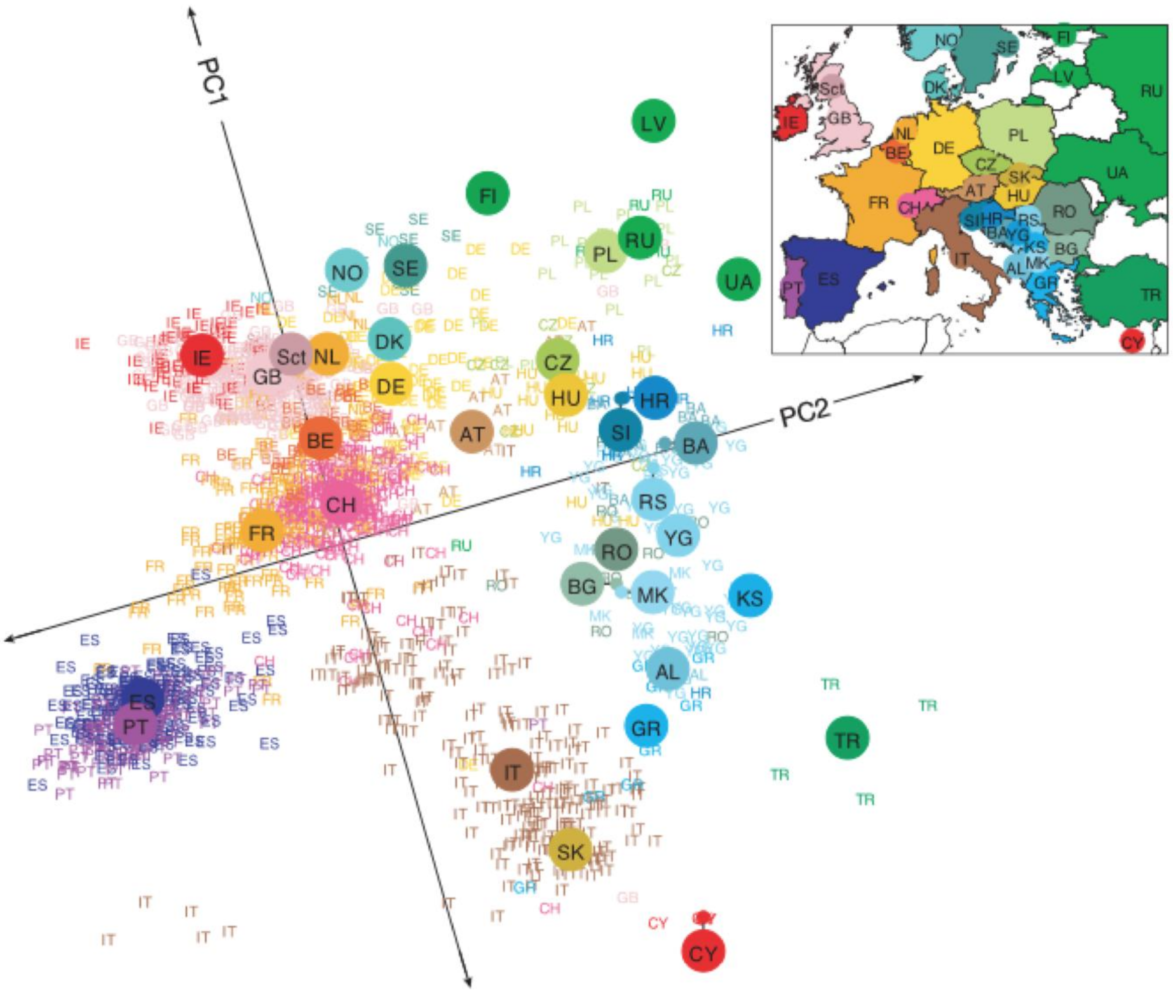


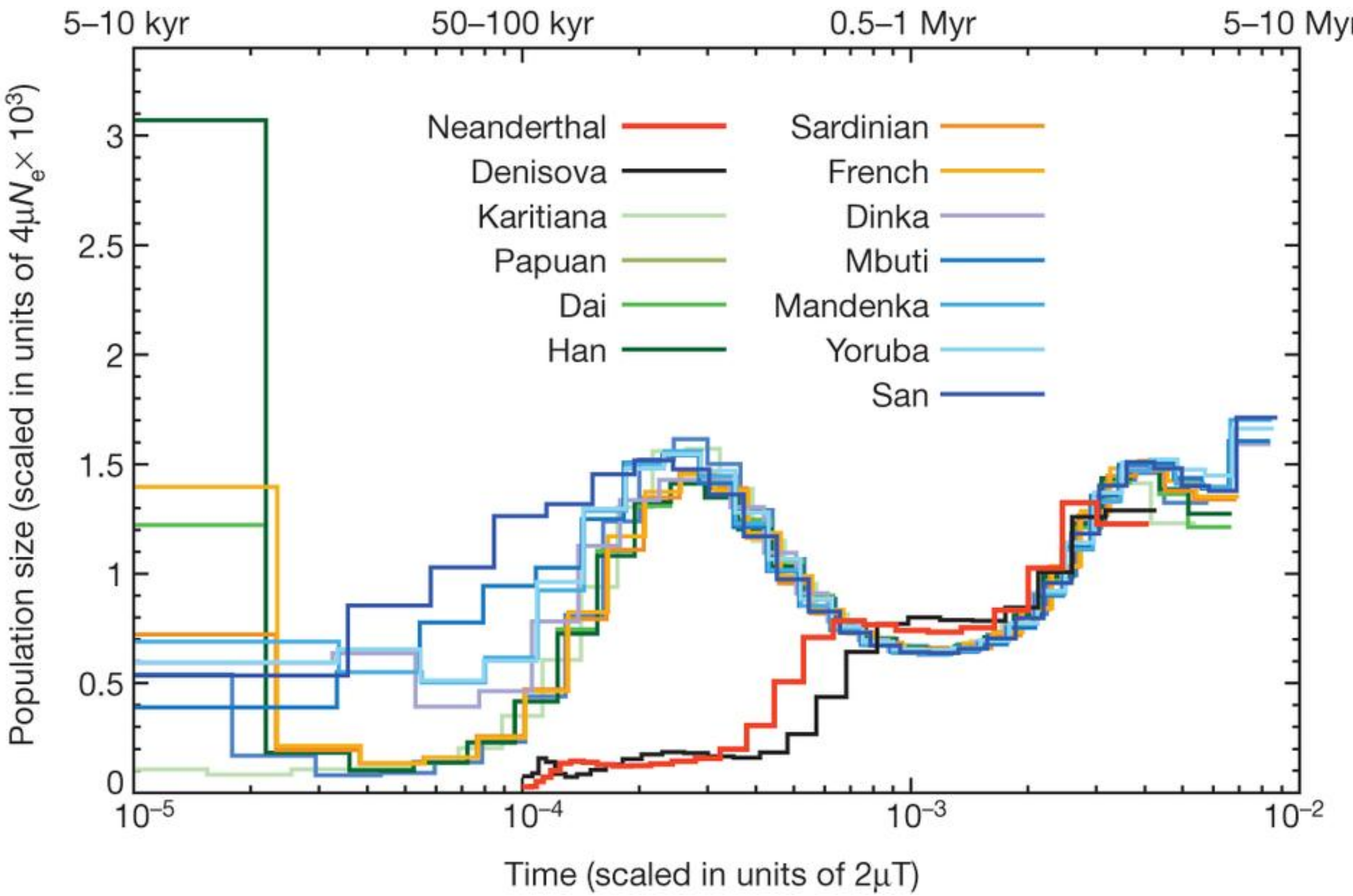
Figure: German Dziebel

Unsupervised learning examples from biology: dimensionality reduction



Genes mirror geography within Europe (2008)

Unsupervised learning examples from biology: structured prediction



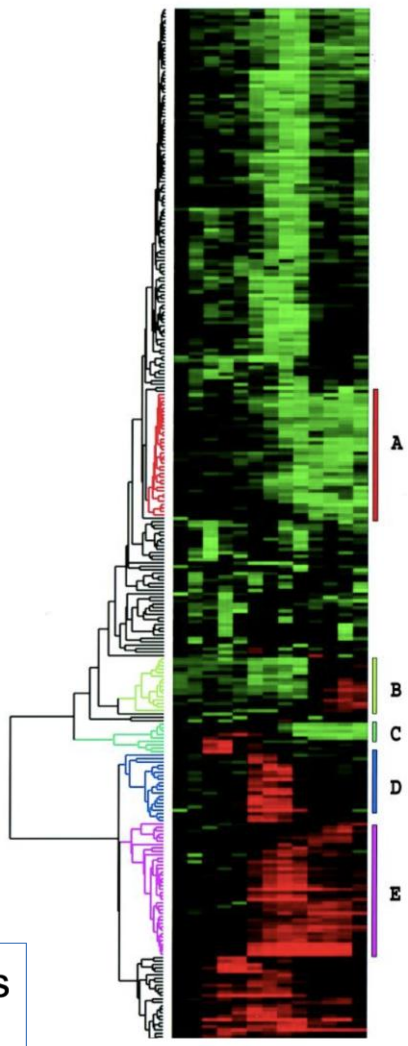
The complete genome sequence of a Neanderthal from the Altai Mountains, Prufer et al (2014)

Clustering

- Learn about the structure in our data
- Cluster new data (prediction)
- Goal: $\mathrm{C} = \{C_1, C_2, \ldots, C_k\}$ such that within cluster difference is minimized

Applications of clustering

- Cluster genes with similar expression patterns



Cluster analysis and display of genome-wide expression patterns

Michael B. Eisen,* Paul T. Spellman,* Patrick O. Brown,† and David Botstein*‡

Applications of clustering

- Image segmentation: cluster similar regions of an image

Image: Jessica Wu

Applications of clustering

- Clustering in social graphs

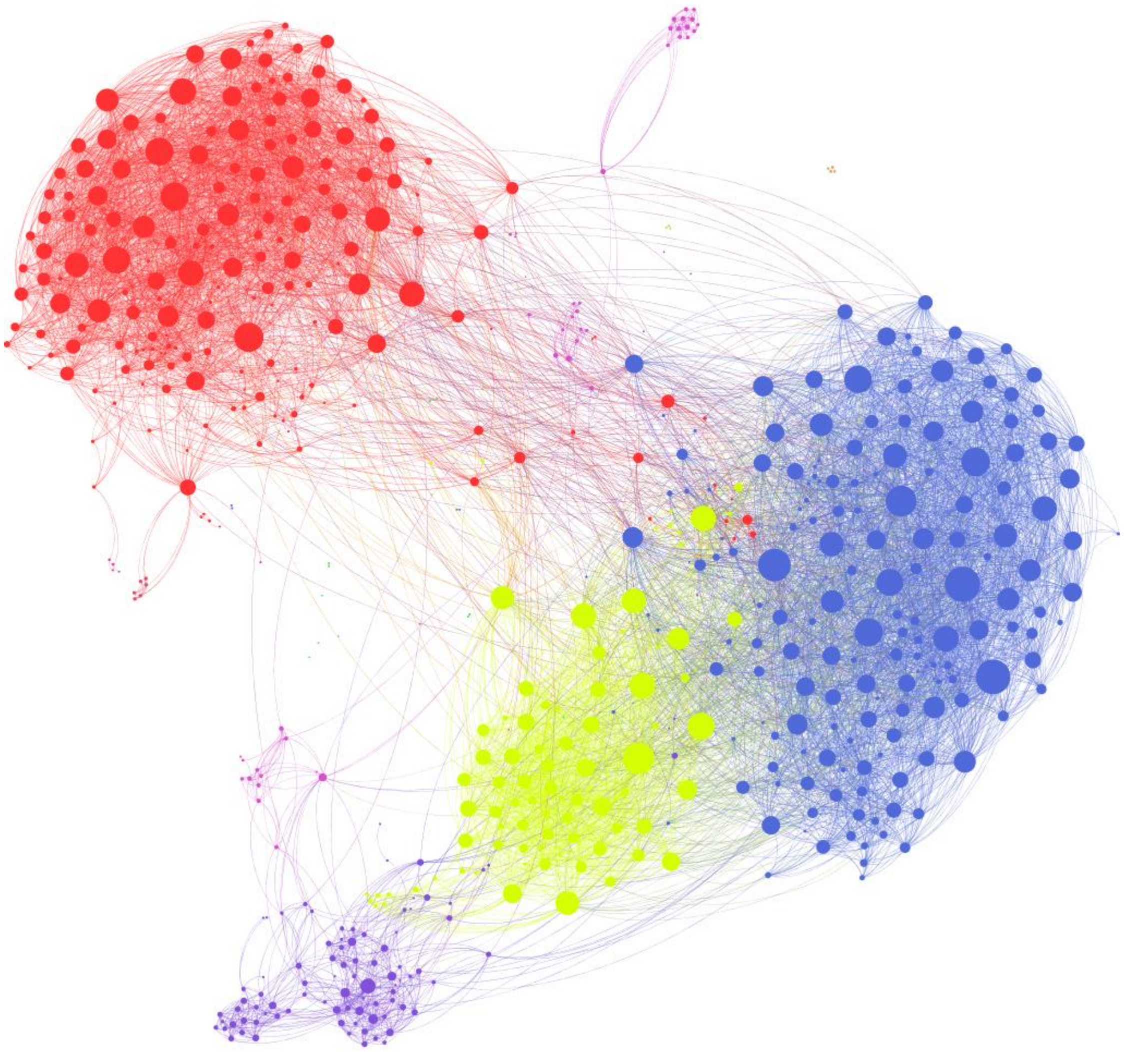


Image: https://griffsgraphs.wordpress.com/2012/07/02/a-facebook-network/