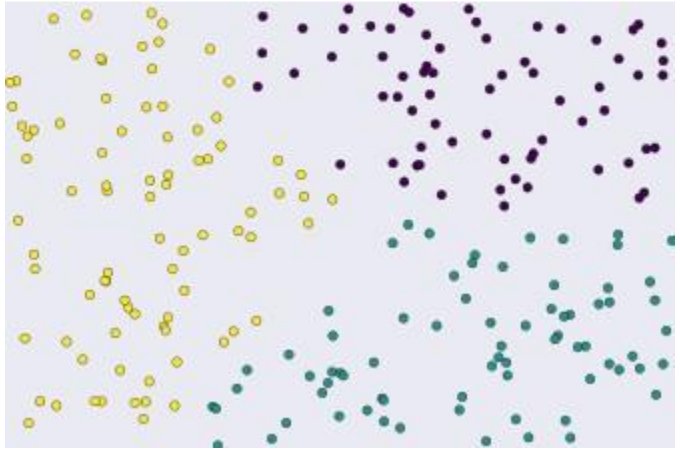
NSERC CREATE for BioZone Machine Learning Bootcamp

Unsupervised Learning

https://developers.google.com/machine-learning/clustering/overview

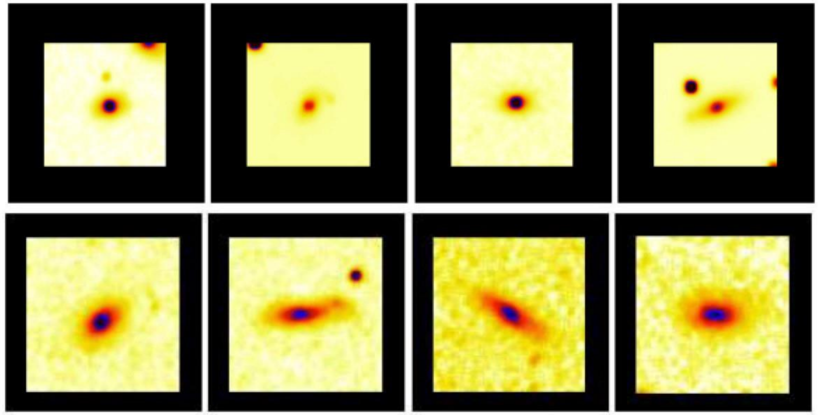


Clustering

The most common type of unsupervised learning

Goal: group “similar” data points together

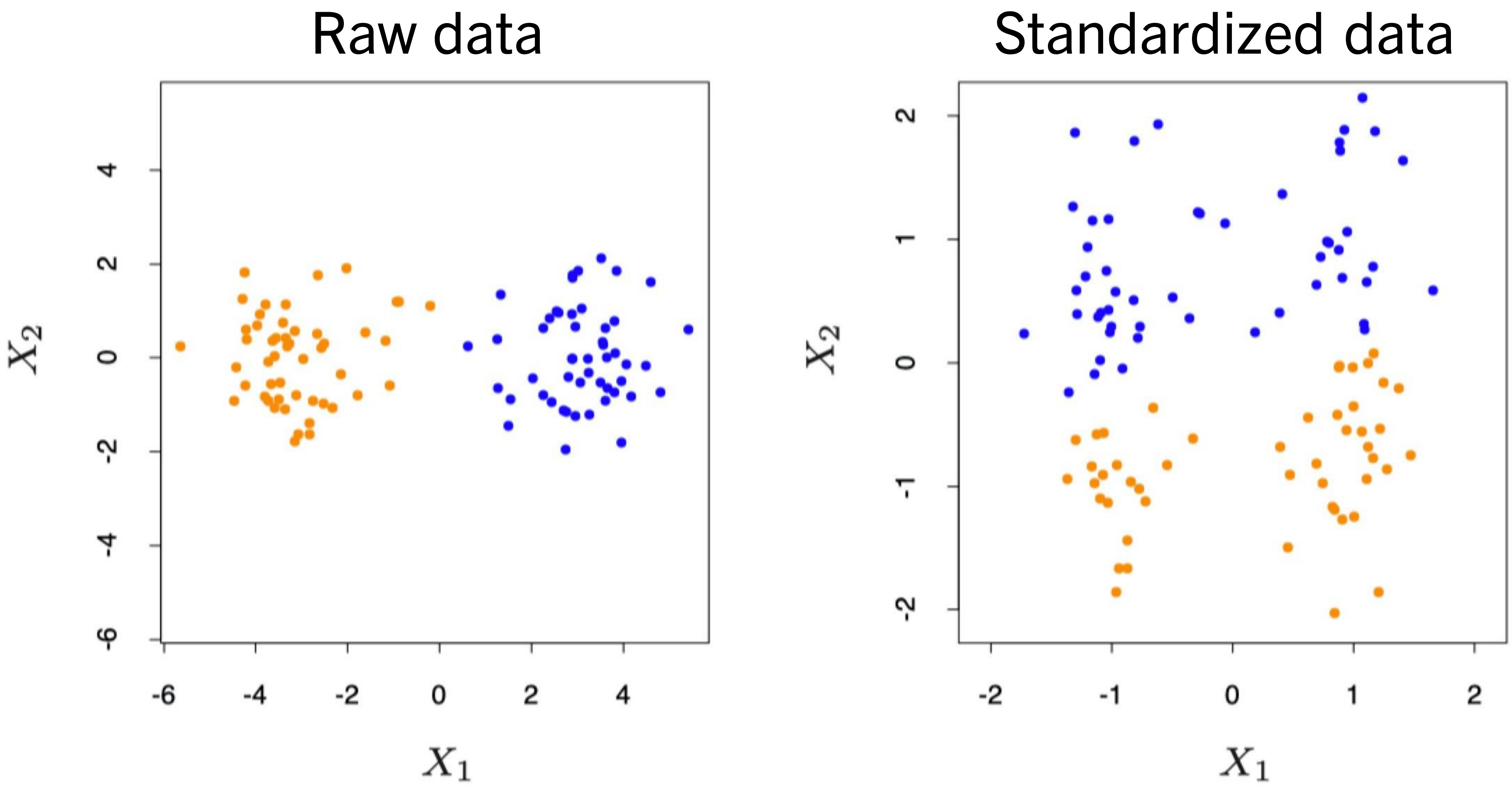
Unsupervised because we don’t label the data as we did in classification/regression: let the features speak for themselves!



Clustering galaxies, from Miller et al. (2005)

Data Preparation for Clustering

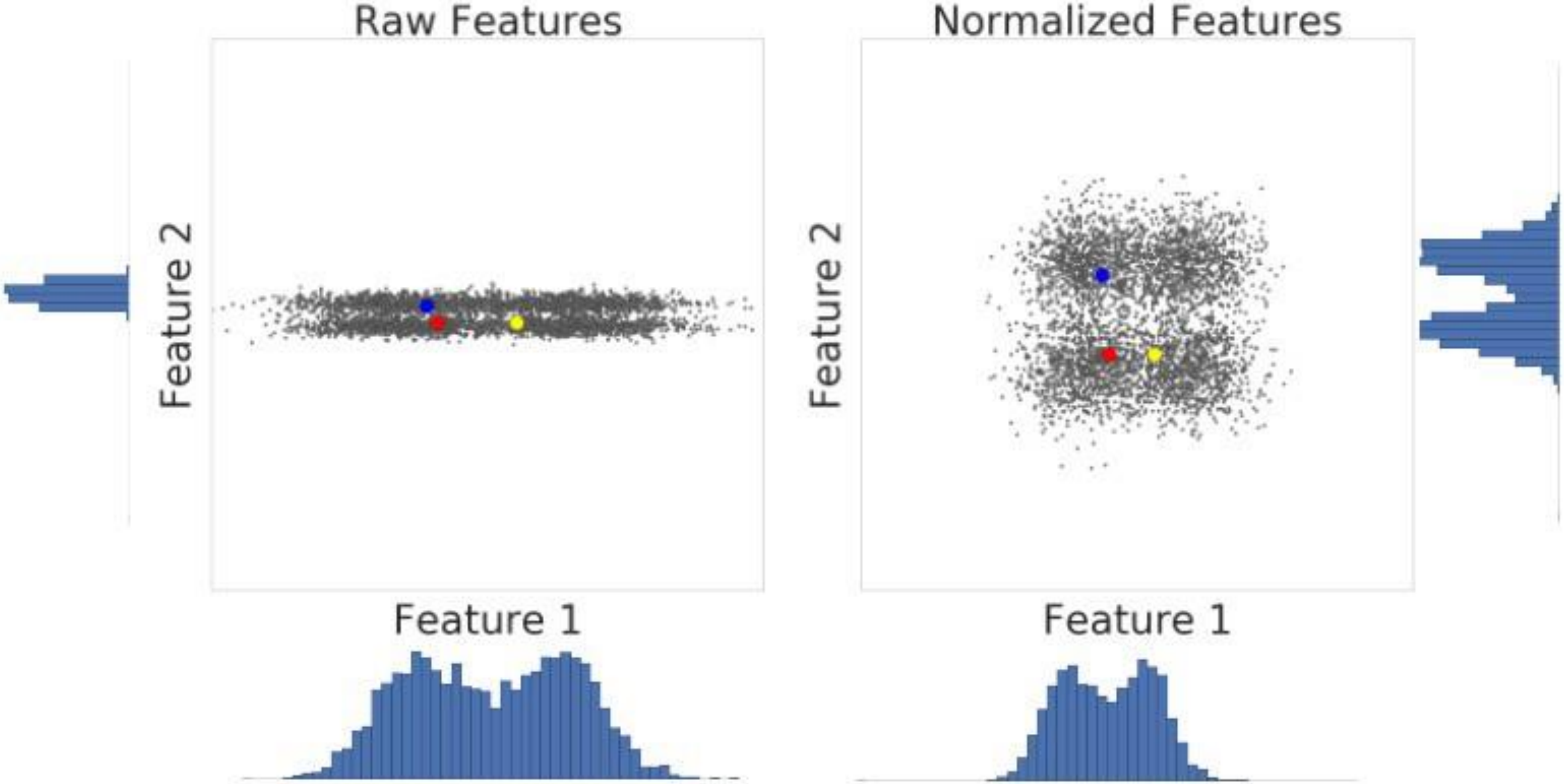
The points are colored by a clustering algorithm



Raw data

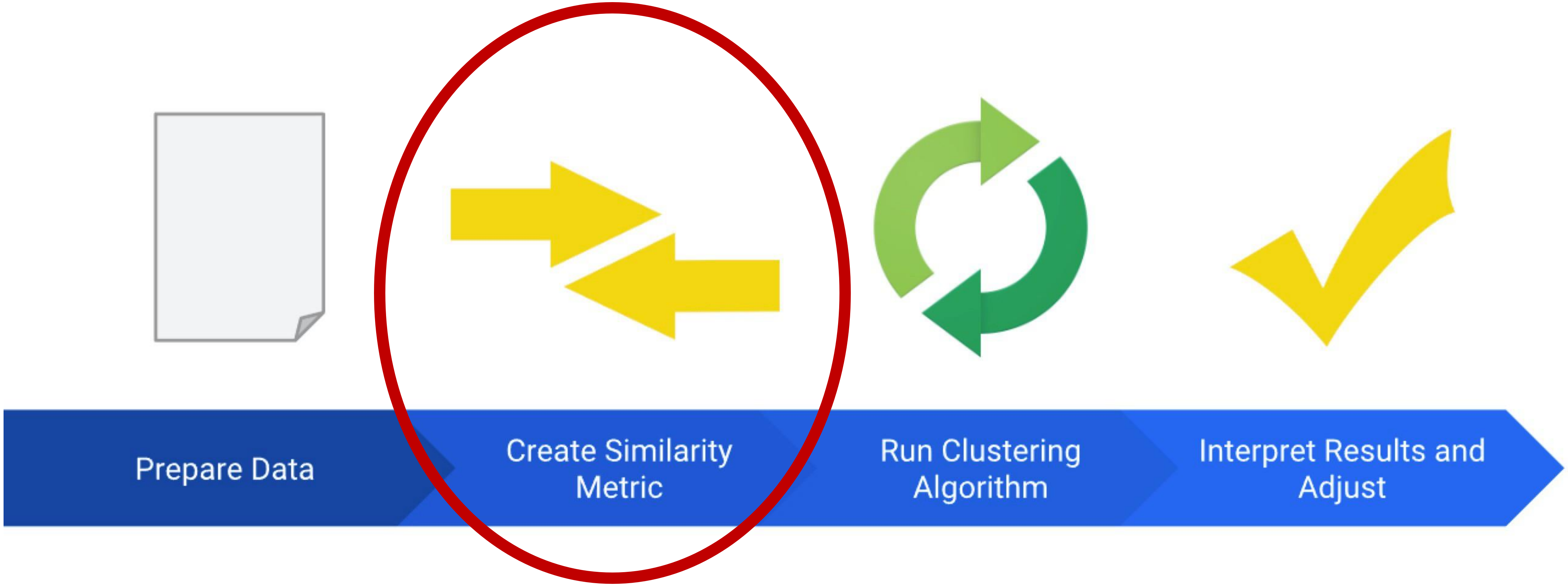
Standardized data

Data Preparation for Clustering



https://developers.google.com/machine-learning/clustering/prepare-data

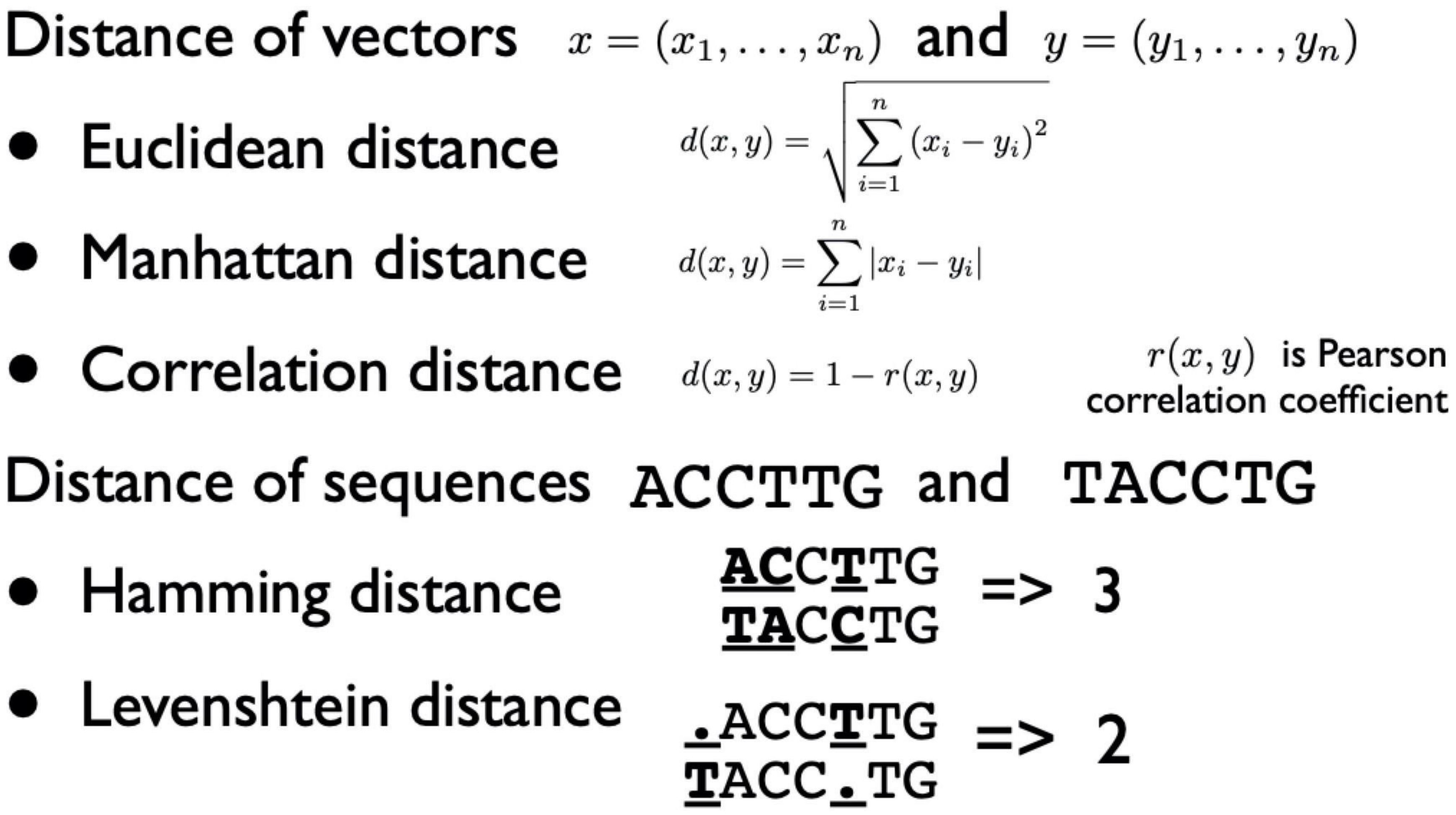
Clustering workflow



From Google's Clustering lesson: https://developers.google.com/machine-learning/clustering/

Distance Metrics

The right distance metric depends on your application!



Distance of vectors $x = (x_1, \ldots, x_n)$ and $y = (y_1, \ldots, y_n)$

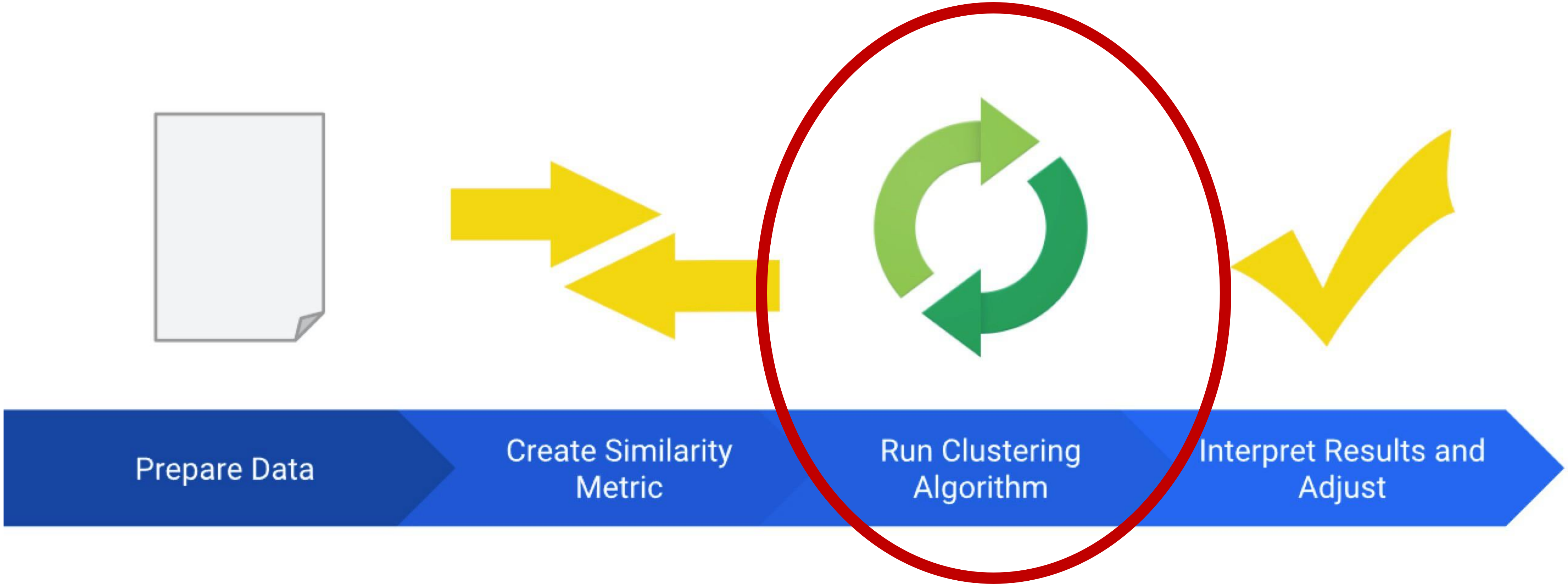
- Euclidean distance $d(x,y) = \sqrt{\sum_{i=1}^{n} (x_i - y_i)^2}$
- Manhattan distance $d(x,y) = \sum_{i=1}^{n} |x_i - y_i|$
- Correlation distance $d(x,y) = 1 - r(x,y)$ — $r(x,y)$ is Pearson correlation coefficient

Distance of sequences ACCTTG and TACCTG

- Hamming distance $\underline{\mathbf{AC}}\mathtt{C}\underline{\mathbf{T}}\mathtt{TG}$ / $\underline{\mathbf{TA}}\mathtt{C}\underline{\mathbf{C}}\mathtt{TG}$ => 3
- Levenshtein distance $\underline{\mathbf{.}}\mathtt{ACC}\underline{\mathbf{T}}\mathtt{TG}$ / $\underline{\mathbf{T}}\mathtt{ACC}\underline{\mathbf{.}}\mathtt{TG}$ => 2

Based on slides by Elena Sügis: http://bioinformaticsinstitute.ru/sites/default/files/preprocessing_unsupervised.pdf

Clustering workflow

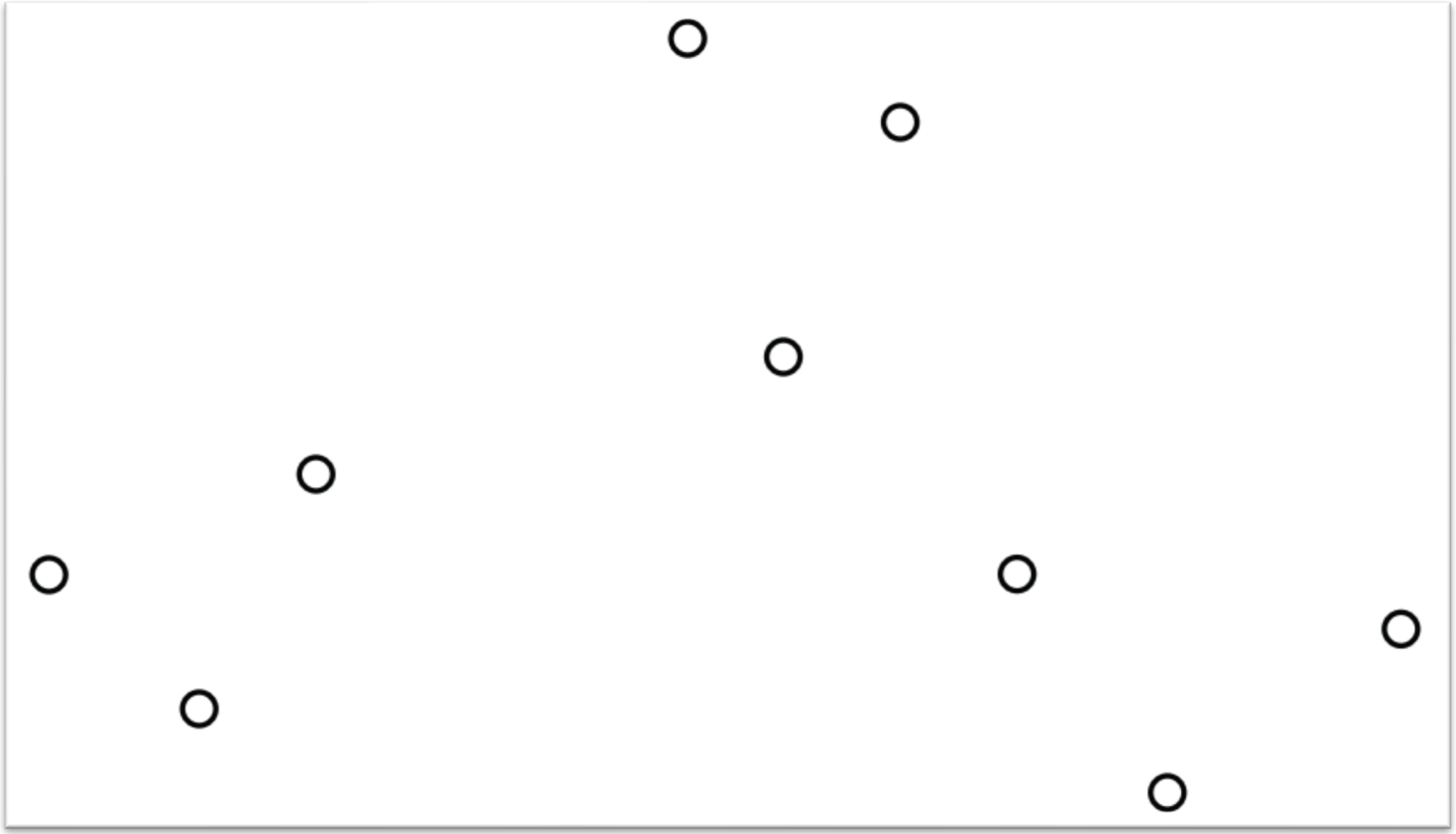


From Google’s Clustering lesson: https://developers.google.com/machine-learning/clustering/

K-means Clustering

Euclidean distance metric

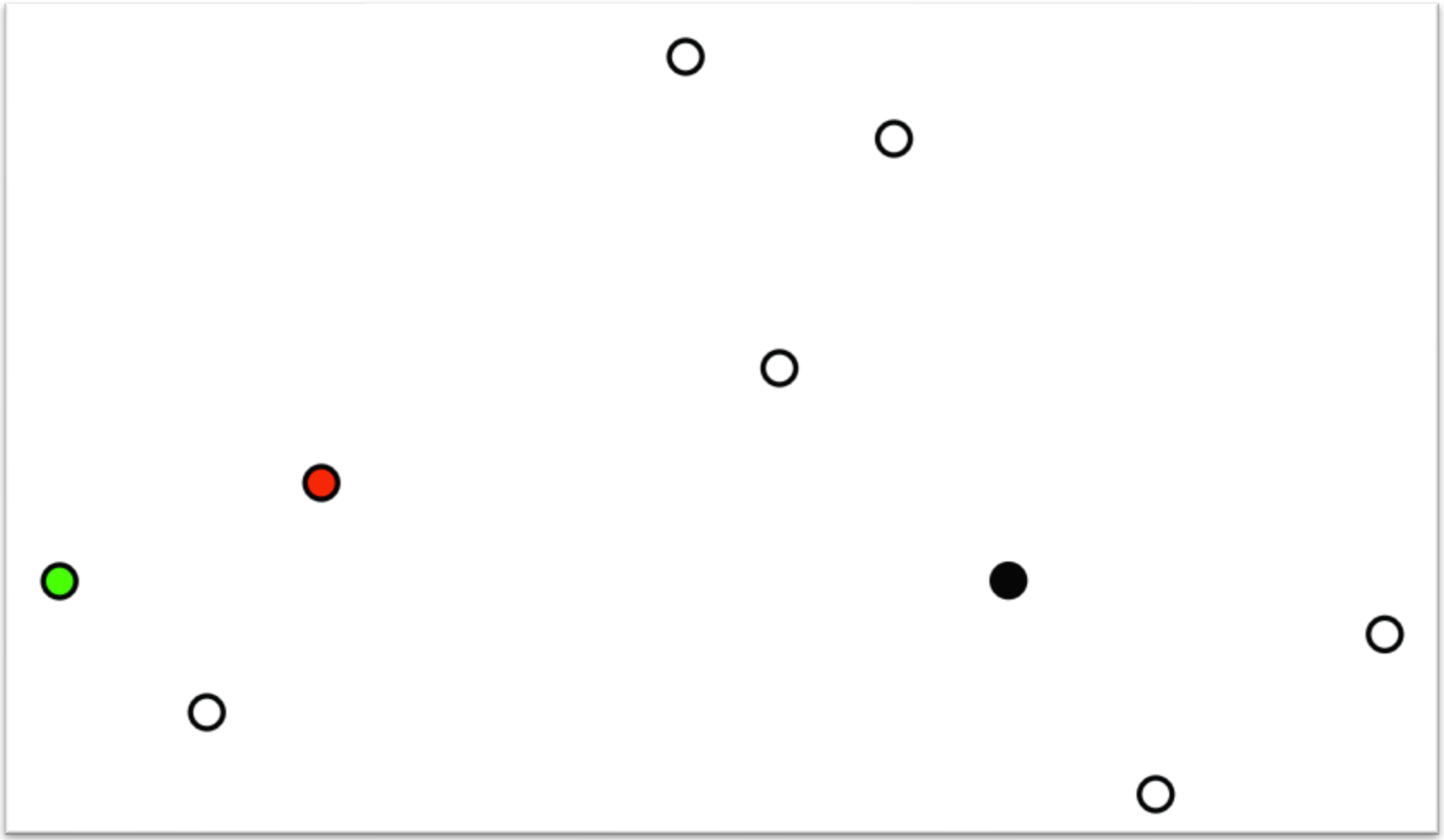
Given a set of data points…



K-means Clustering

Euclidean distance metric

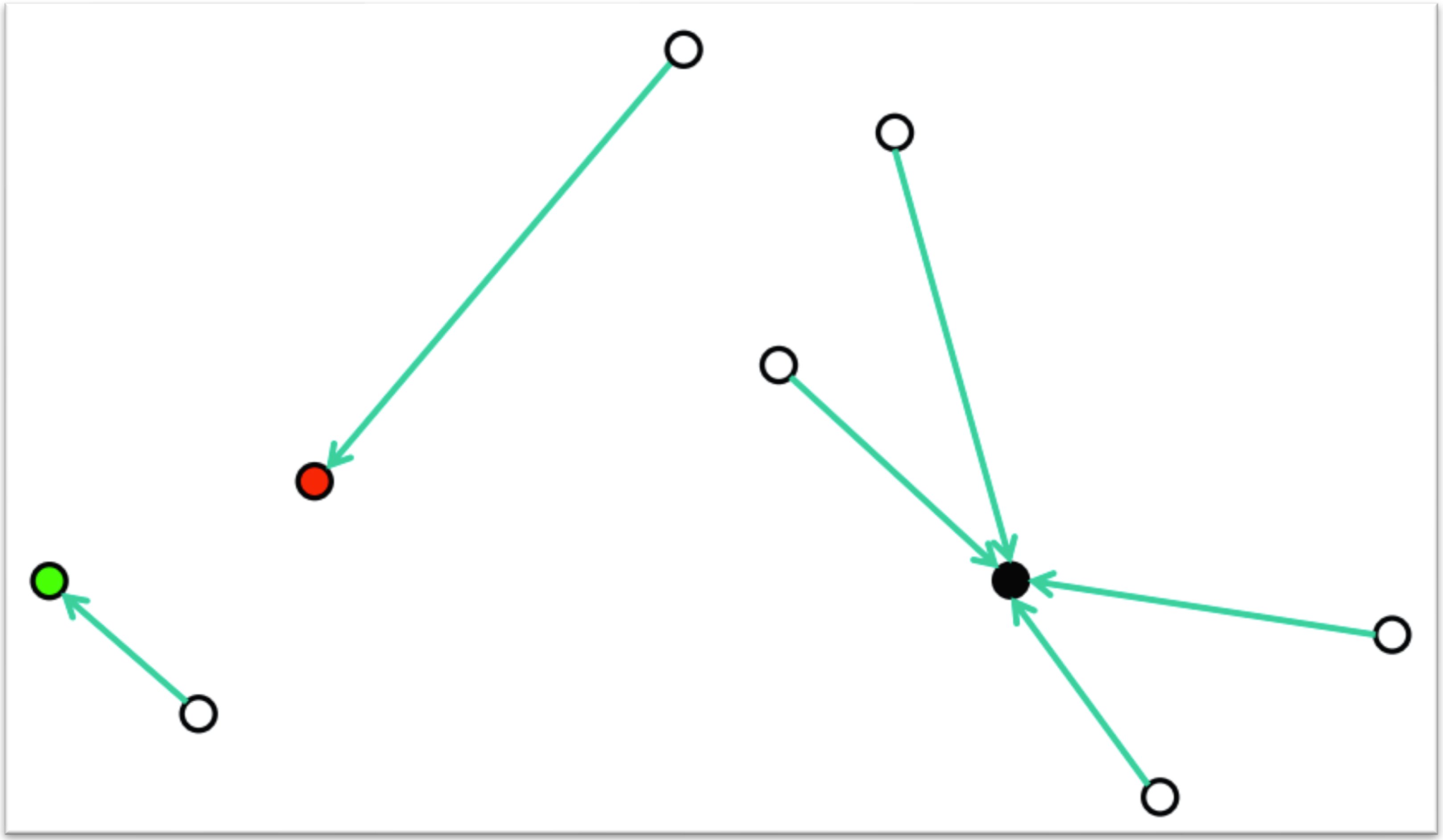
Select k=3 initial centers at random



K-means Clustering

Euclidean distance metric

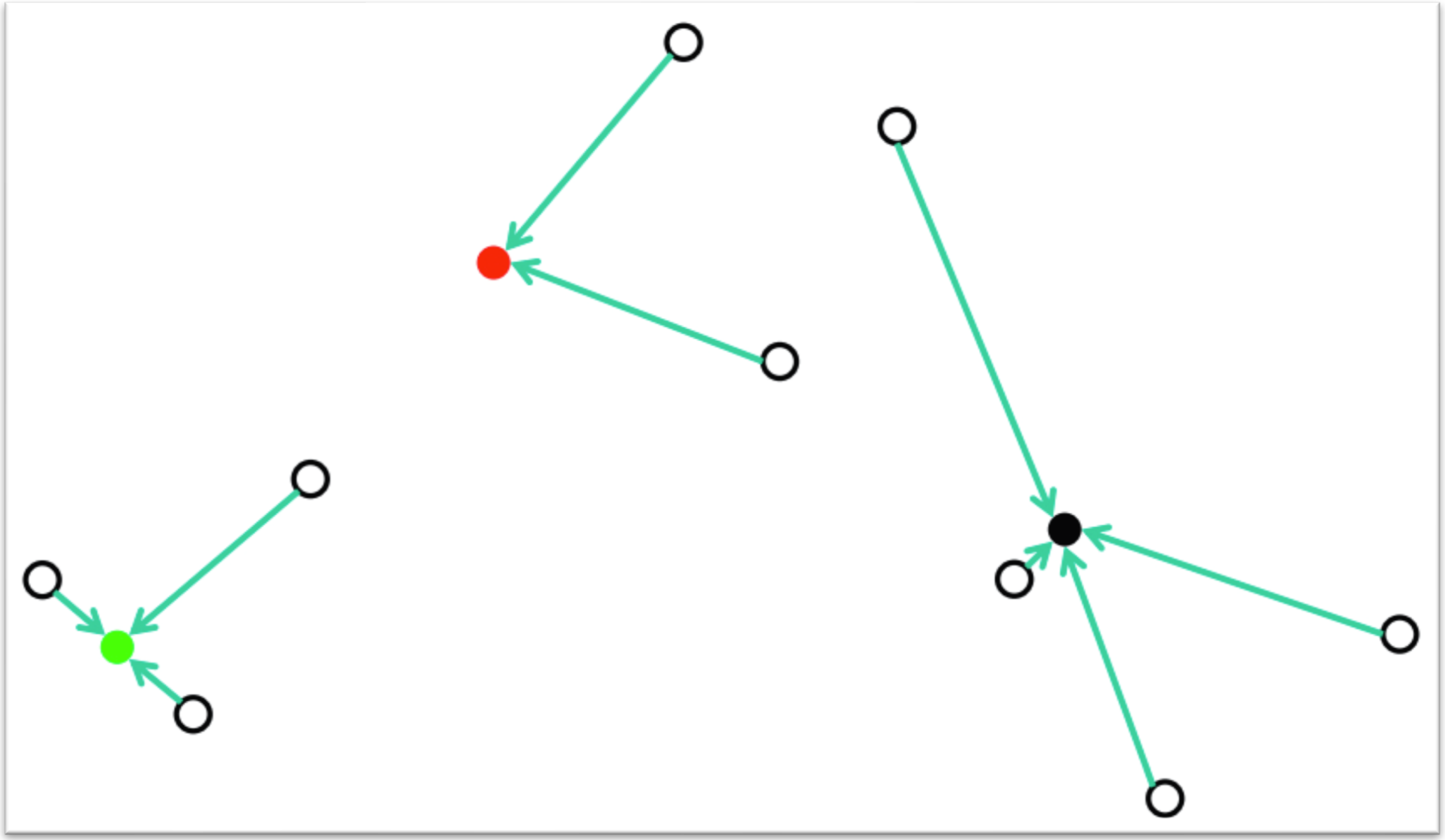
Recompute optimal centers given a fixed clustering



K-means Clustering

Euclidean distance metric

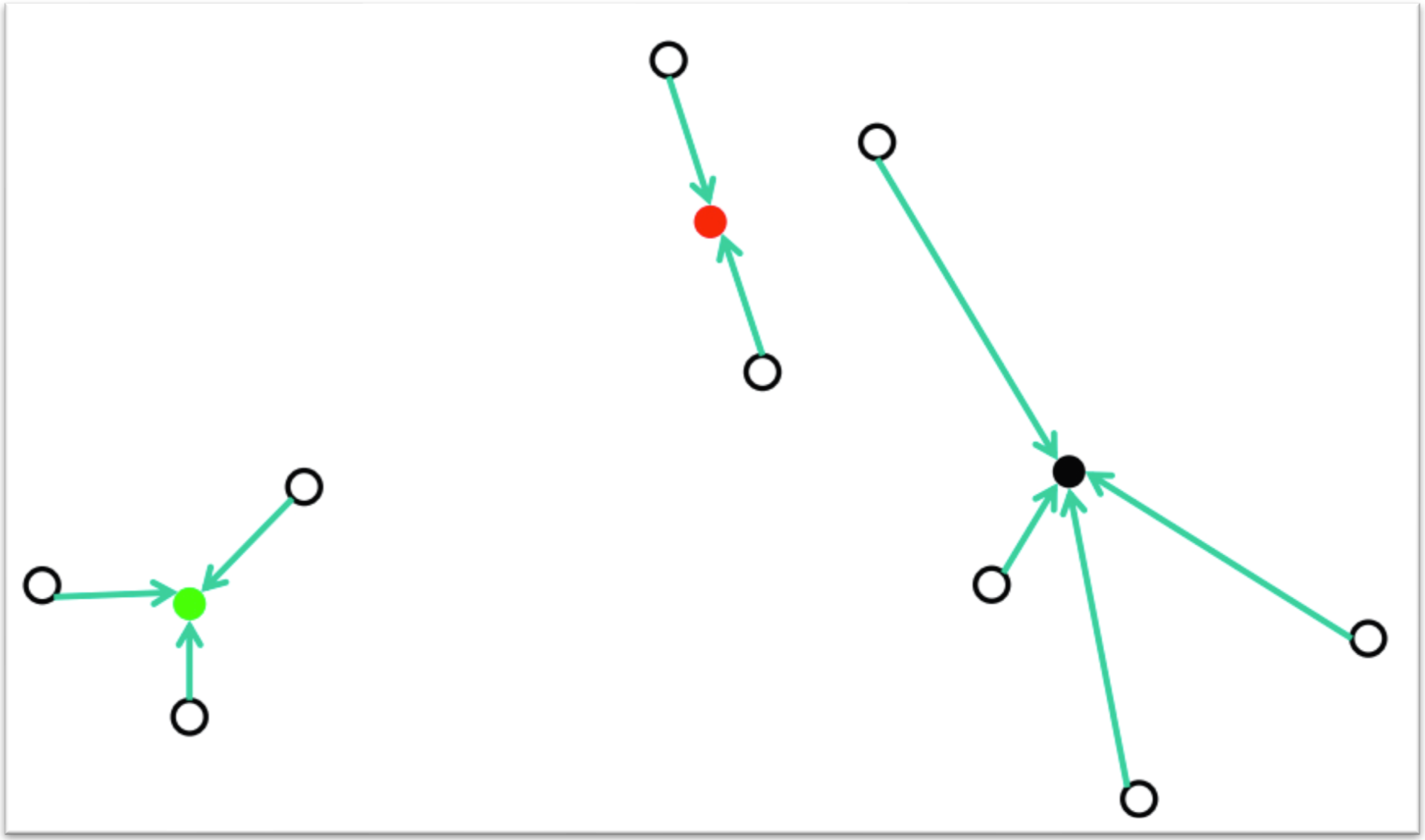
Assign each point to its nearest center



K-means Clustering

Euclidean distance metric

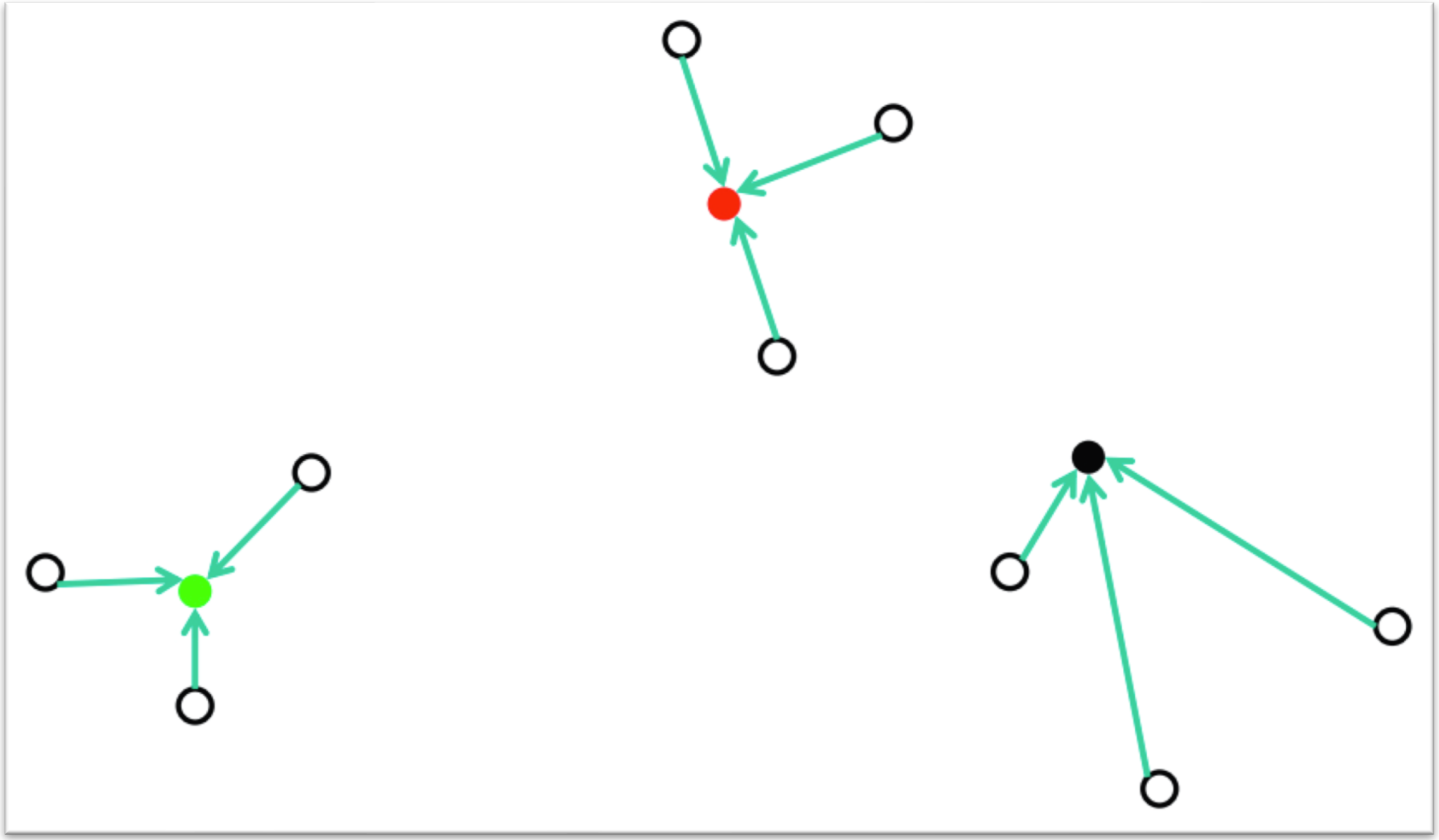
Recompute optimal centers given a fixed clustering



K-means Clustering

Euclidean distance metric

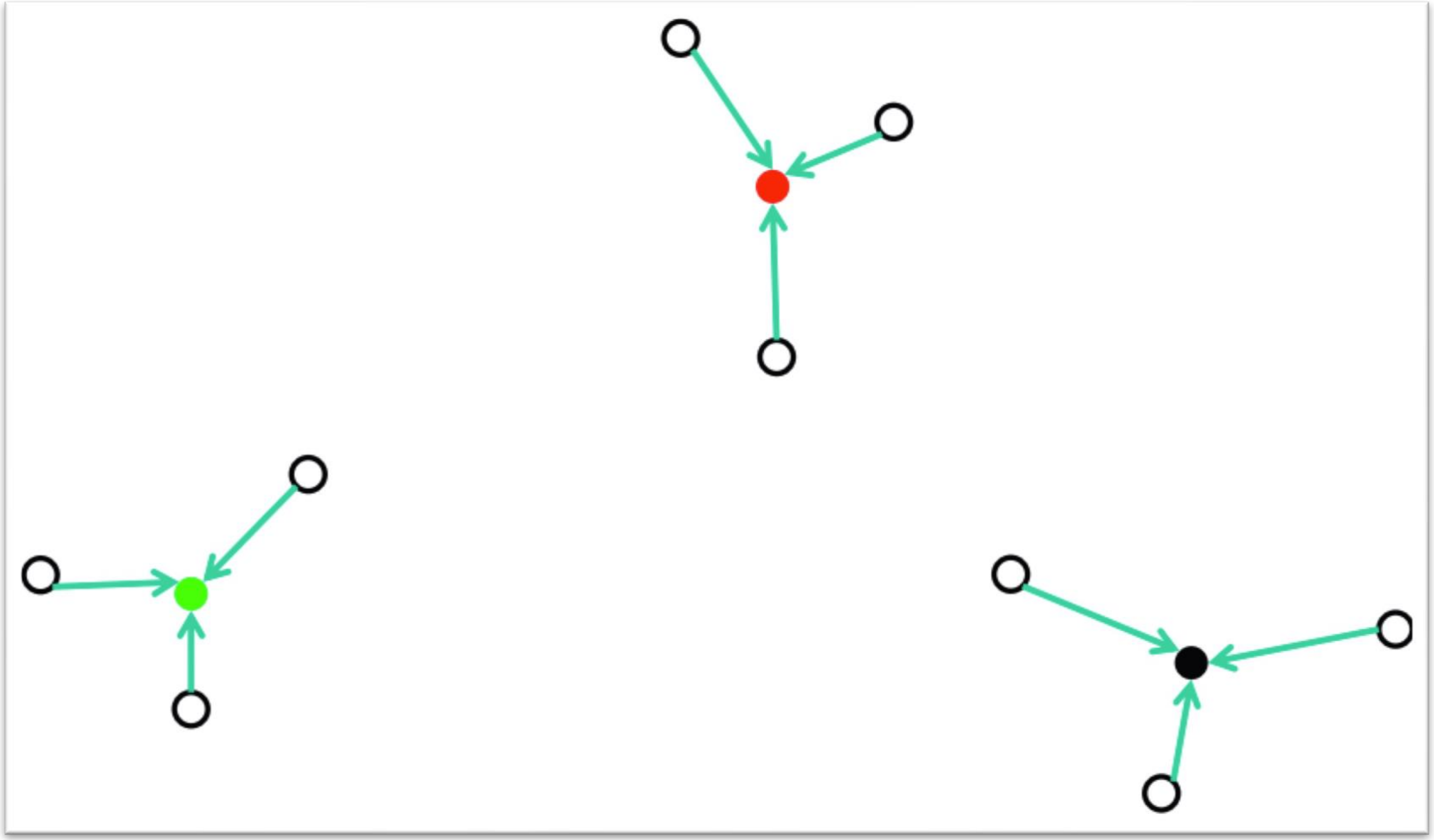
Assign each point to its nearest center



K-means Clustering

Euclidean distance metric

Recompute optimal centers given a fixed clustering



Selecting the number of clusters

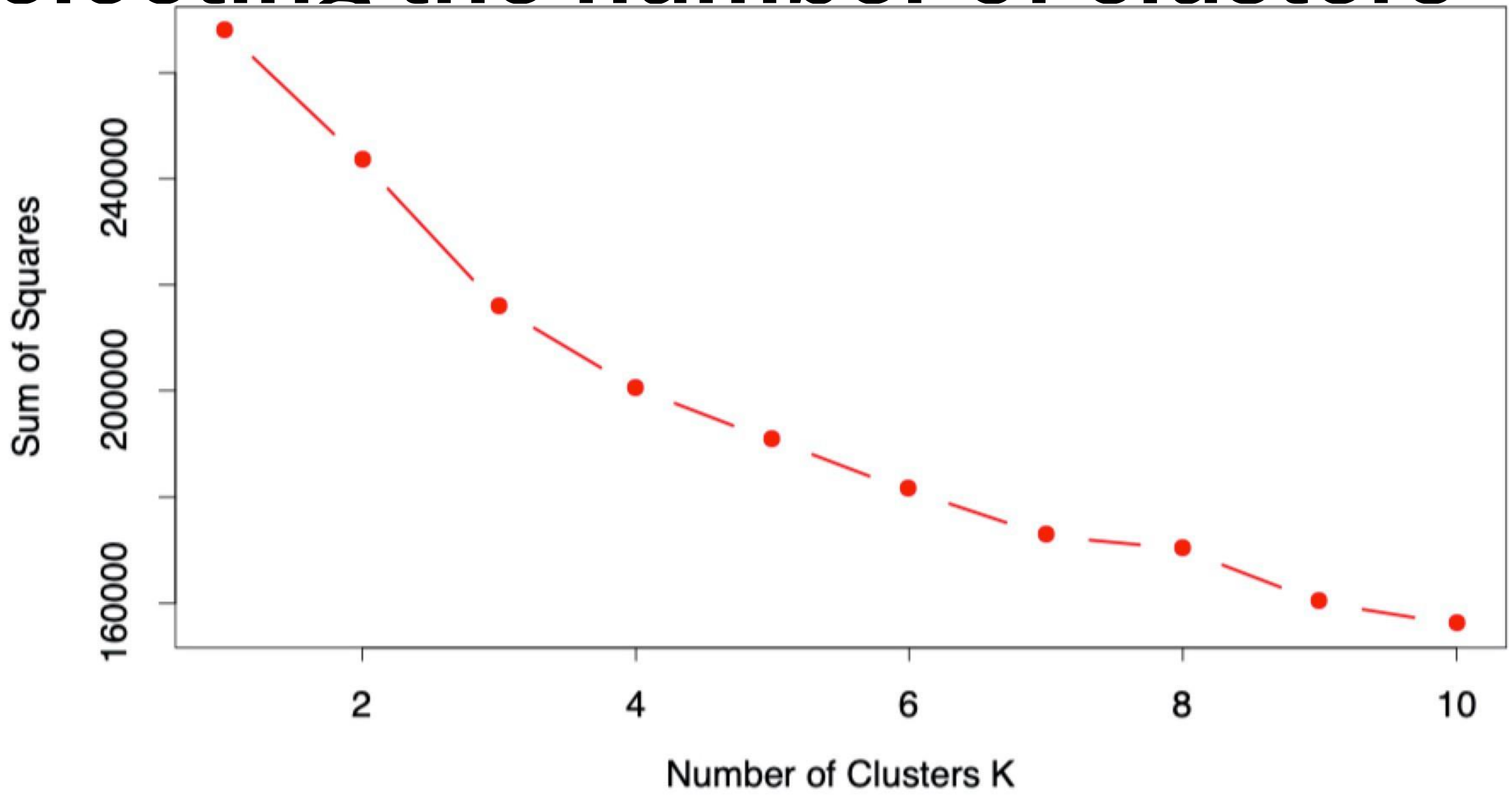
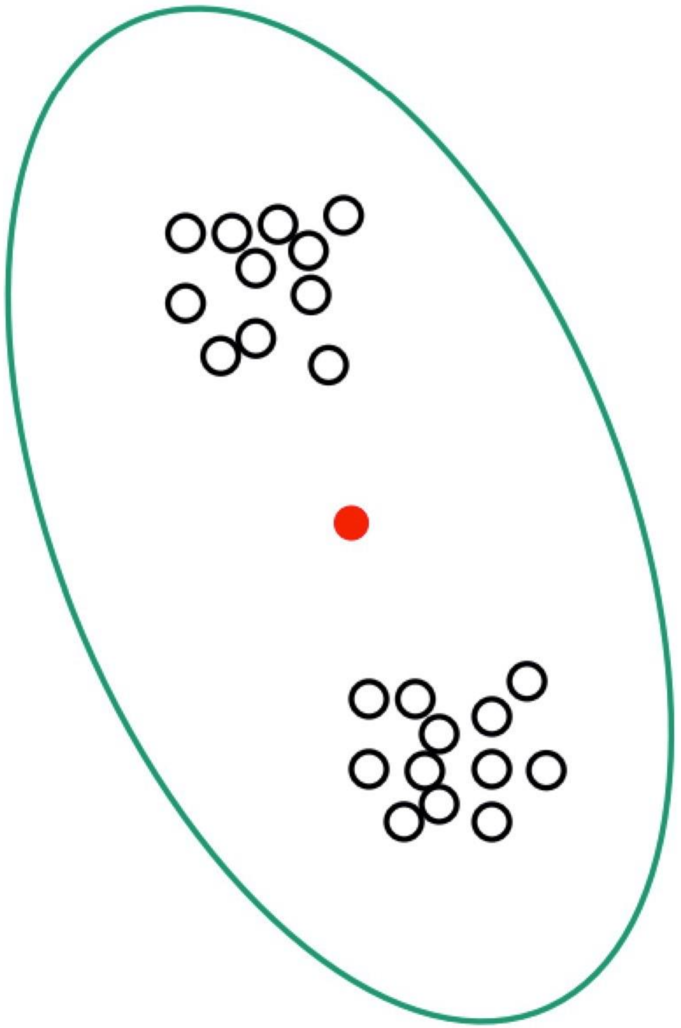
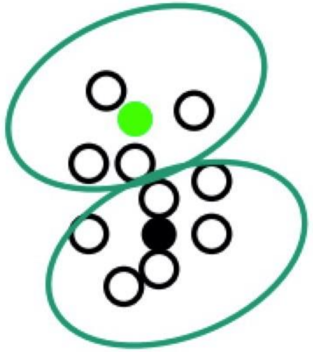


FIGURE 14.8. *Total within-cluster sum of squares for K-means clustering applied to the human tumor microarray data.*

K-means can fail

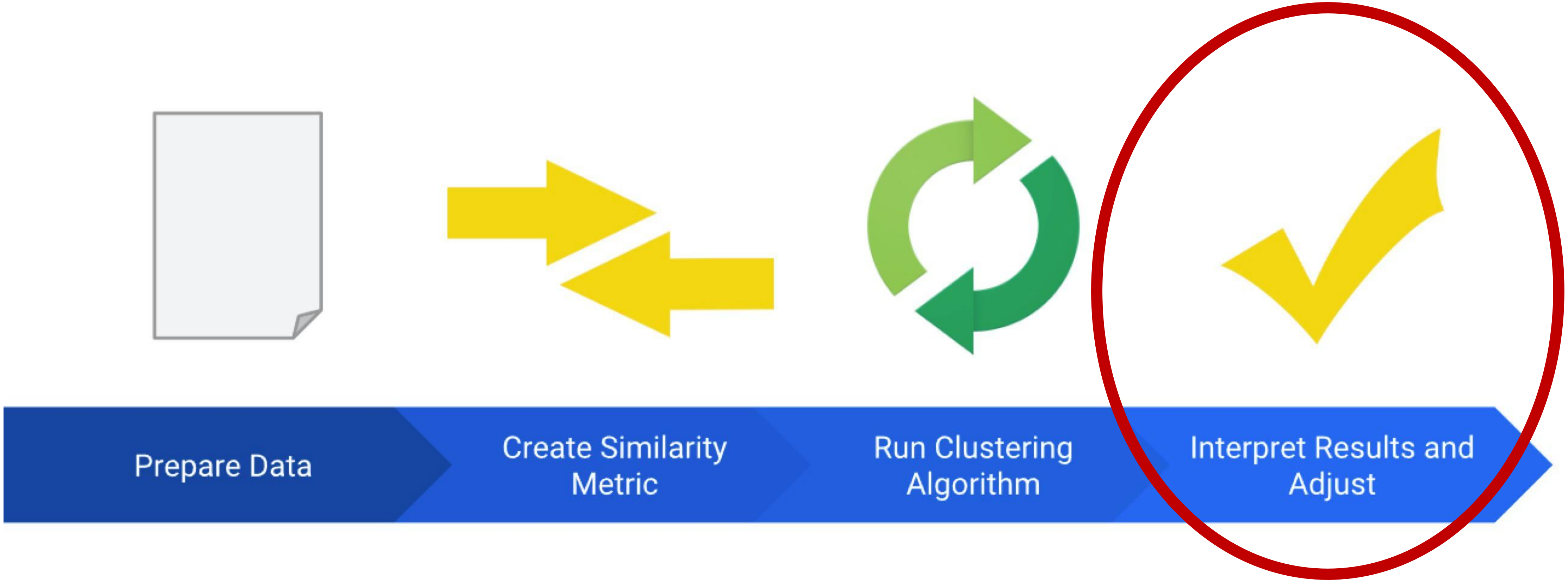


This is a heuristic!
No guarantees it'll find optimum



In practice, smarter centroid initialization solves this

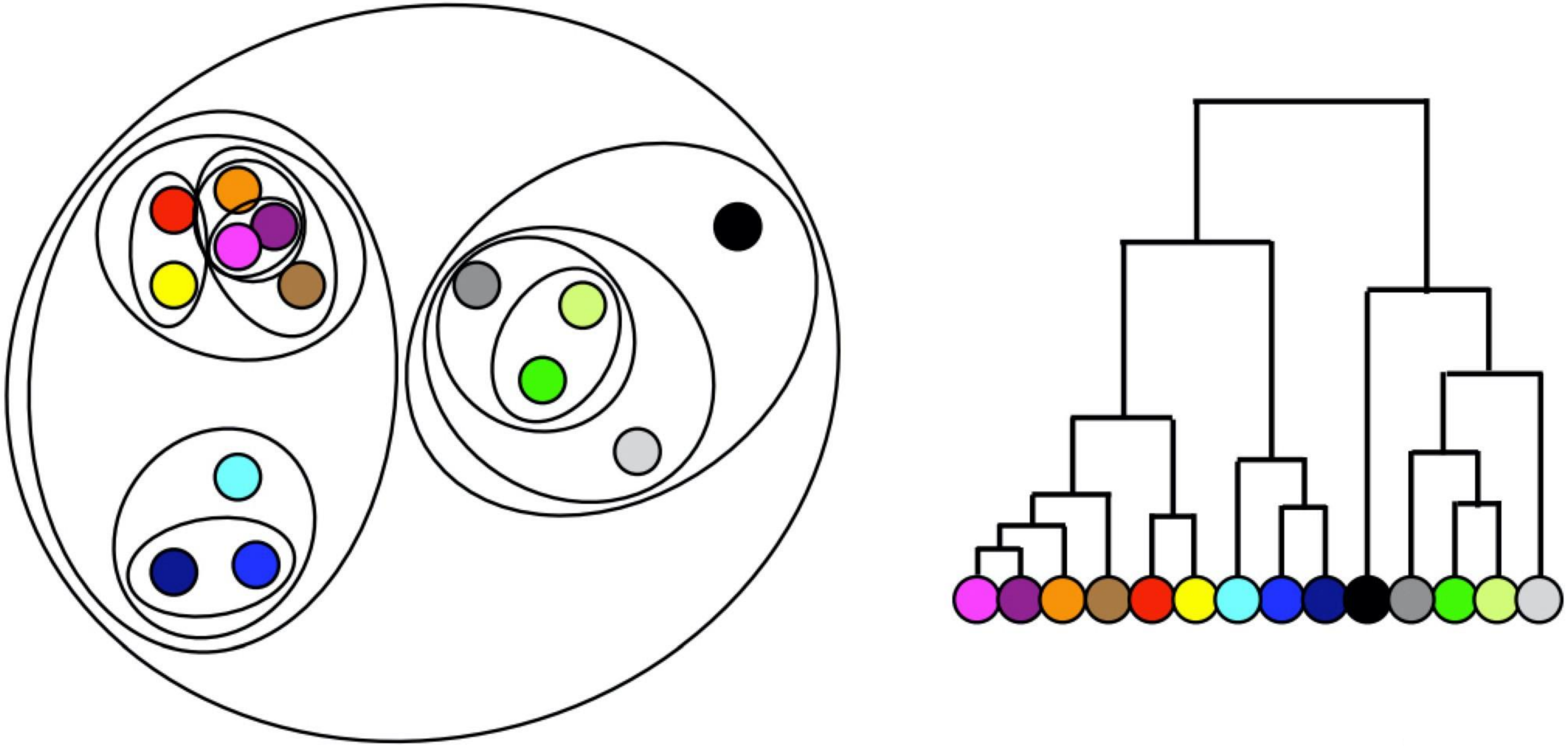
Clustering workflow



From Google’s Clustering lesson: https://developers.google.com/machine-learning/clustering/

Hierarchical Clustering

High-level idea: build a tree (hierarchy) of clusters



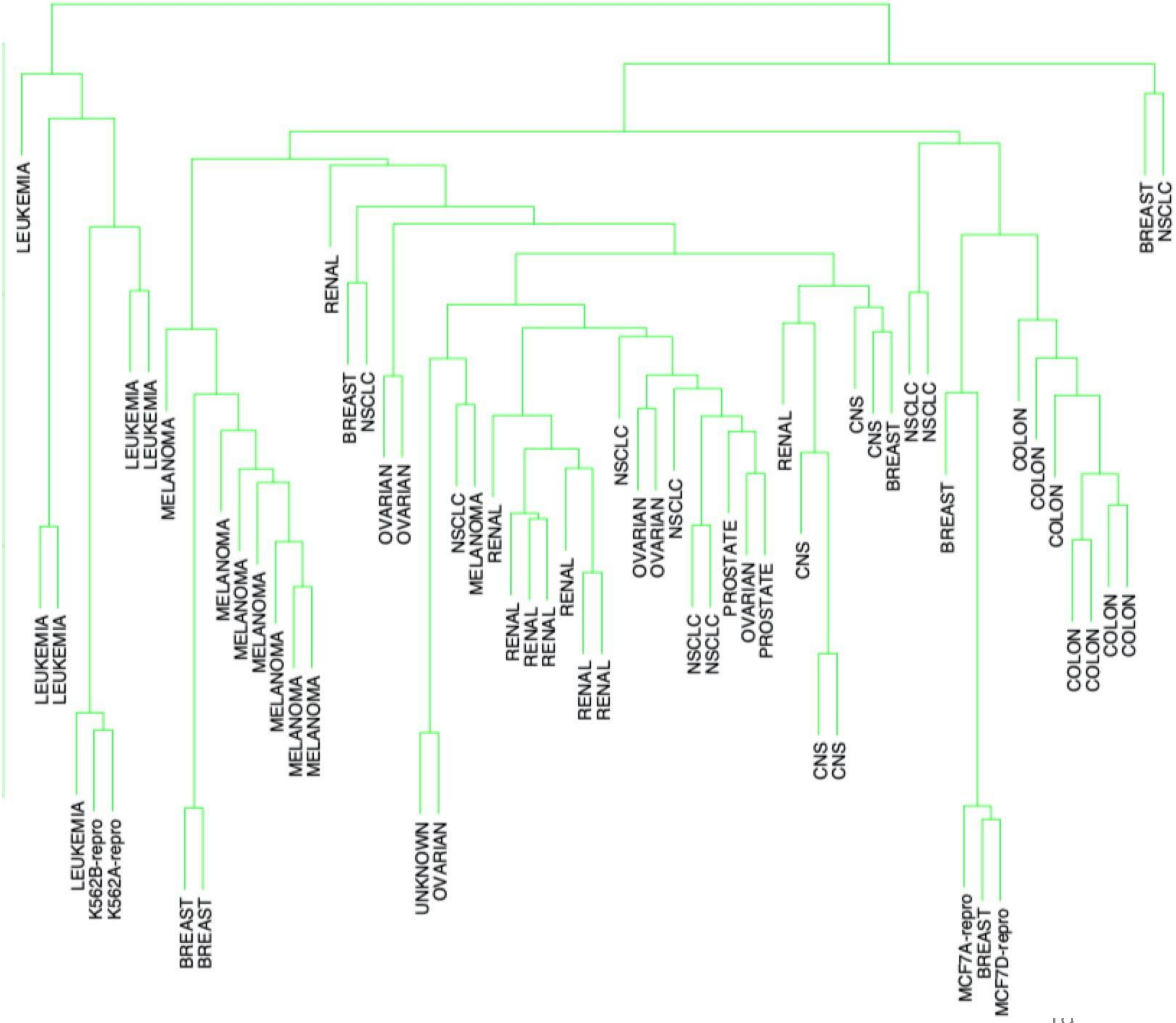
Based on slides by Elena Sügis: http://bioinformaticsinstitute.ru/sites/default/files/preprocessing_unsupervised.pdf

Hierarchical Clustering

Human Tumor Microarray Data

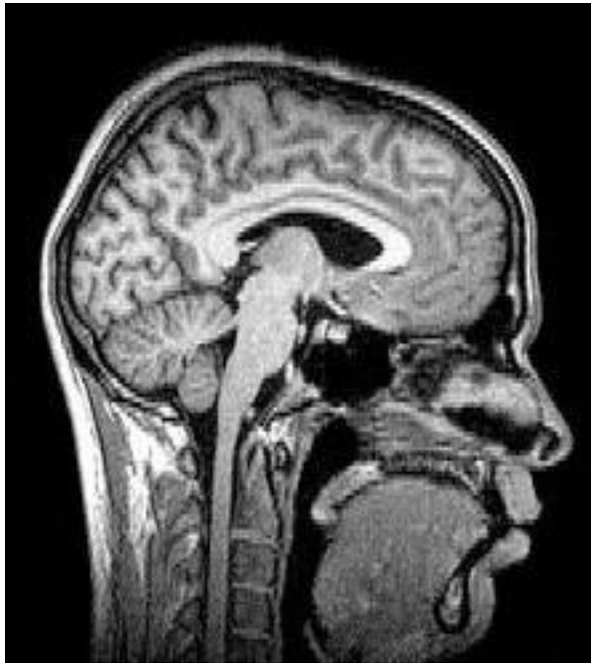
64 samples, 6830 features (gene expression levels)

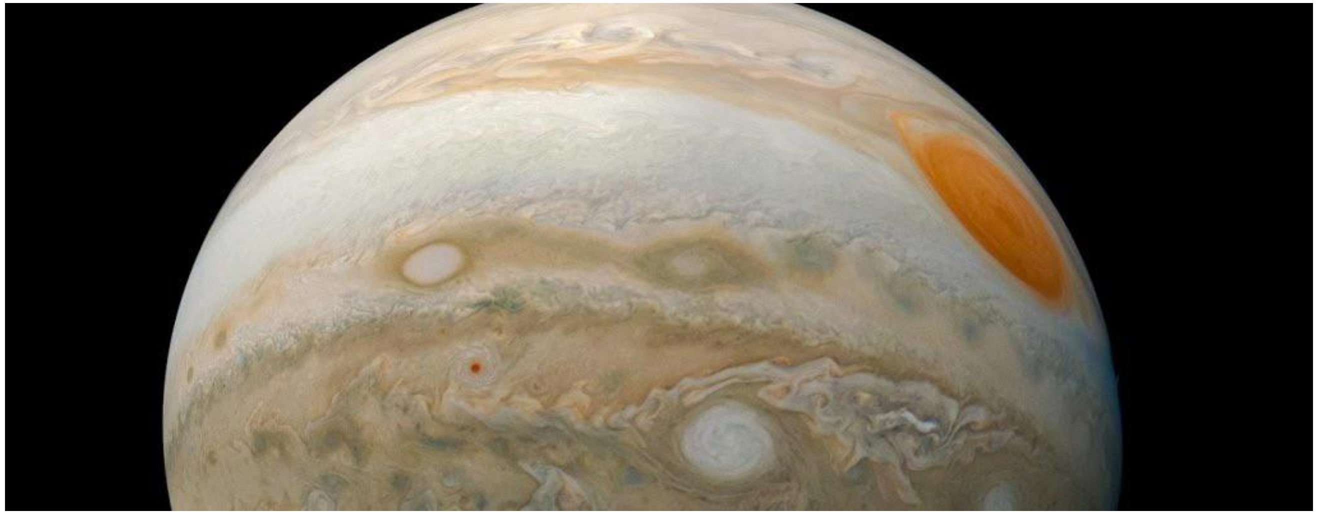
Elements of Statistical Learning, Chapter 14.3.8

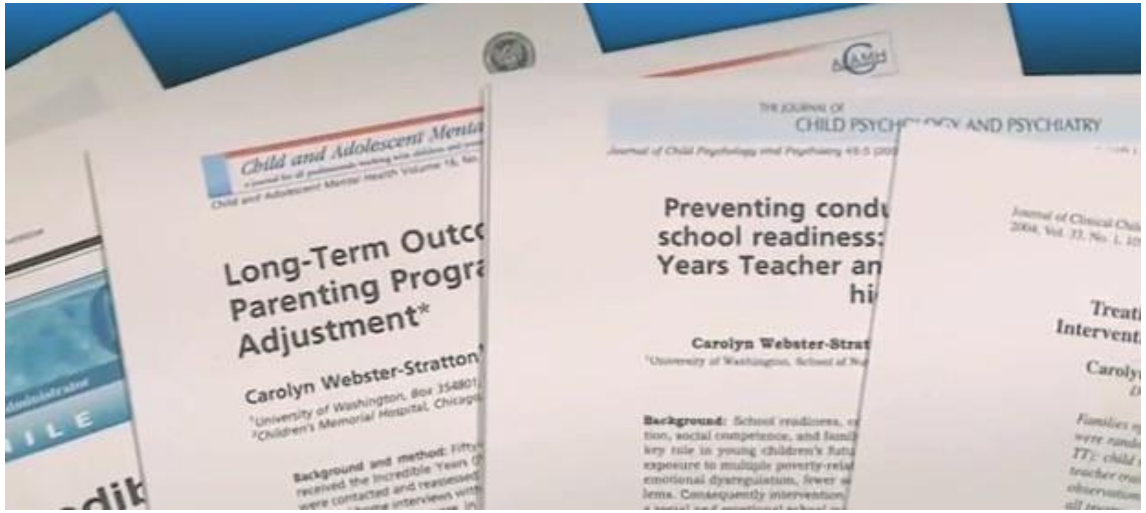


Dimensionality Reduction

or dealing with very high-dimensional data



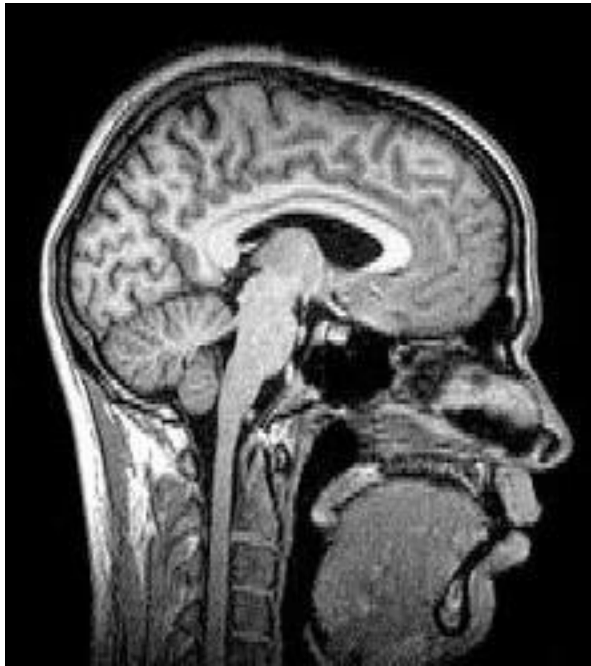




Dimensionality Reduction

Examples: Principal Component Analysis (PCA), t-SNE, …

Powerful unsupervised learning techniques for extracting hidden (potentially lower dimensional) structure from high dimensional datasets.



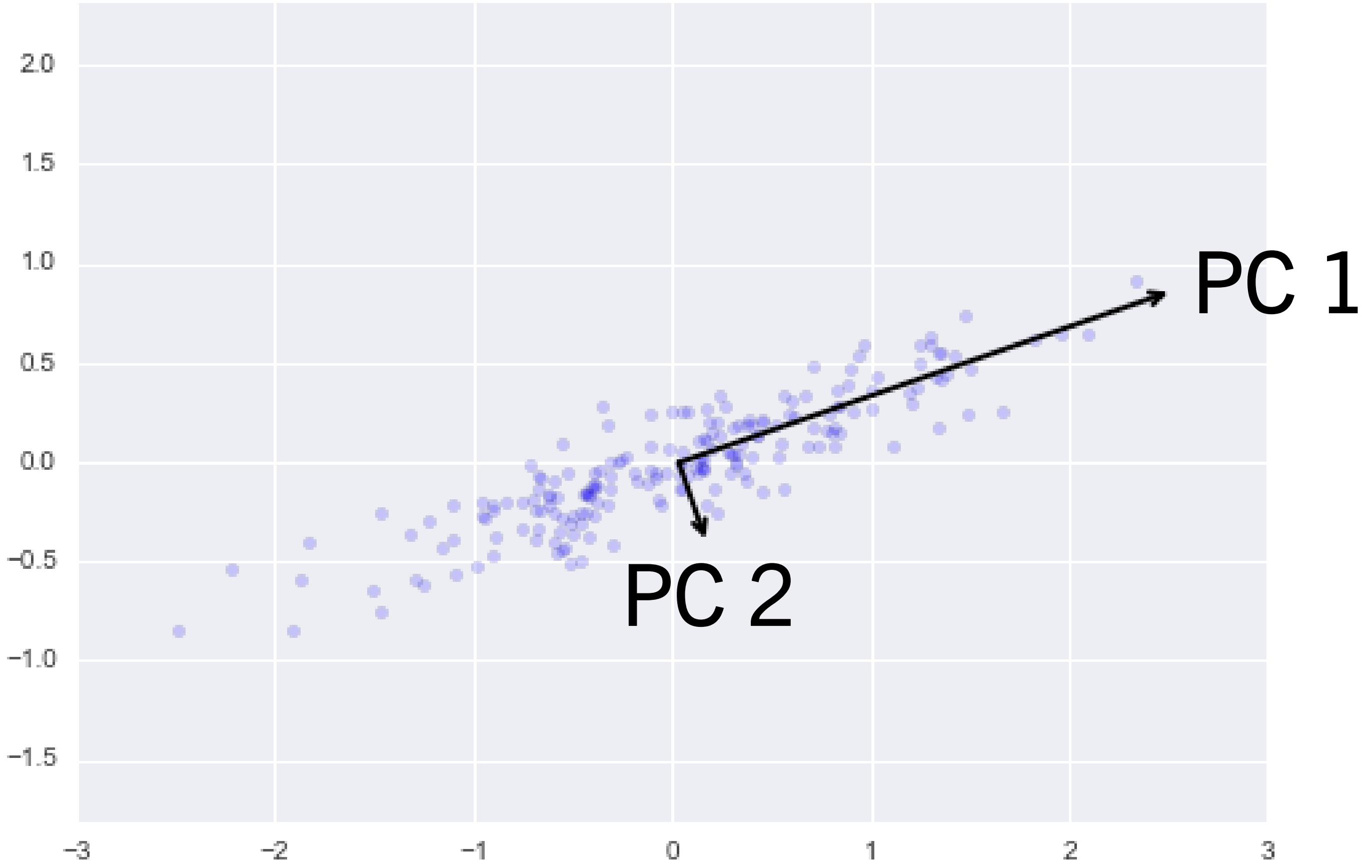
Useful for:

- Visualization
- Data compression for faster supervised learning
- Noise removal

Based on slide by Nina Balcan

Principal Component Analysis (PCA)

- Principal Components (PC) are orthogonal directions that capture most of the variance in the data.



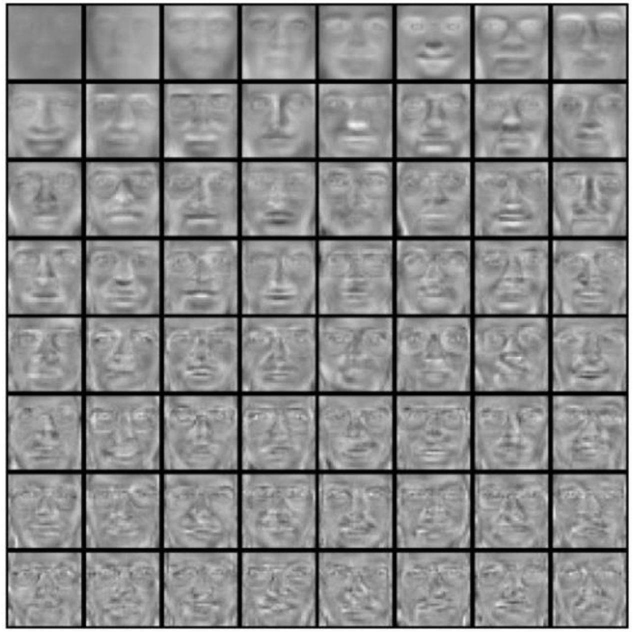
PCA for Face Reconstruction

Eigenfaces, slide based on Derek Hoeim's, UIUC CS543

Image dataset

PCA algorithm

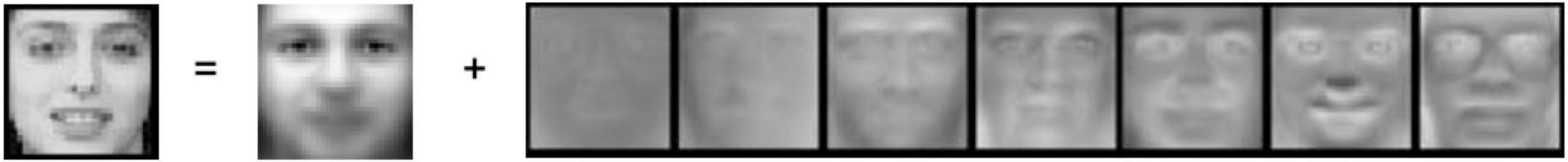
64 Principal Components



PCA for Face Reconstruction

Eigenfaces, slide based on Derek Hoeim’s, UIUC CS543

Face Reconstruction using the Principal Components

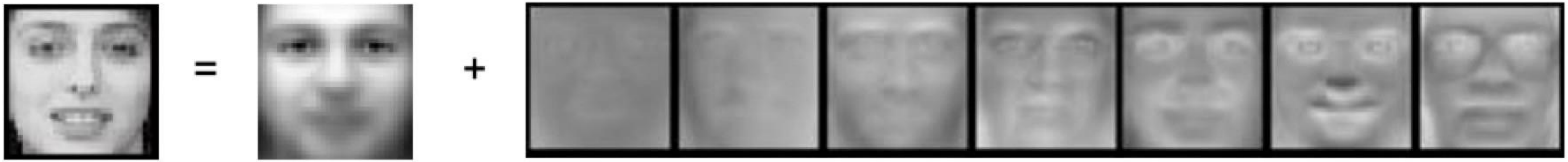


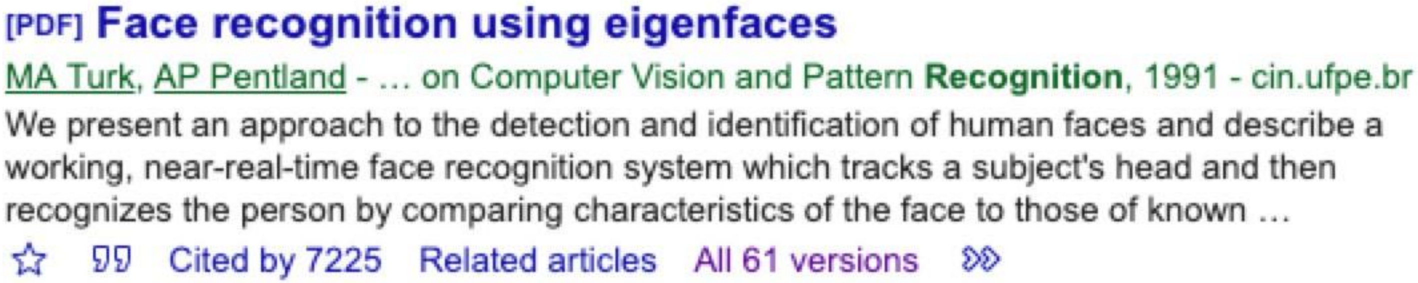
PCA for Face Reconstruction

Eigenfaces, slide based on Derek Hoeim’s, UIUC CS543

Face Recognition using PCA:

1. Given face image datasets, extract Principal Components $v_{!}, v_{"}, \ldots, v_{\#}$.
2. Given new image, project onto PCs.
3. Find closest (projected) image in training dataset





[PDF] **Face recognition using eigenfaces**

MA Turk, AP Pentland - … on Computer Vision and Pattern **Recognition**, 1991 - cin.ufpe.br

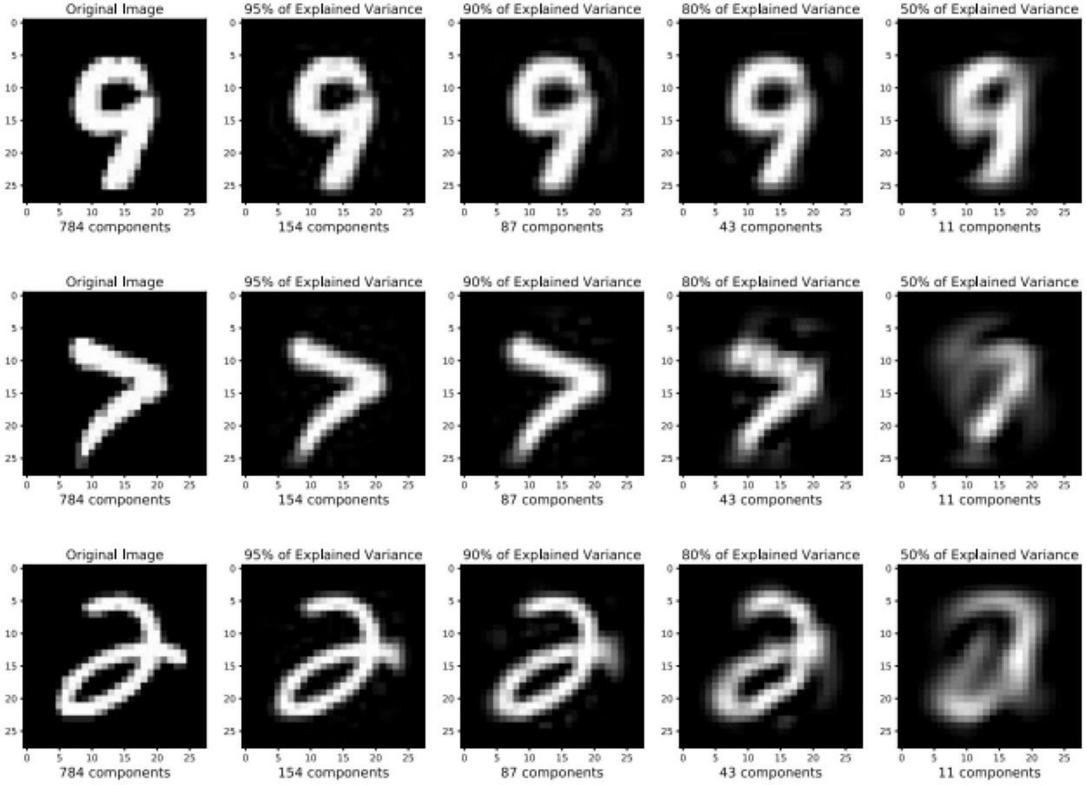
We present an approach to the detection and identification of human faces and describe a working, near-real-time face recognition system which tracks a subject's head and then recognizes the person by comparing characteristics of the face to those of known …

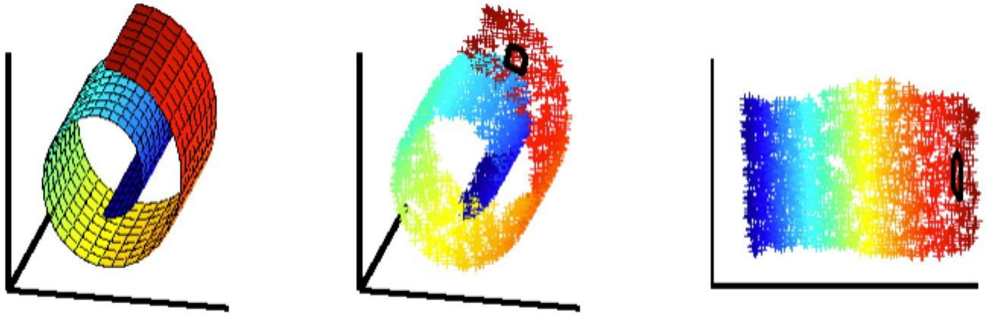
☆ 99 Cited by 7225 Related articles All 61 versions »

Final words on PCA

- Advantages
  - Fast to compute an optimal solution: an eigenvector problem
  - No hyper-parameters to tune

- Caveats
  - Discards information
  - Limited to linear projections





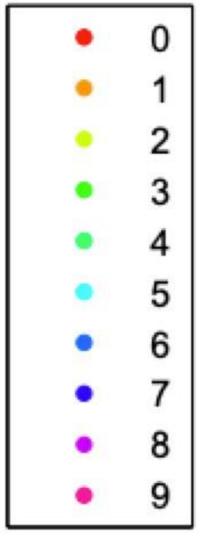
- From Michael Guerzhoy's slides, UofT CSC320

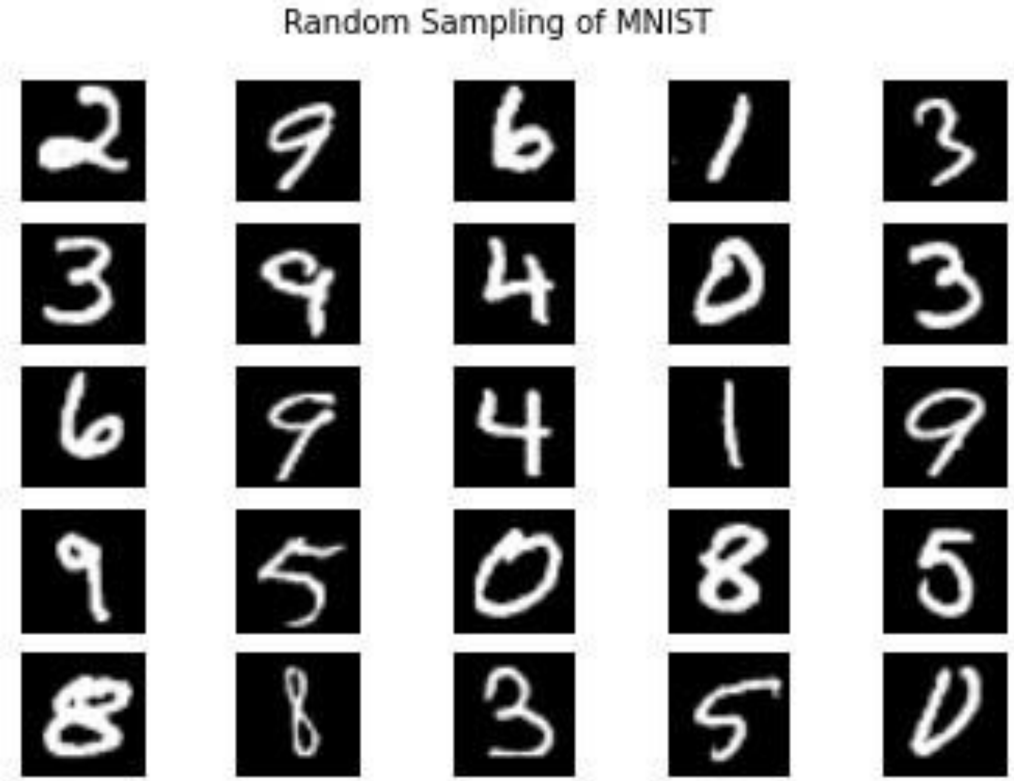
t-SNE

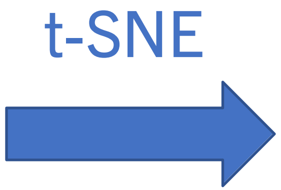
t-Distributed Stochastic Neighbor Embedding

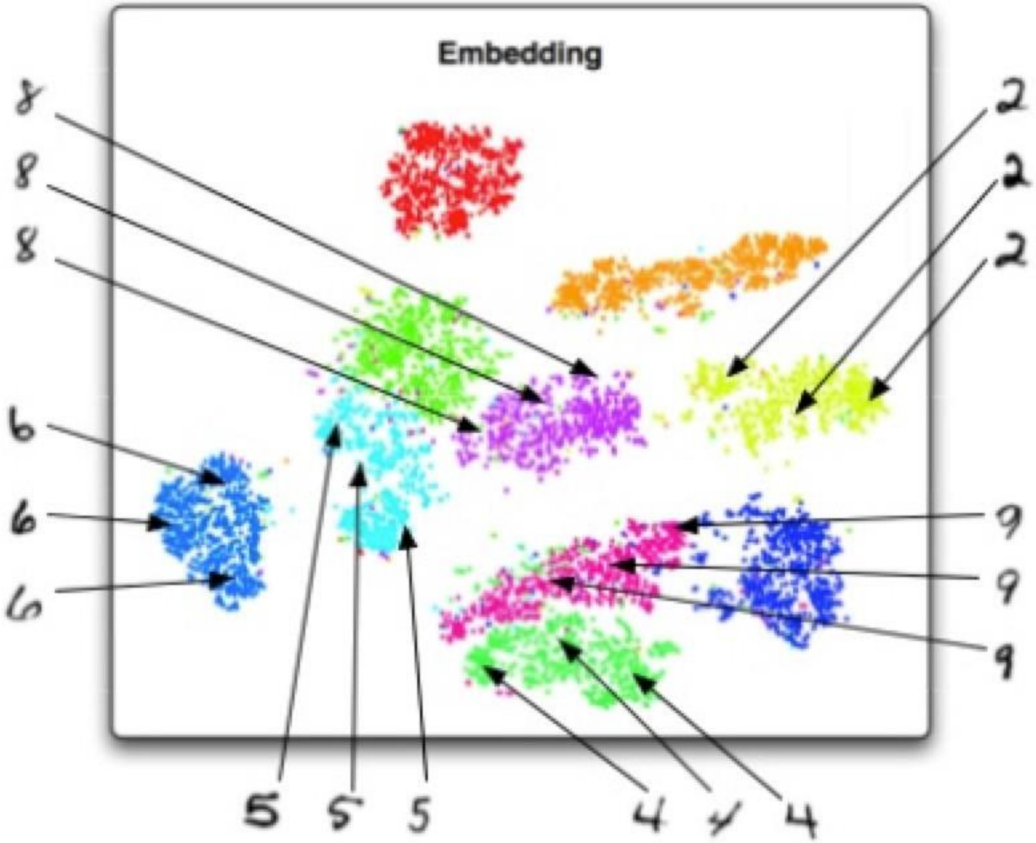
784 dimensions = 28x28 pixels

2 dimensions







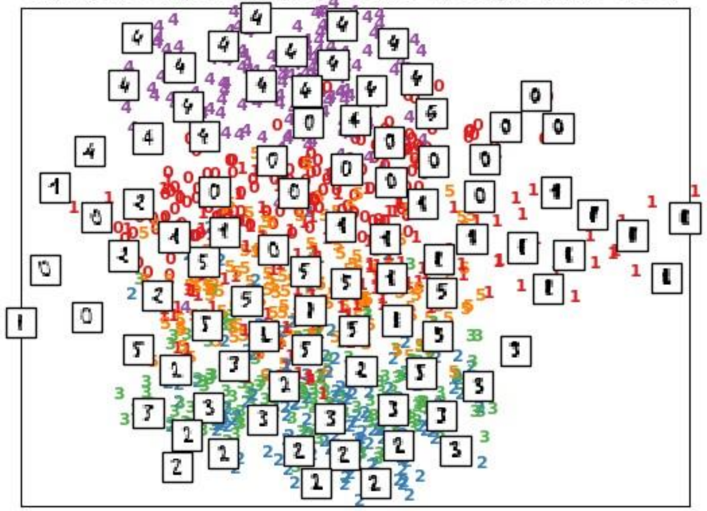


t-SNE
t-Distributed Stochastic Neighbor Embedding

A selection from the 64-dimensional digits dataset

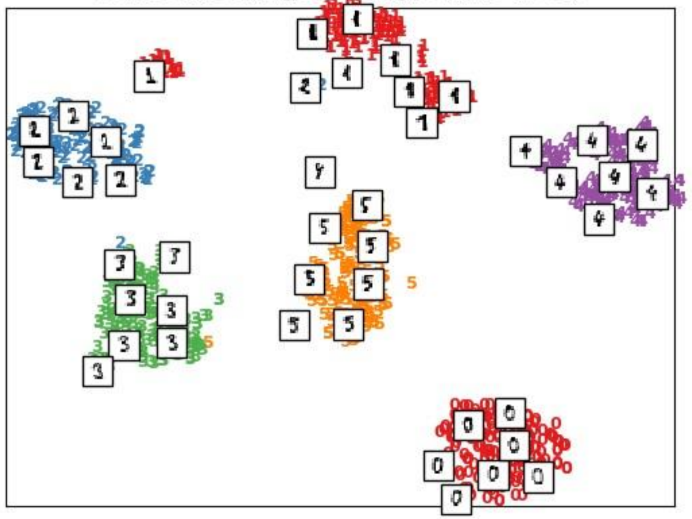
PCA

Principal Components projection of the digits (time 0.00s)



t-SNE

t-SNE embedding of the digits (time 4.60s)



From https://scikit-learn.org/stable/auto_examples/manifold/plot_lle_digits.html

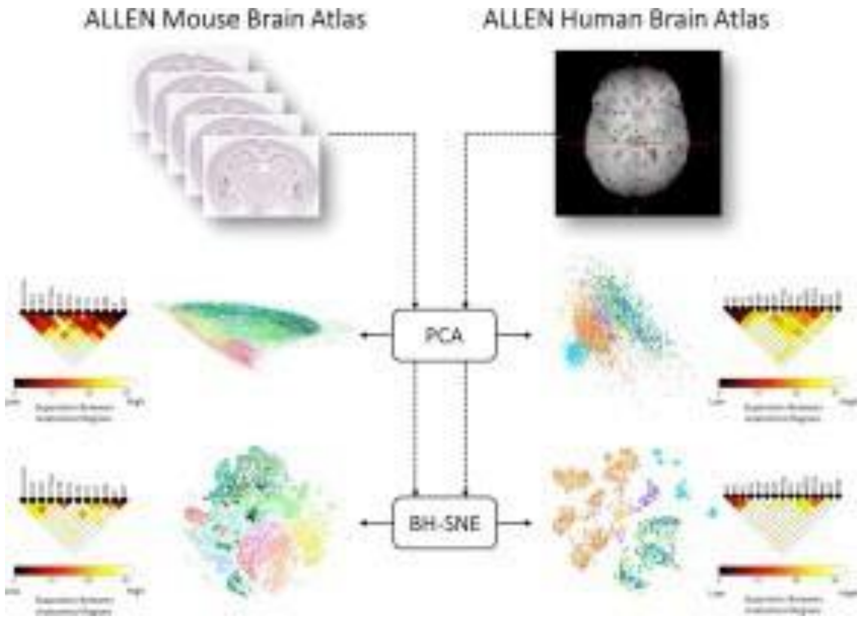
Final words on t-SNE

Advantages

- Conserves local and global patterns in the data
- Handles highly non-linear data

Caveats

- Slow to compute
- Requires careful hyper-parameter tuning
- Cannot project a new point



Visualizing the spatial gene expression organization in the brain through non- linear similarity embeddings. Mahfouz et al. (2015)

Interactive dimensionality reduction

- https://projector.tensorflow.org/
  - You can use the “LOAD” button to upload your own data and interactively visualize the results of PCA or t-SNE, in the browser

- https://distill.pub/2016/misread-tsne/
  - t-SNE has some tricky hyper-parameters that must be tuned to the dataset you care about. This interactive study looks at how the hyper-parameters behave and gives guidelines for tuning them to get the best outcomes