Course material at:
https://github.com/lyeskhalil/mlbootcamp2022

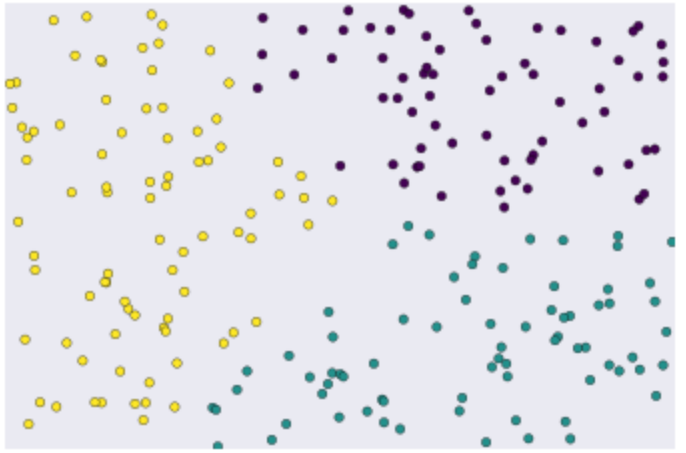
Unsupervised Learning

Tuesday, Lecture 2

FASE ML Bootcamp

Based on material from:
Elements of Statistical Learning by Hastie, Tibshirani, Friedman,
Nina Balca, CMU 10-601
Google's ML course
Elena Sügis' slides
Derek Hoeim's slides

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



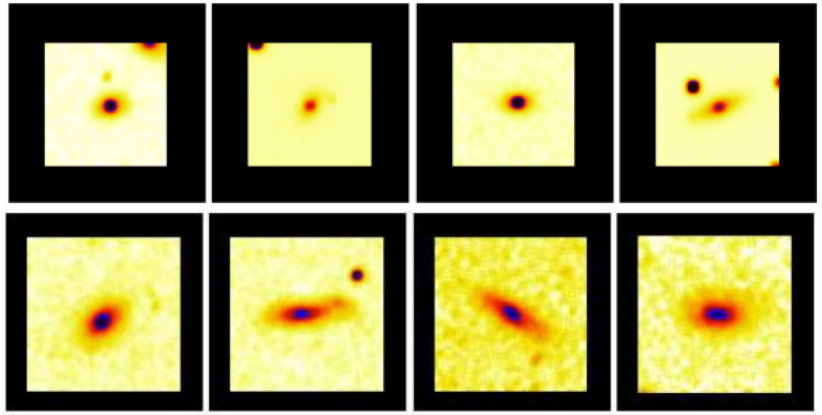
Clustering

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!

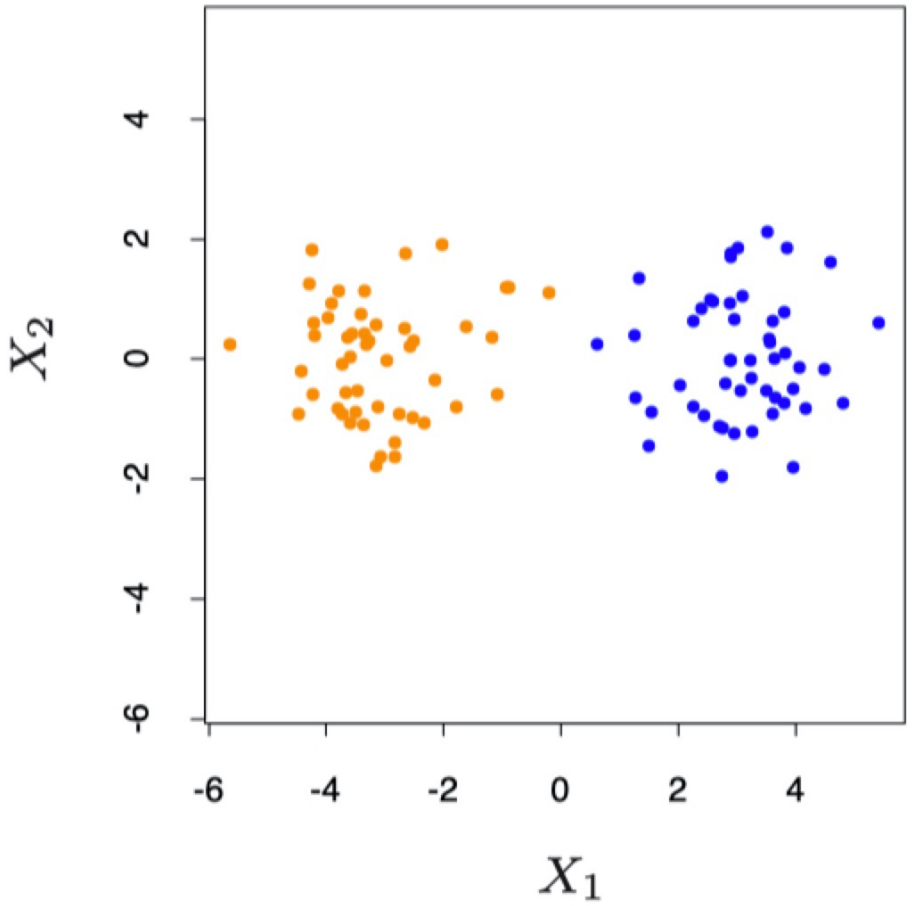
Clustering galaxies, from Miller et al. (2005)



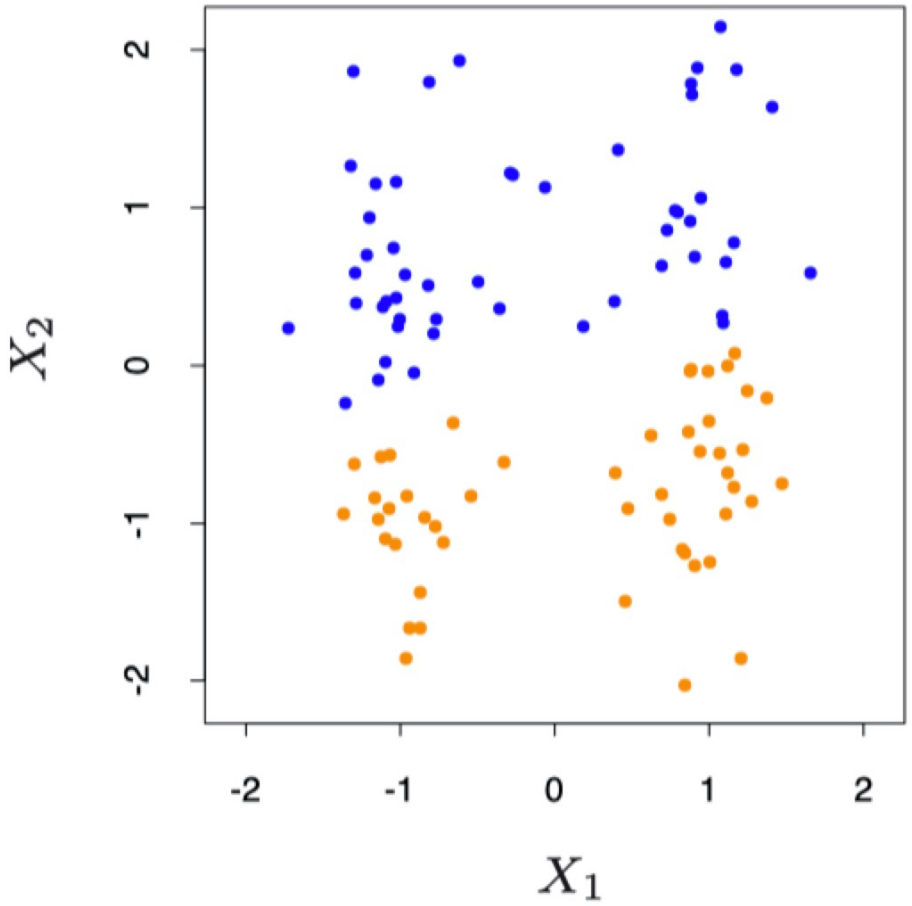
Data Preparation for Clustering

The points are colored by a clustering algorithm

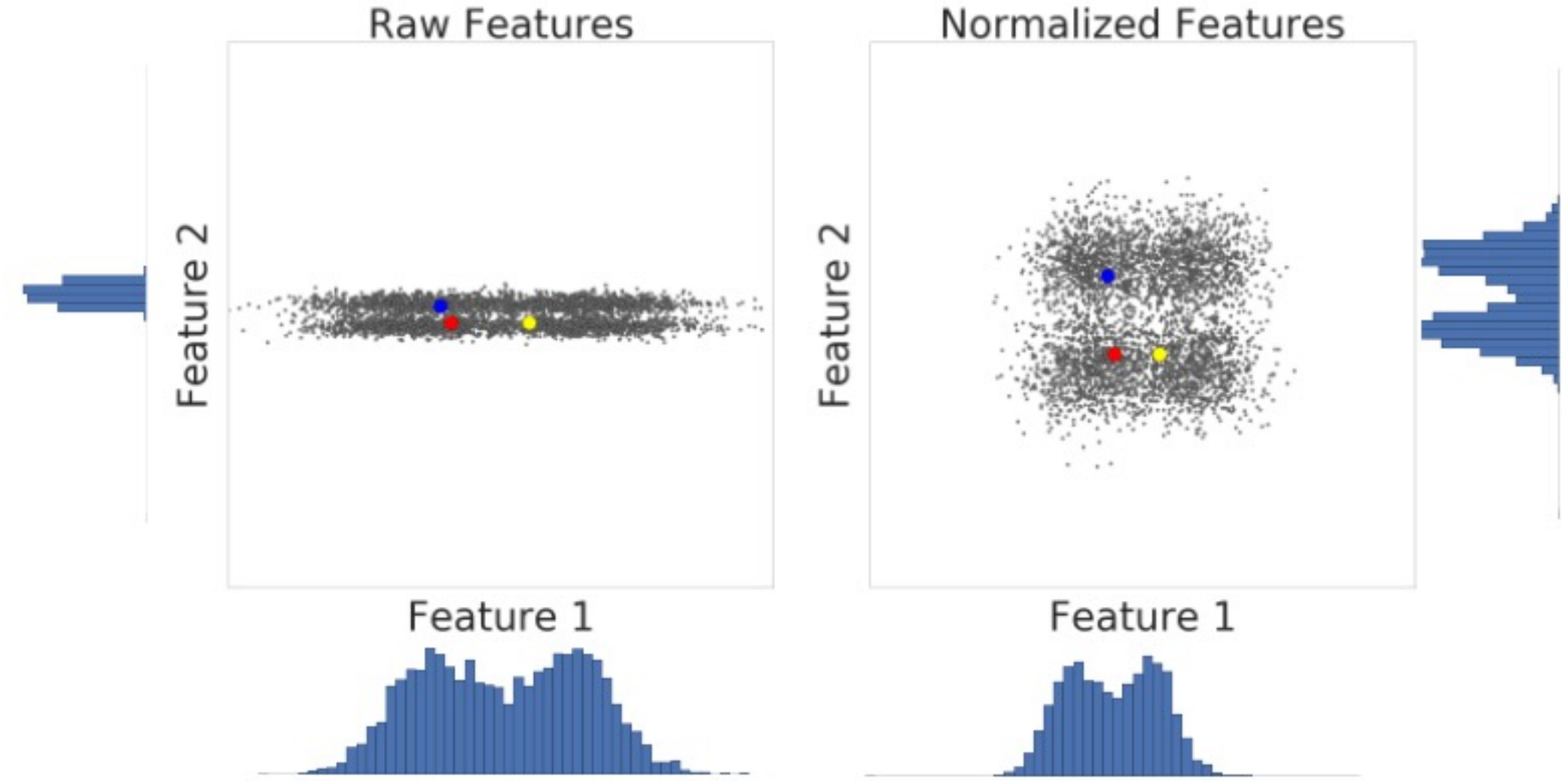
Raw data



Standardized data

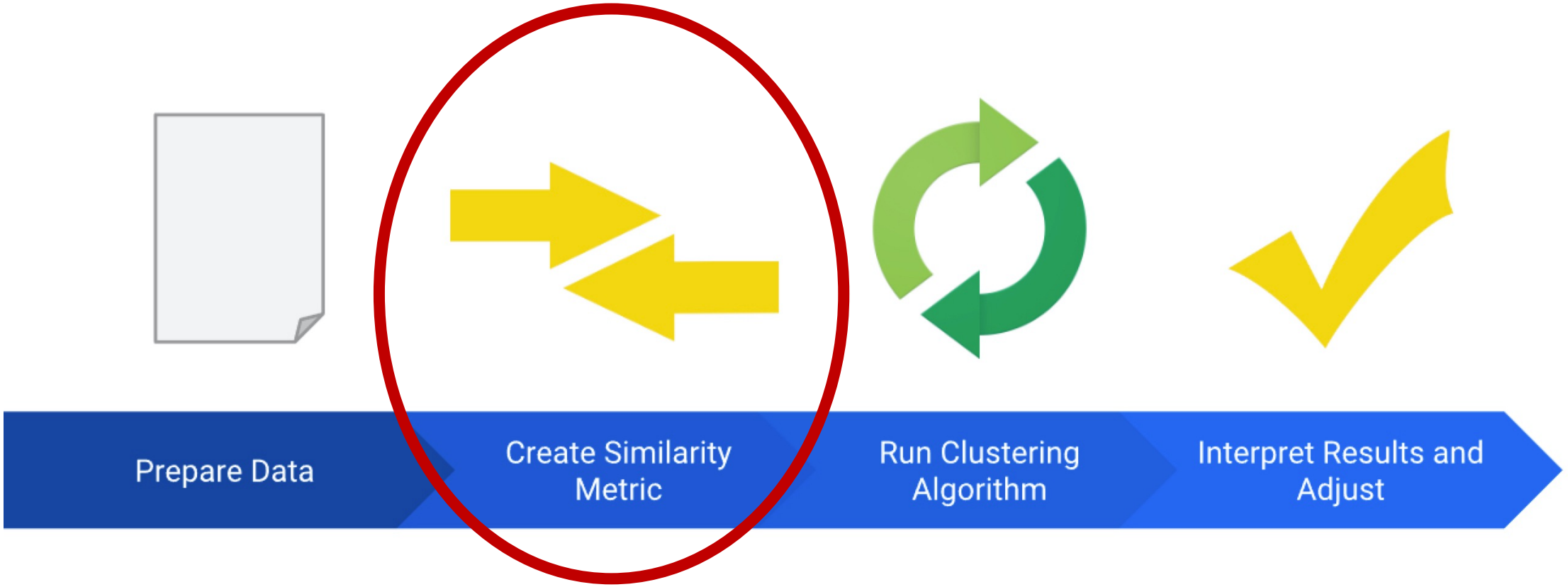


Data Preparation for Clustering



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

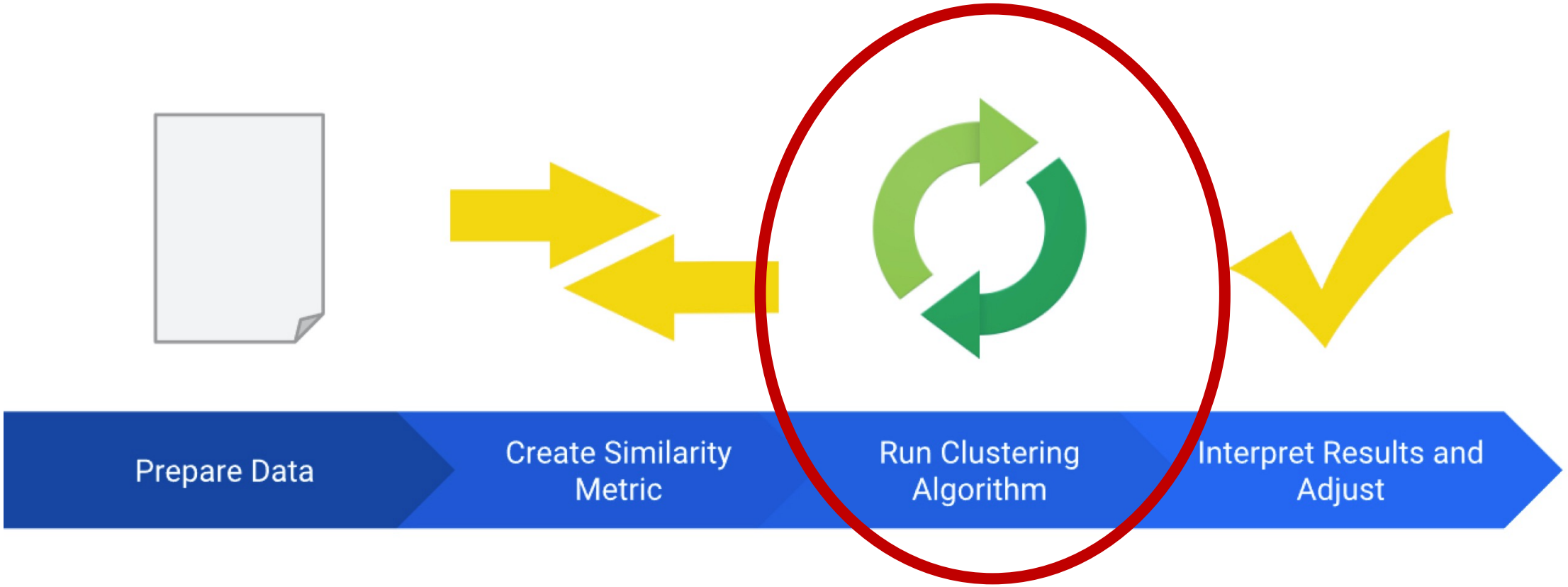
```
ACCTTG
TACCTG   => 3
```

- Levenshtein distance

```
.ACCTTG
TACC.TG  => 2
```

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

Clustering workflow

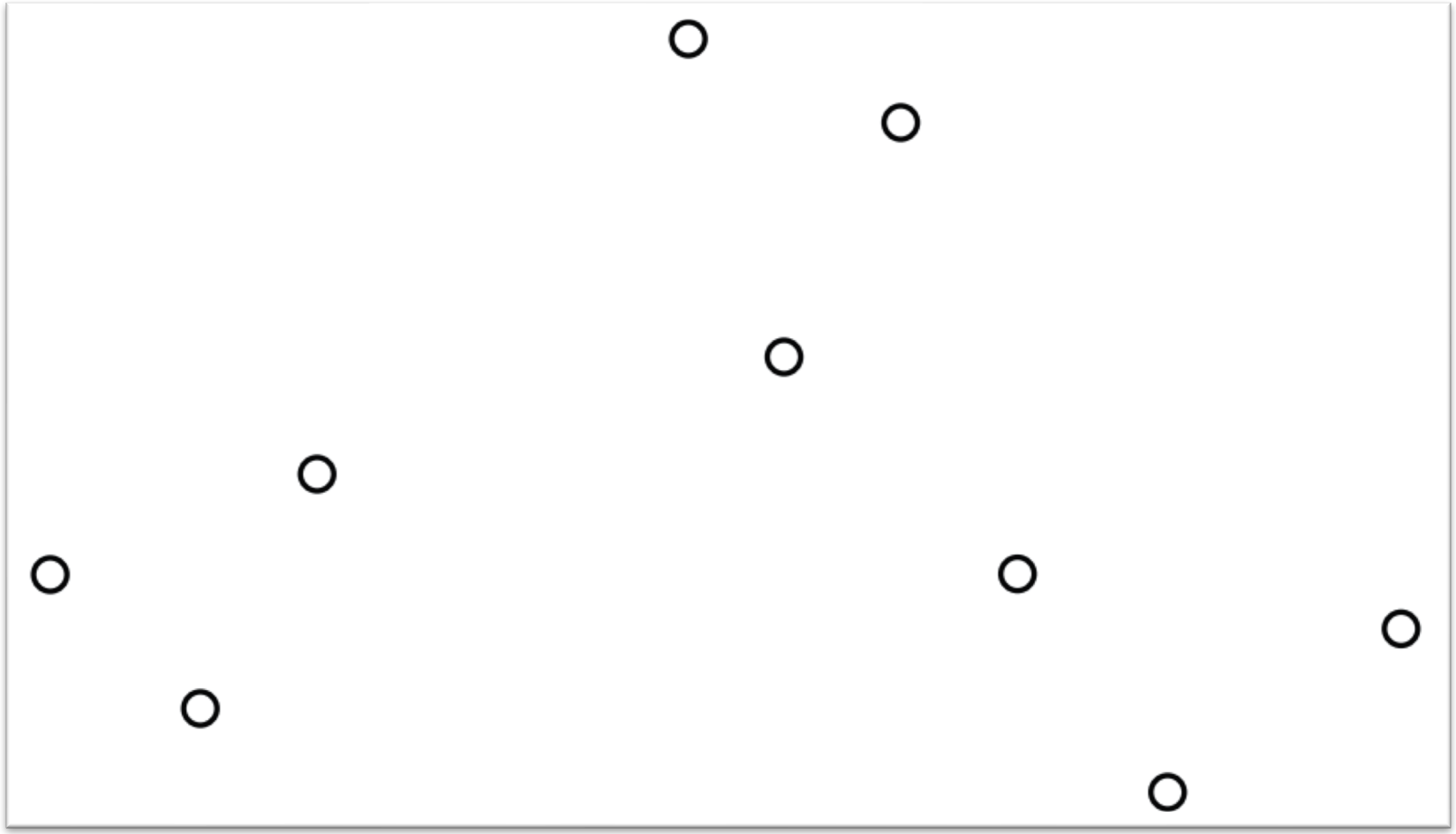


From Google's Clustering lesson: https://developers.google.com/machine-learning/clustering/

K-means Clustering

Euclidean distance metric

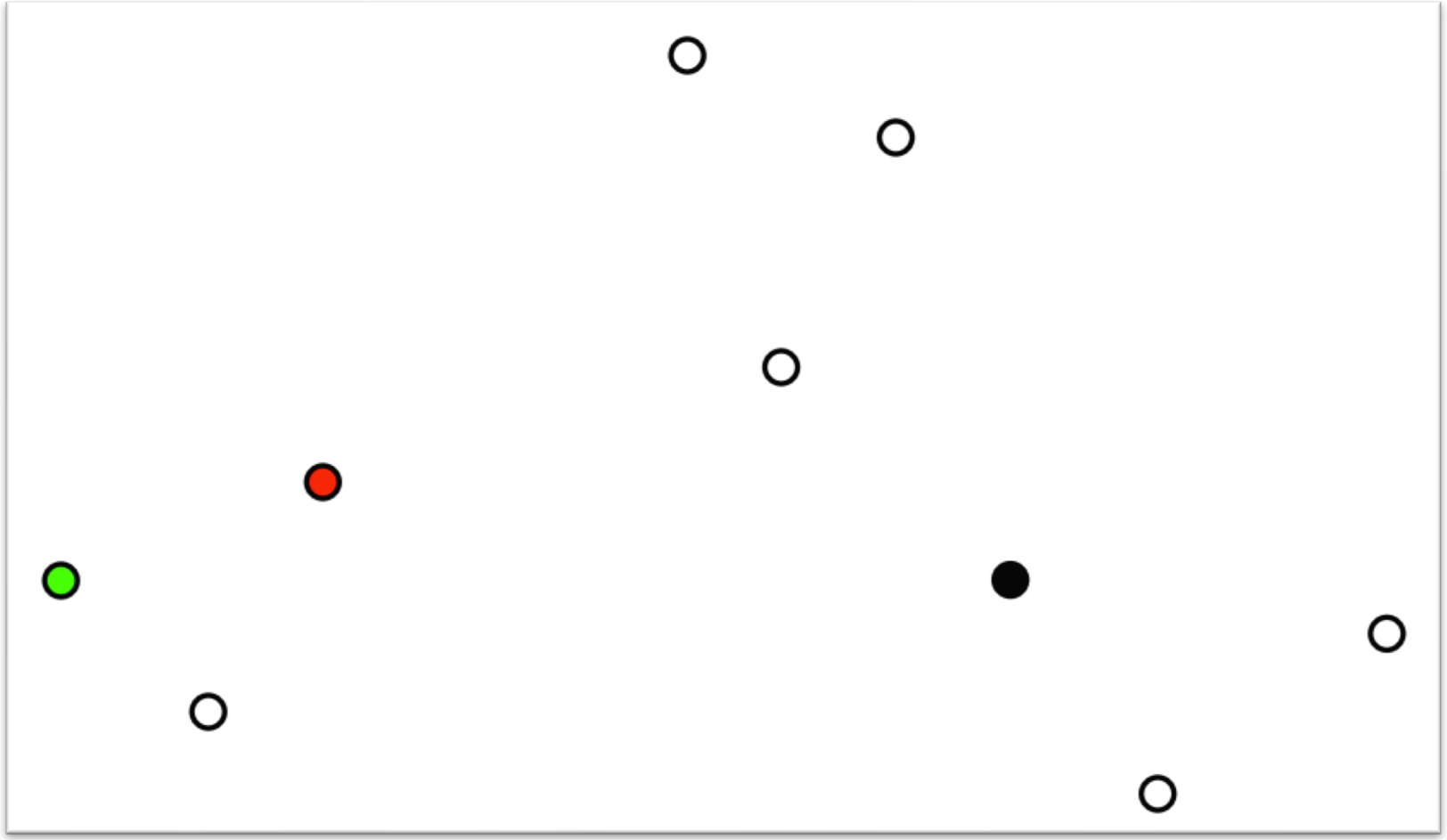
Given a set of data points…



K-means Clustering

Euclidean distance metric

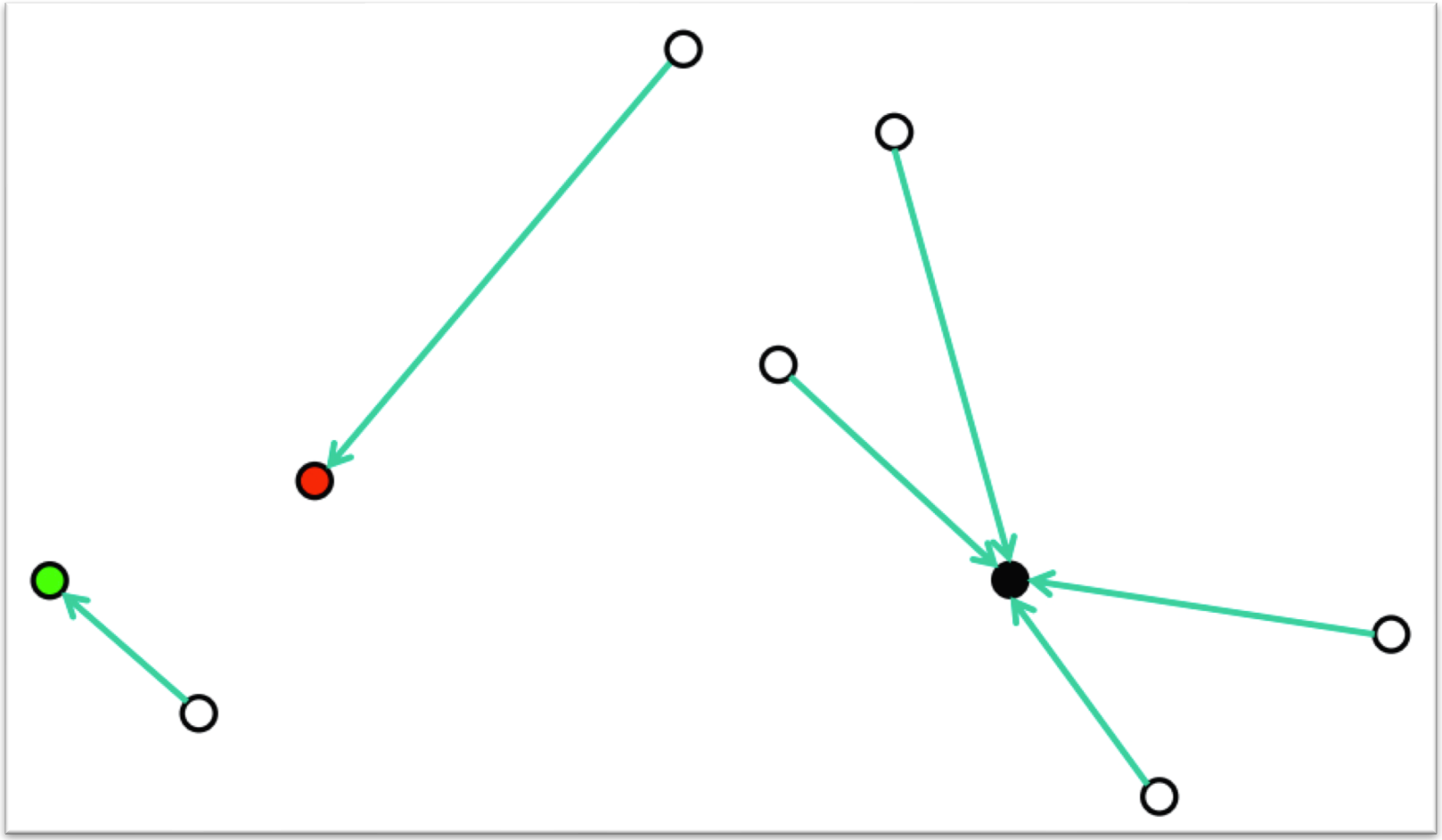
Select **k=3** initial centers at random



K-means Clustering

Euclidean distance metric

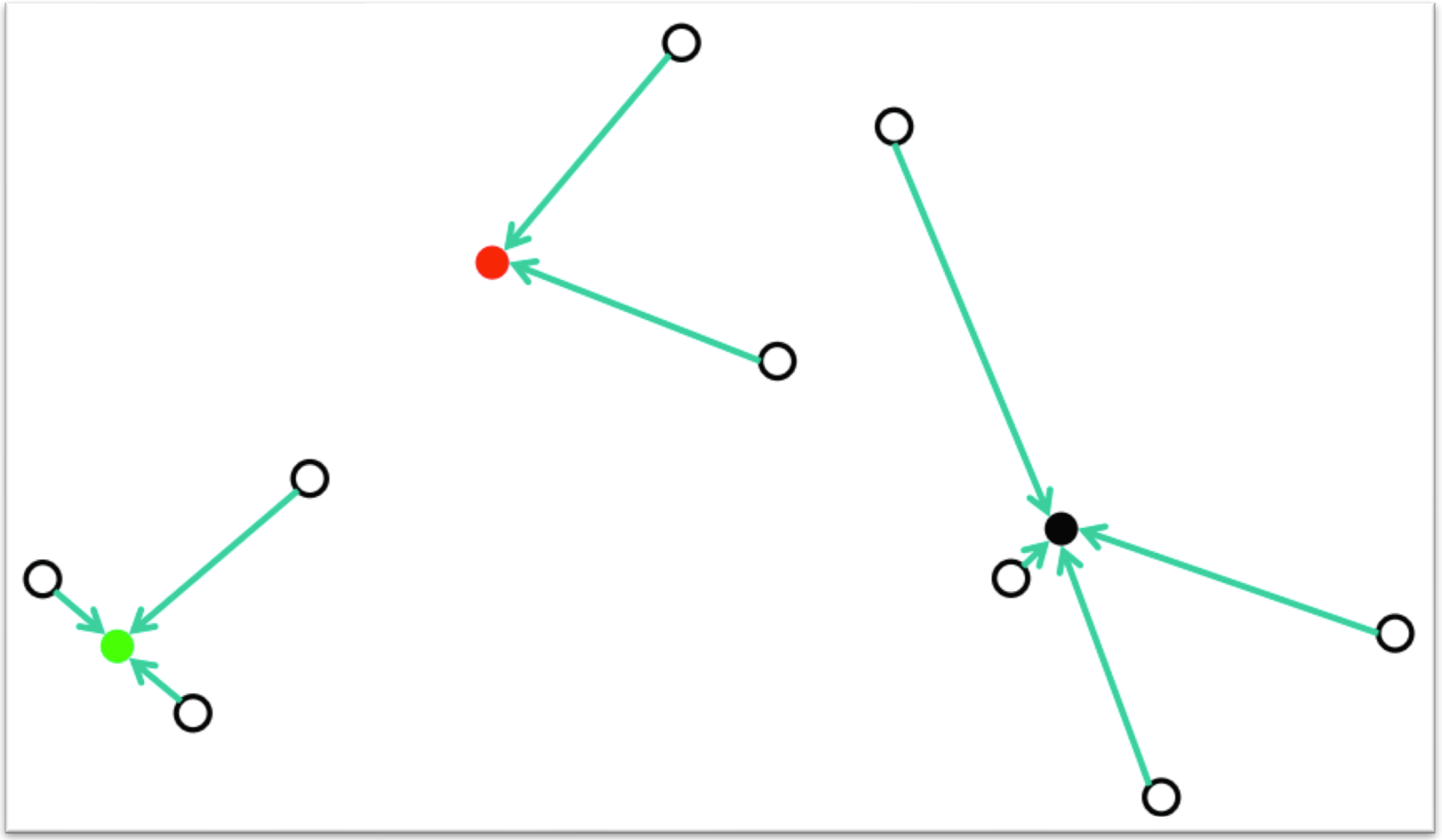
Recompute optimal centers given a fixed clustering



K-means Clustering

Euclidean distance metric

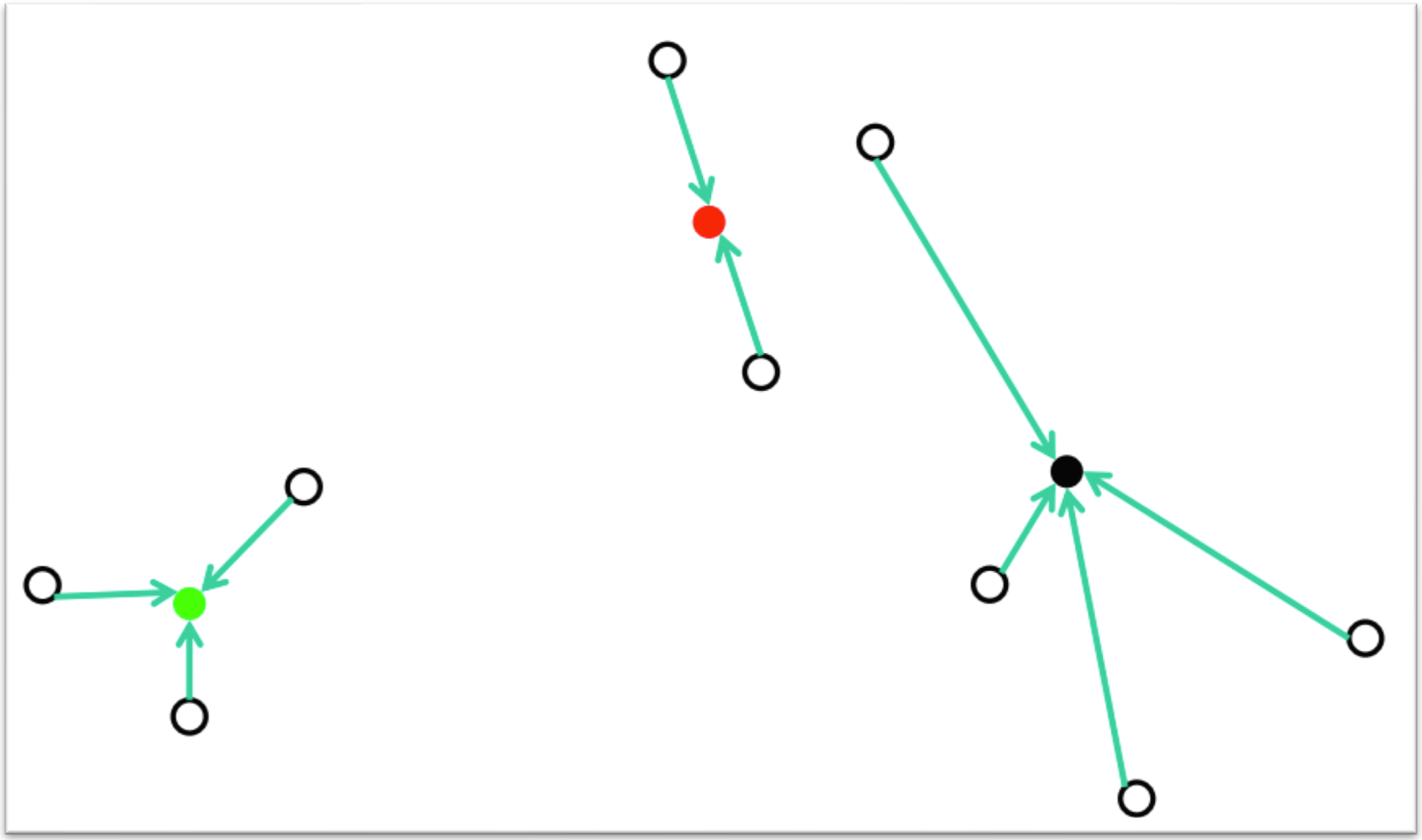
Assign each point to its nearest center



K-means Clustering

Euclidean distance metric

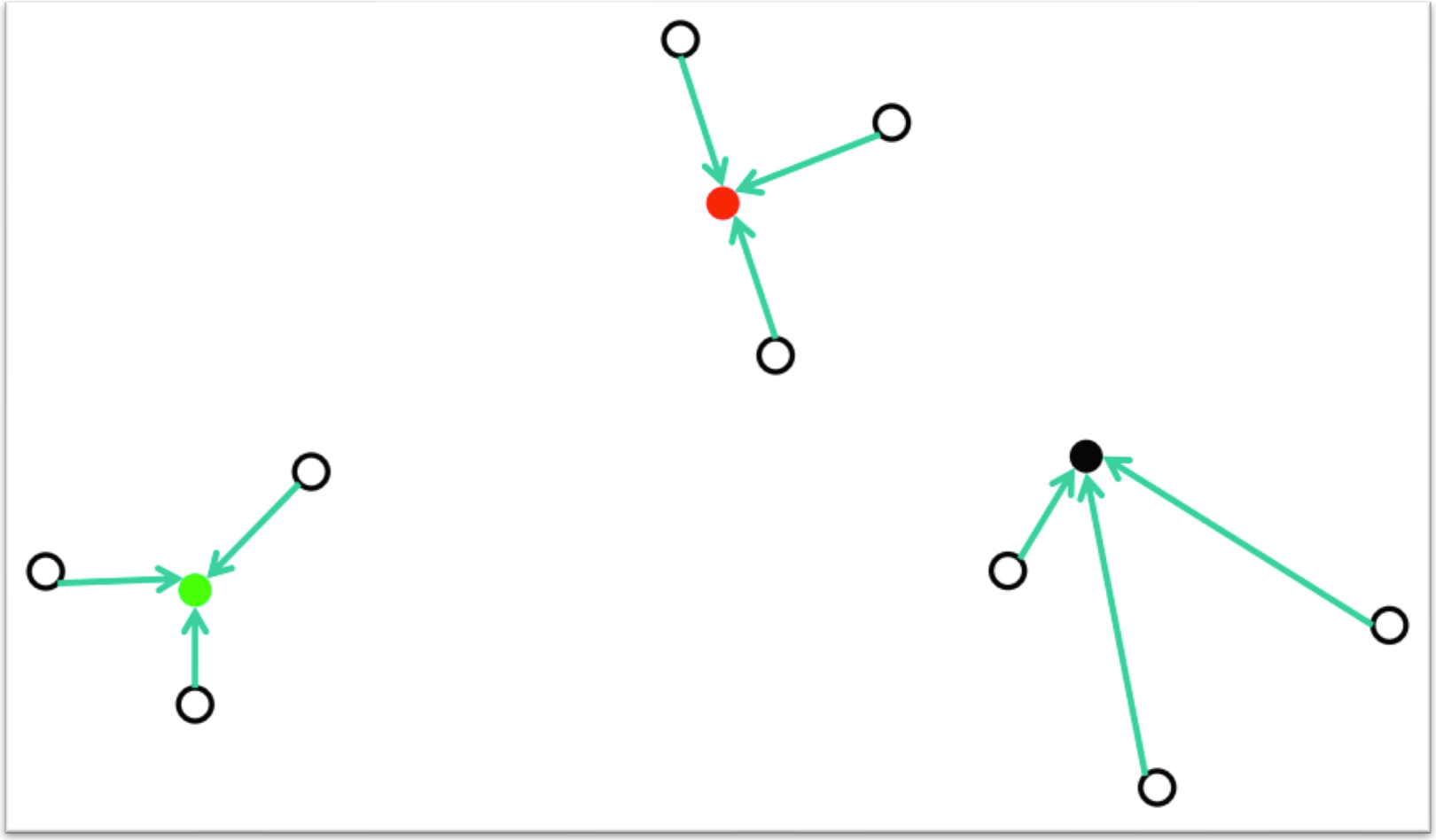
Recompute optimal centers given a fixed clustering



K-means Clustering

Euclidean distance metric

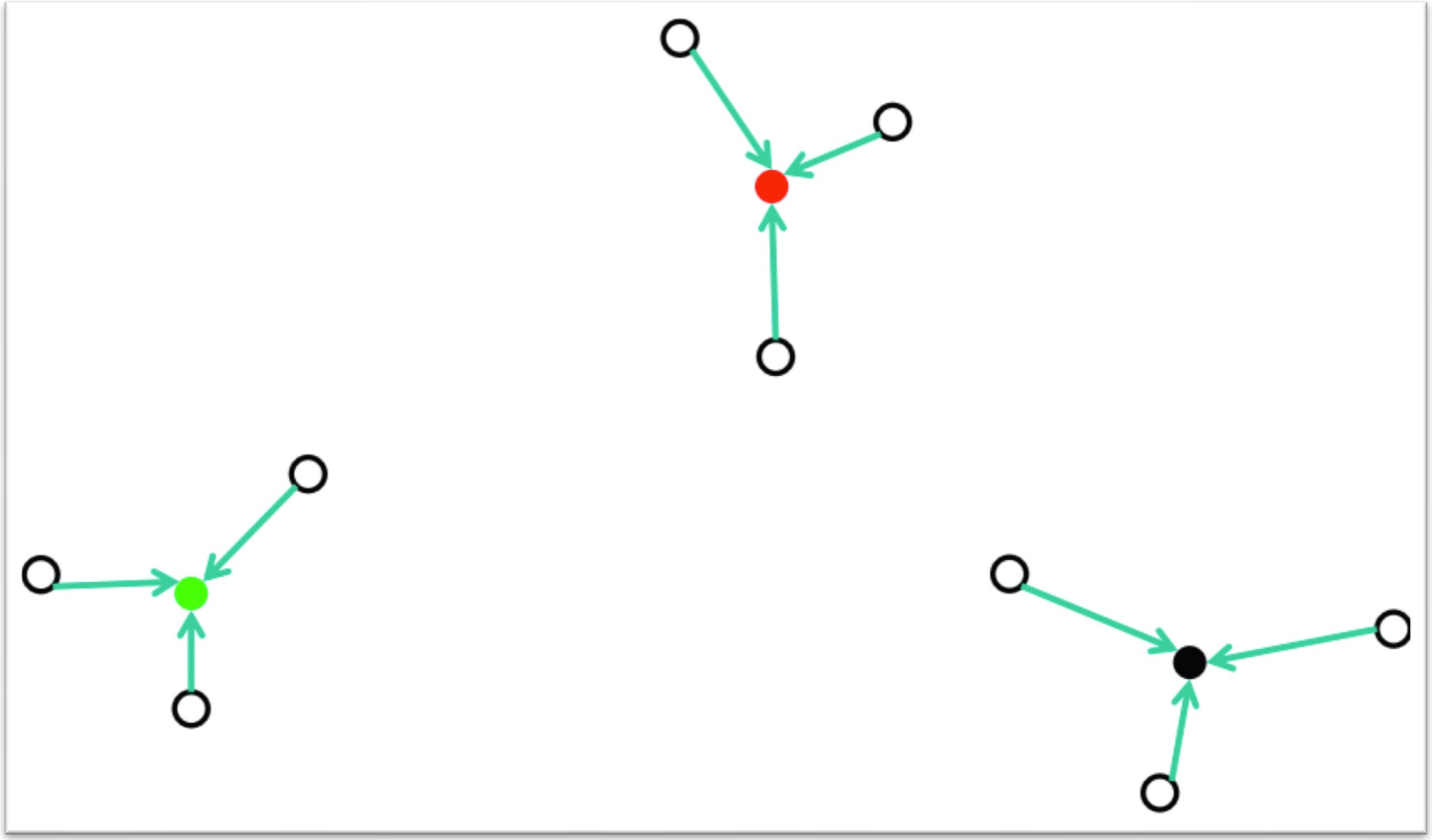
Assign each point to its nearest center



K-means Clustering

Euclidean distance metric

Recompute optimal centers given a fixed clustering



Selecting the number of clusters

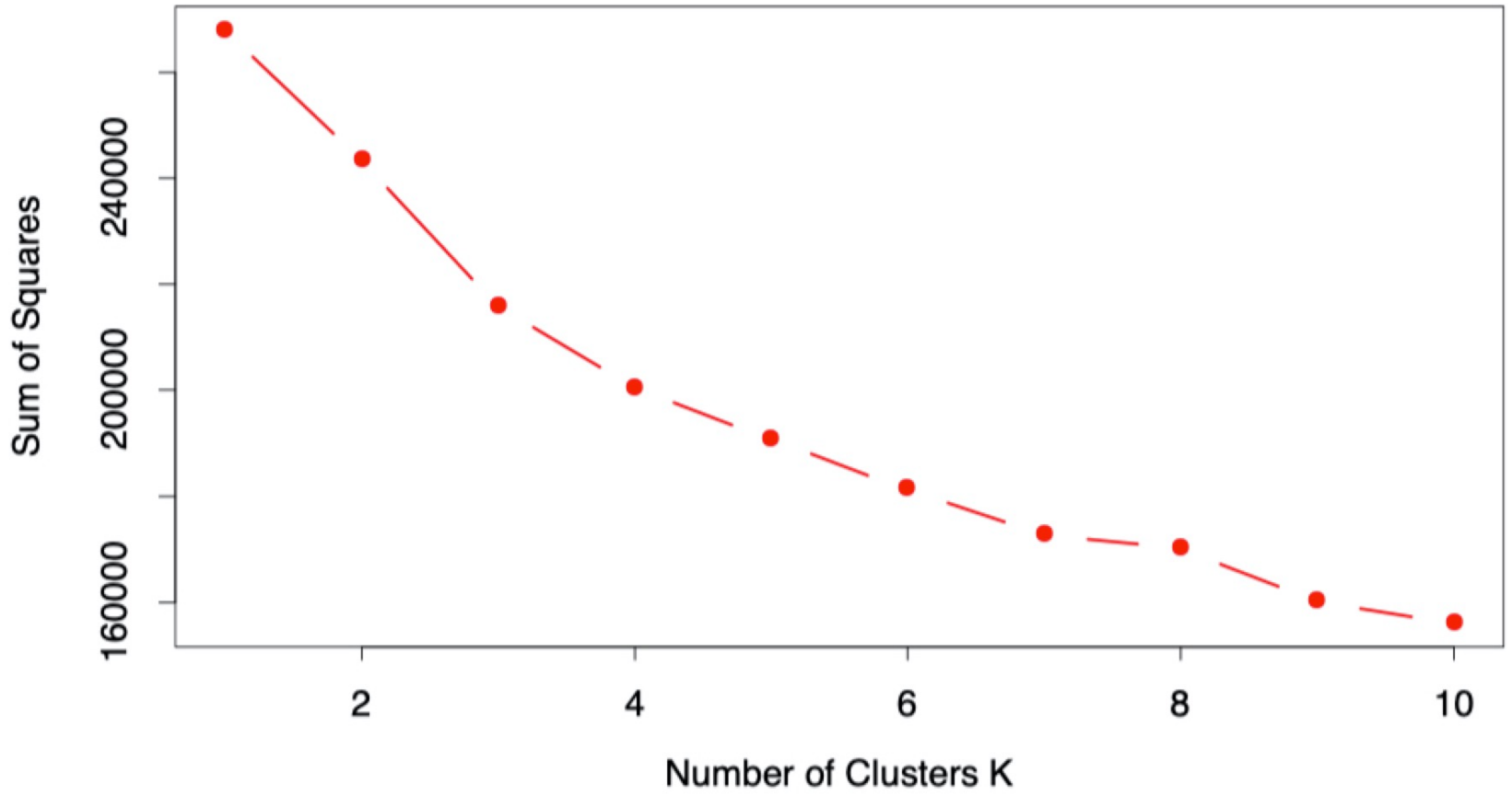
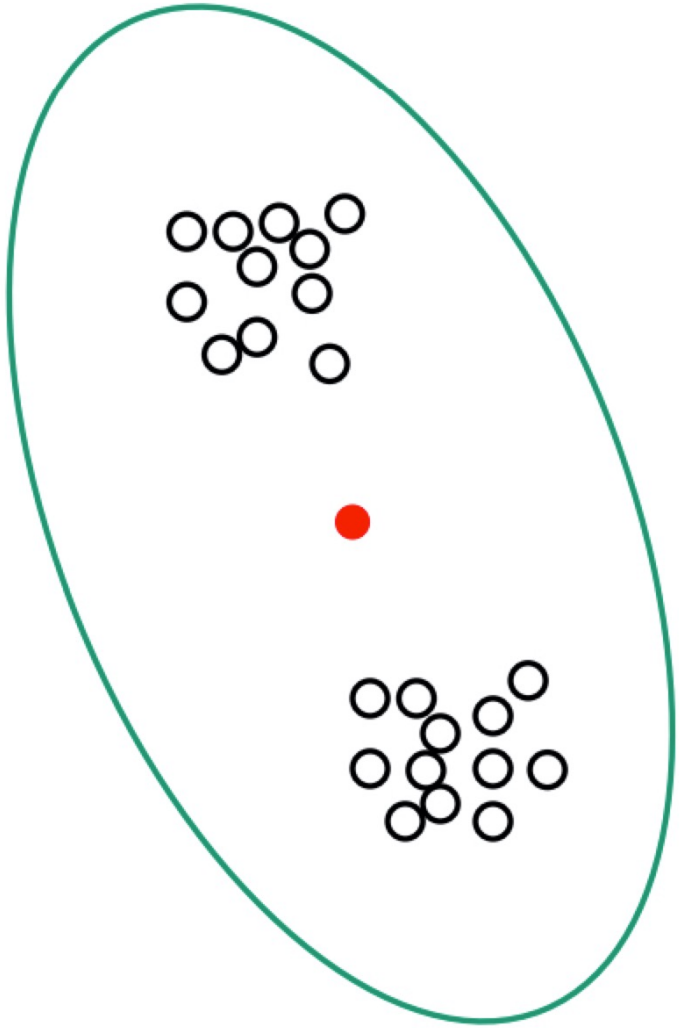
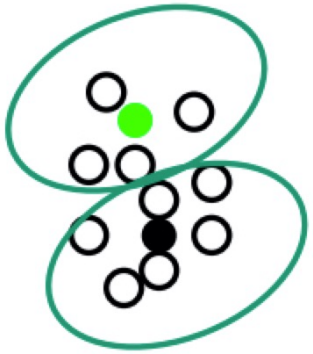


FIGURE 14.8. *Total within-cluster sum of squares for K-means clustering applied to the human tumor microarray data.*

K-means can **fail**

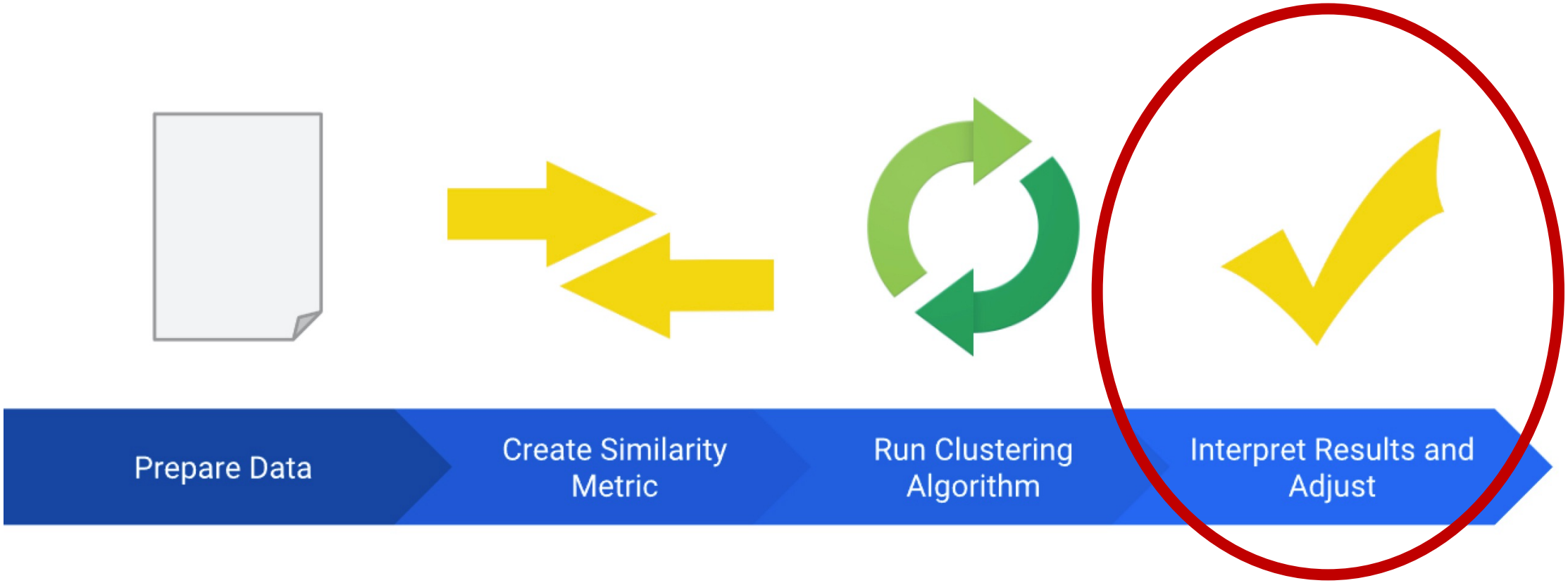


This is a **heuristic!**
No guarantees it'll find optimum

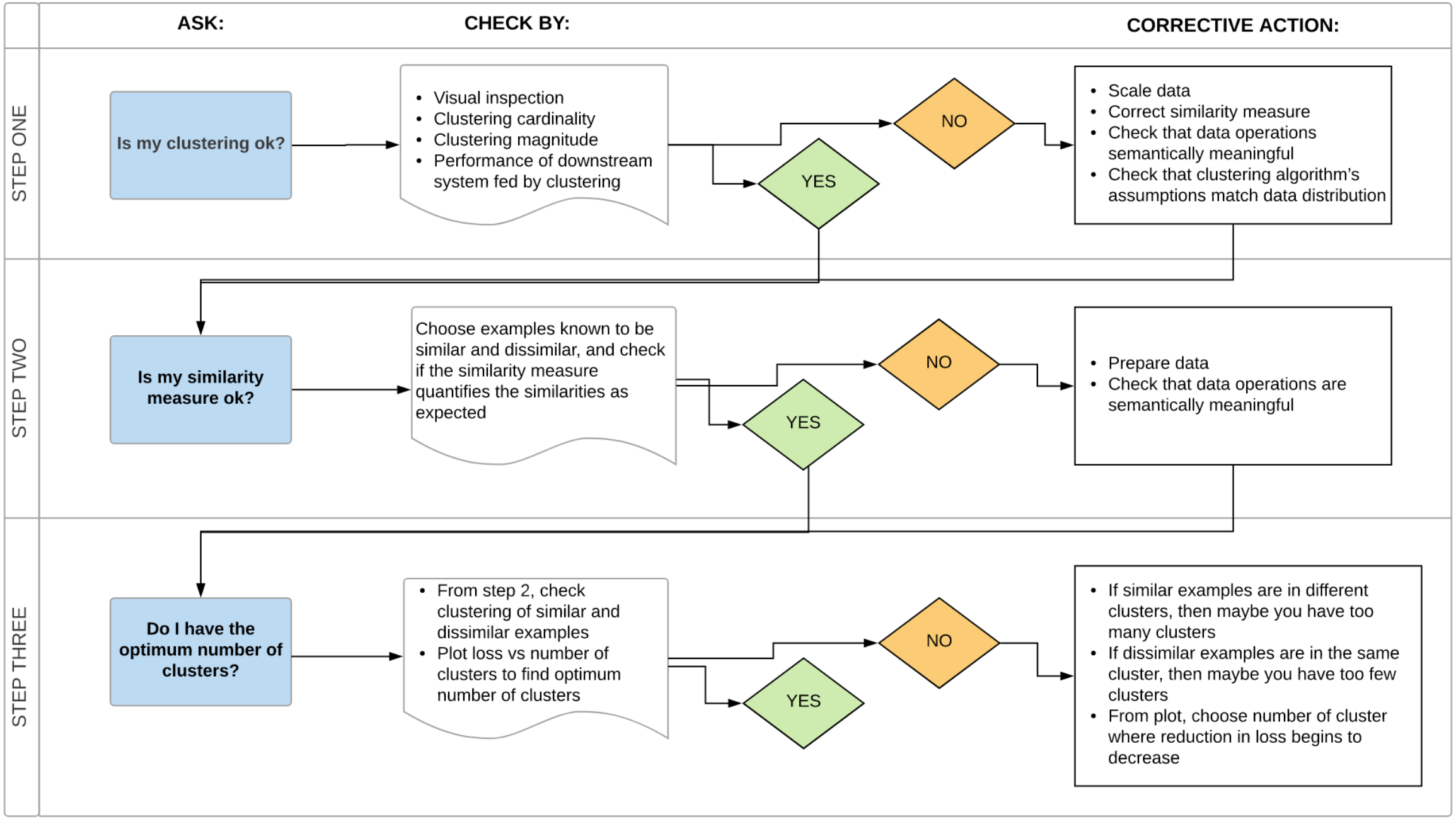


In practice, **smarter centroid initialization** solves this

Clustering workflow



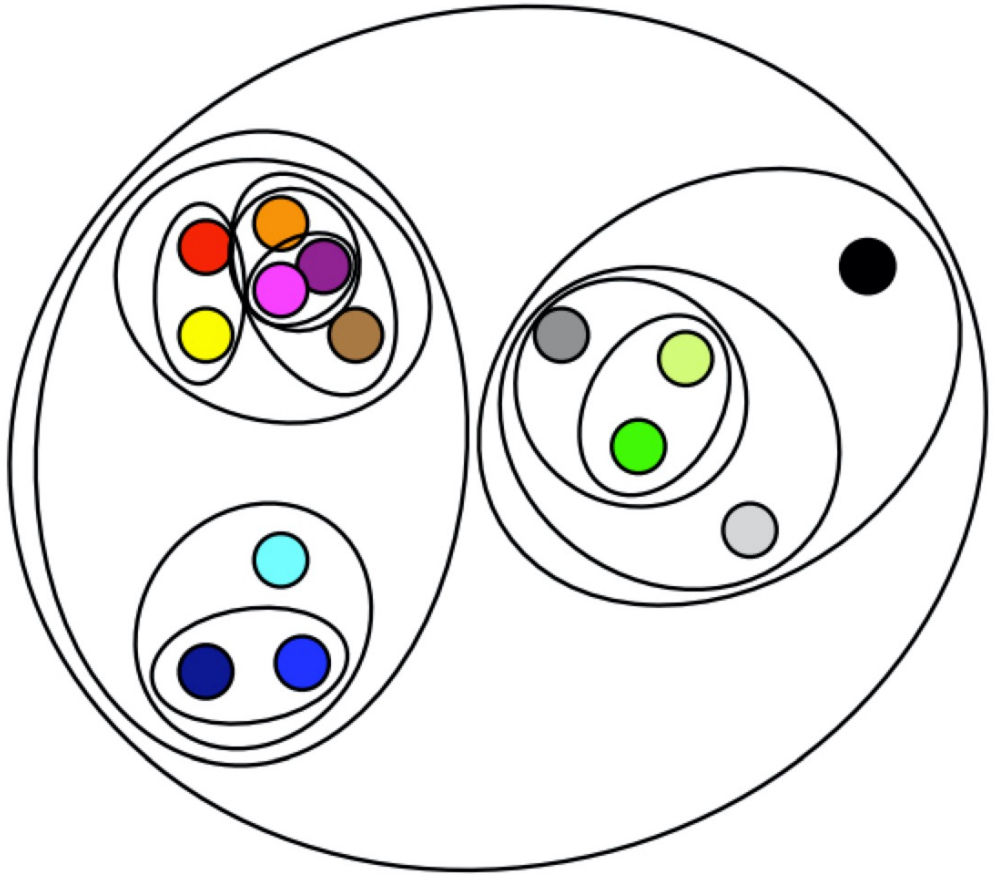
From Google's Clustering lesson: https://developers.google.com/machine-learning/clustering/

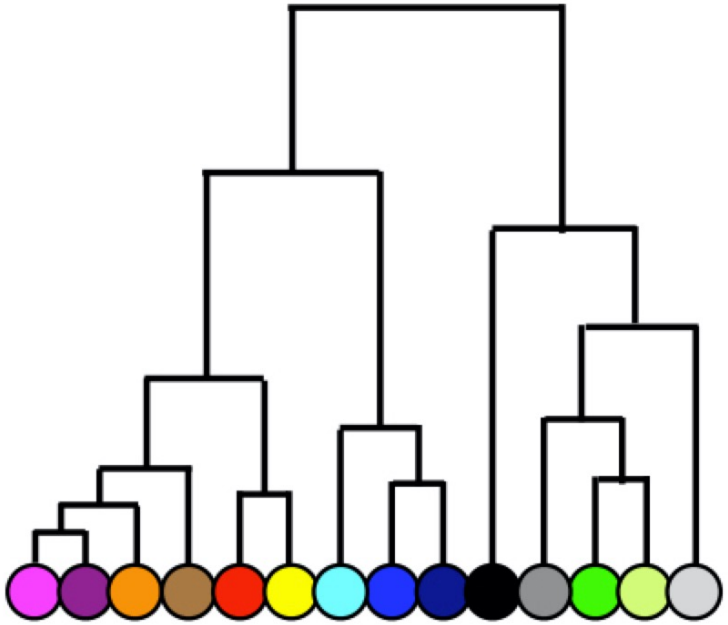


From Google's Clustering lesson: https://developers.google.com/machine-learning/clustering/

Hierarchical Clustering

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





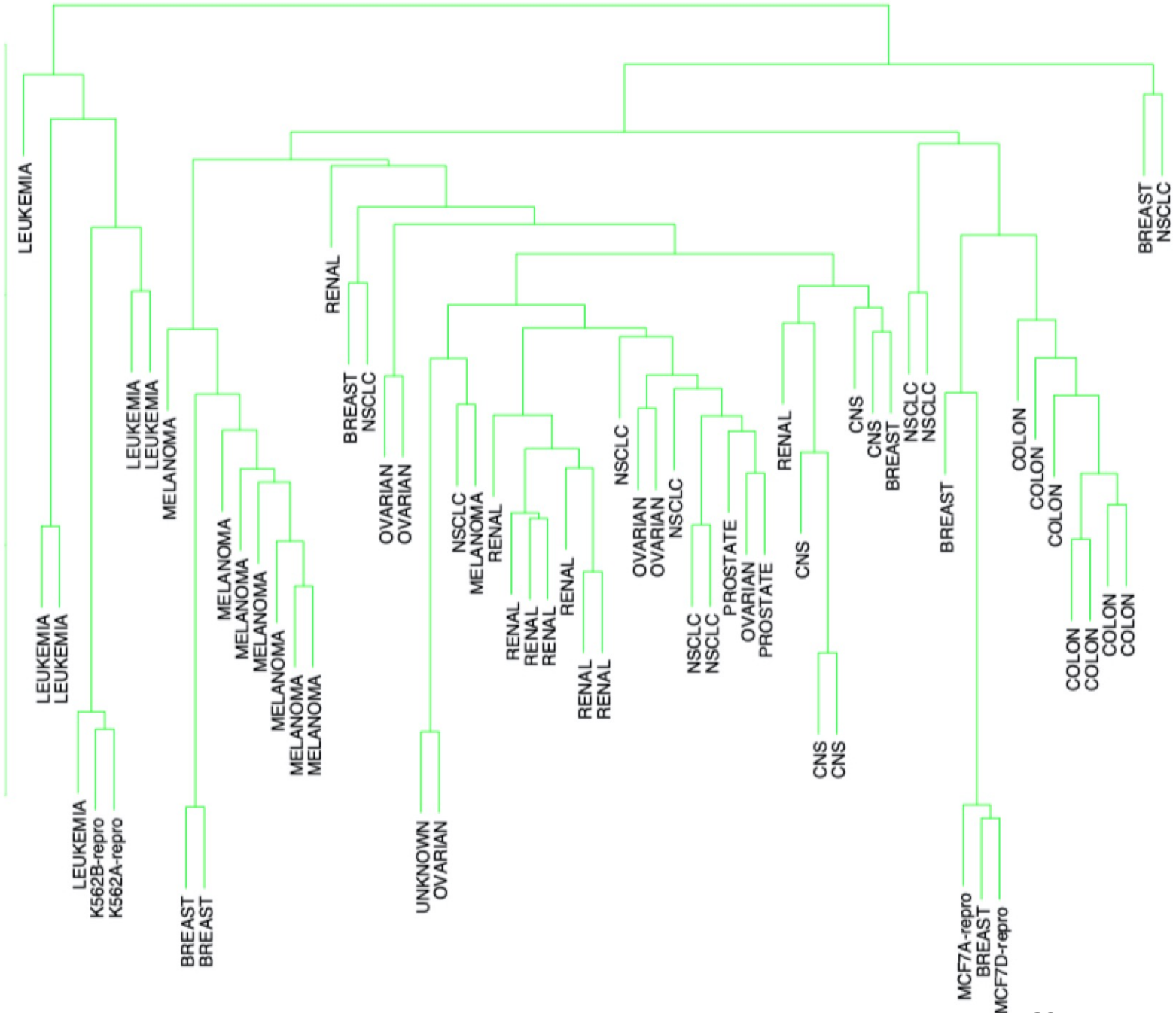
Based on slides by Elena Sügis: http://bioinformaticsinstitute.ru/sites/default/files/preprocessing_unsupervised.pdf

Hierarchical Clustering

Human Tumor Microarray Data

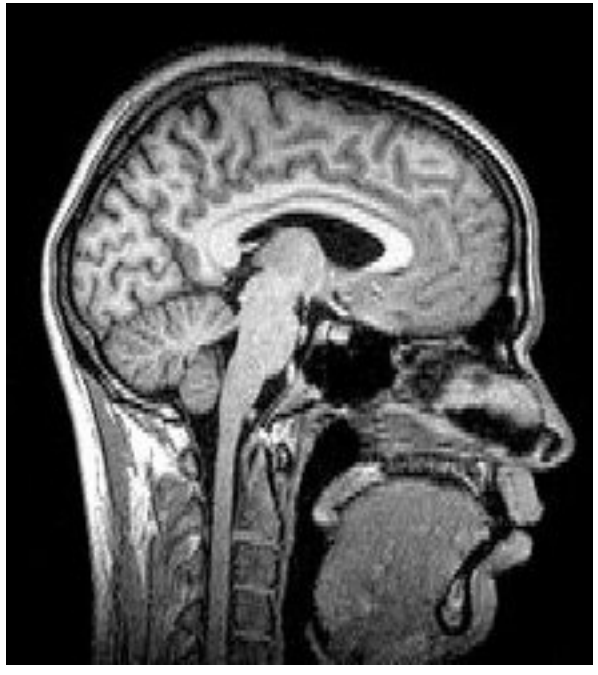
64 samples, 6830 features (gene expression levels)

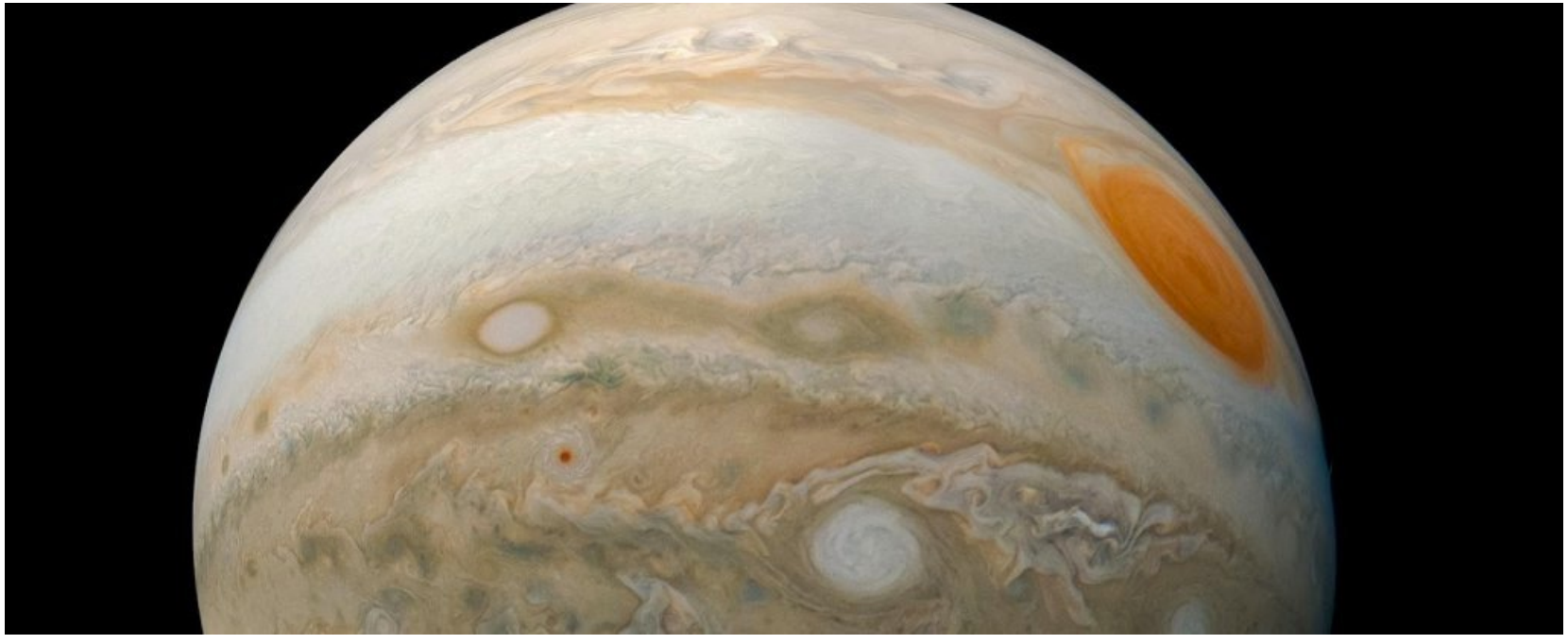
Elements of Statistical Learning, Chapter 14.3.8

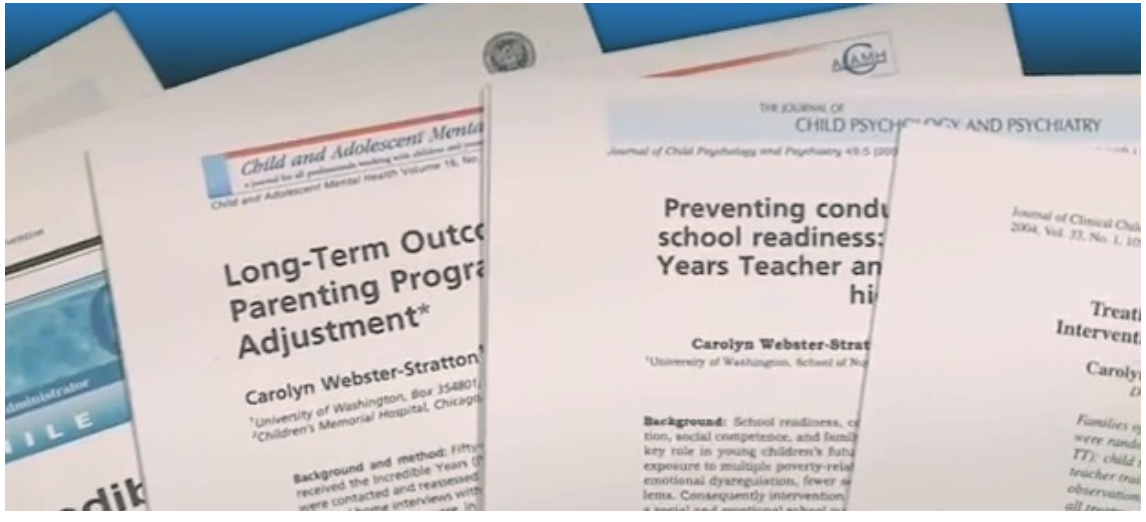


Dimensionality Reduction

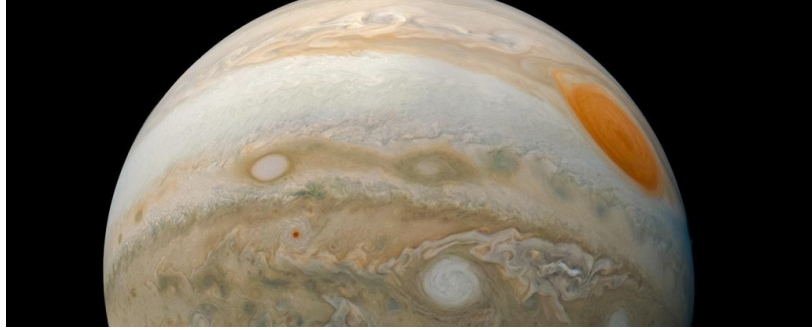
or dealing with very high-dimensional data





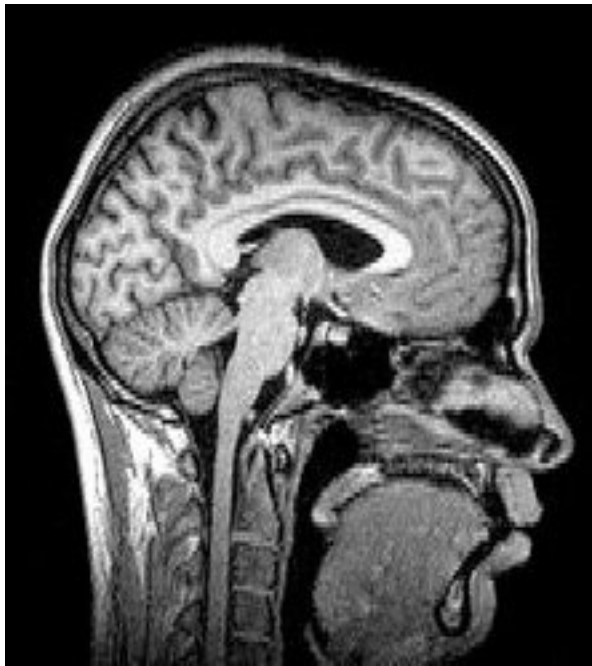


Dimensionality Reduction



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

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



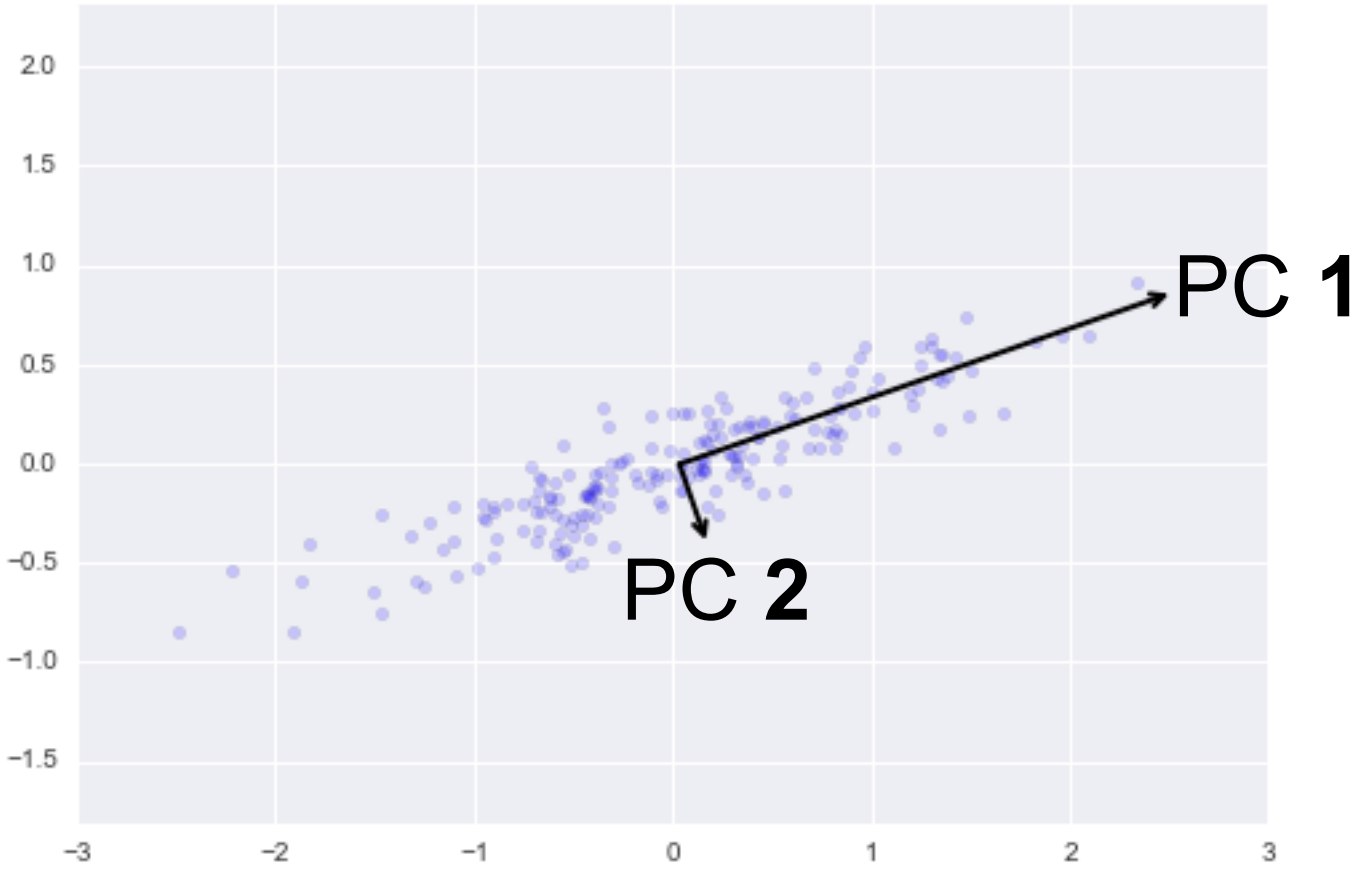
Useful for:

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

Based on slide by Nina Balcan

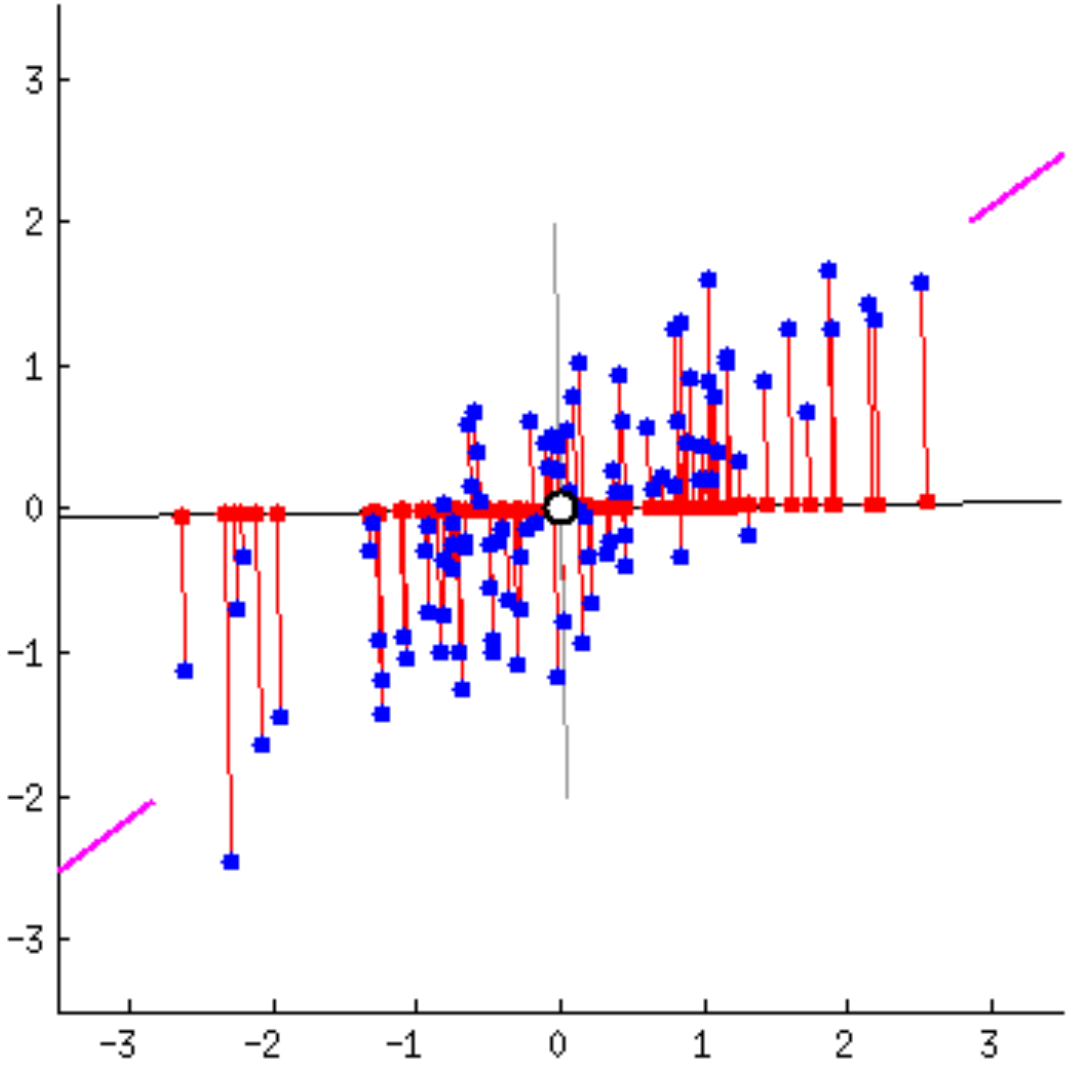
Principal Component Analysis (PCA)

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



Principal Component Analysis (PCA)

From https://stats.stackexchange.com/a/140579



Principal Component Analysis (PCA)

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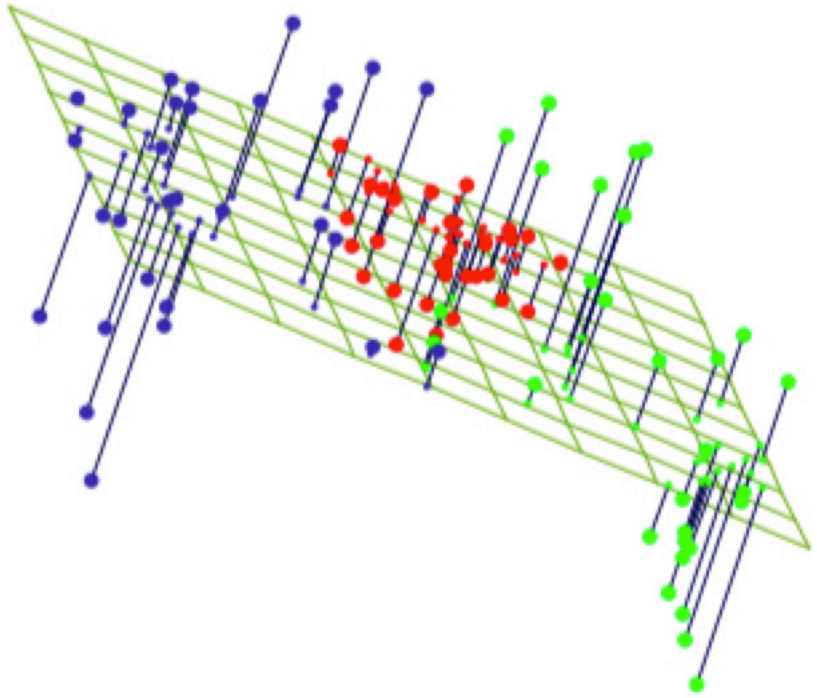
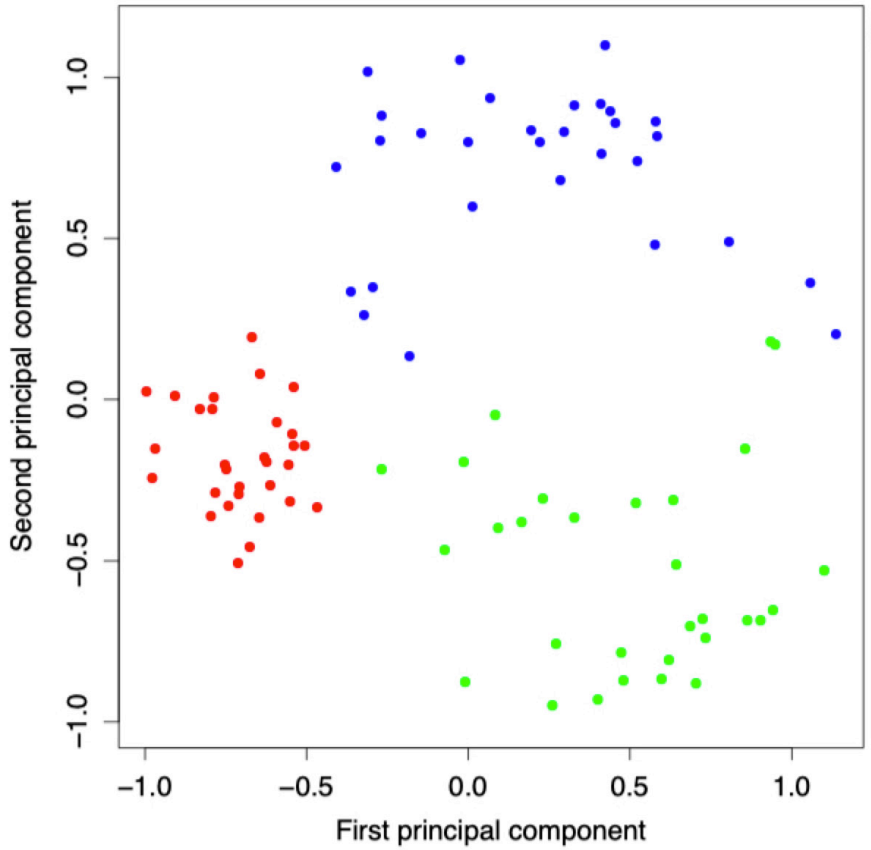


PC **2**



PC **1**

Principal Component Analysis (PCA)

Dataset $S = \{x_i\}_{i = 1,\ldots,n}$

- x_i: data example with d attributes
- μ: mean data point

PCA **approximates x with $\hat{x}_k$ by finding projection directions** $v_0, v_1, \ldots, v_k$ such that:

$$\hat{x}_k = \mu + ((x - \mu) \cdot v_0)v_0 + ((x - \mu) \cdot v_1)v_1 + \cdots + ((x - \mu) \cdot v_k)v_k$$

and the reconstruction error $(x - \hat{x}_k)^2$ is minimized

$v_0, v_1, \ldots, v_k$ are **orthogonal** unit vectors.

PCA for Face Reconstruction

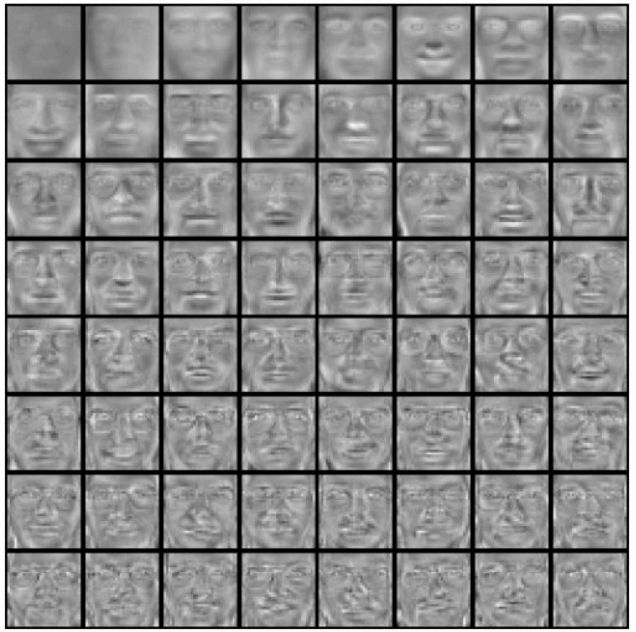
Eigenfaces, slide based on Derek Hoeim's, UIUC CS543

Image dataset, $\{x_i\}_{i=1,\ldots,n}$

PCA algorithm

64 Principal Components

$v_0, v_1, \ldots, v_{63}$

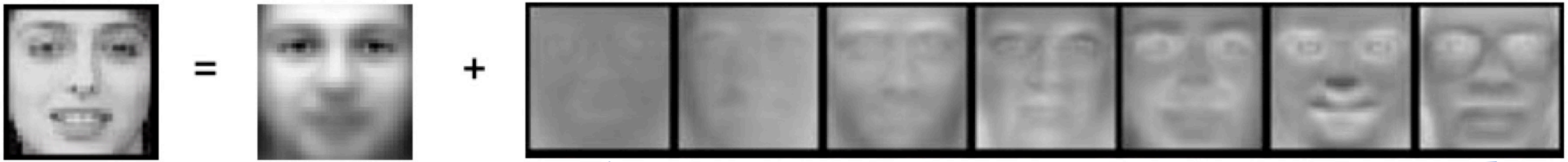


PCA for Face Reconstruction

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

Face Reconstruction using the Principal Components

x



$$\hat{x}_8 = \mu + ((x-\mu)\cdot v_0)v_0 + \dots + ((x-\mu)\cdot v_7)v_7$$

PCA for Face Reconstruction

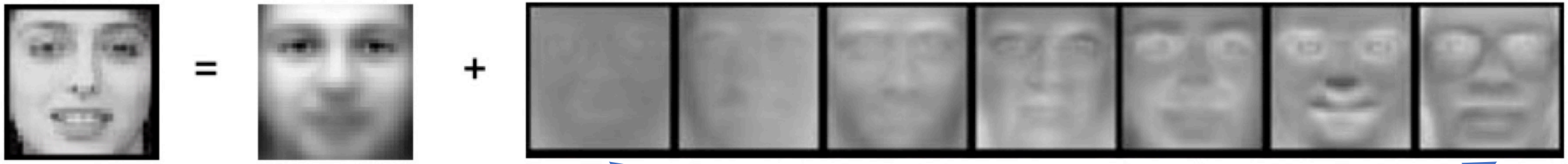
Eigenfaces, slide based on Derek Hoeim's, UIUC CS543

Face Recognition using PCA:

1- Given face image datasets, **extract Principal Components** $v_0, v_1, \ldots, v_k$.

2- Given new image, **project** onto PCs.

3- **Find closest** (projected) image in training dataset



$$\hat{x}_8 = \mu + ((x-\mu)\cdot v_0)v_0 + \ldots + ((x-\mu)\cdot v_7)v_7$$

[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 …

☆ Cited by 7225 Related articles All 61 versions »

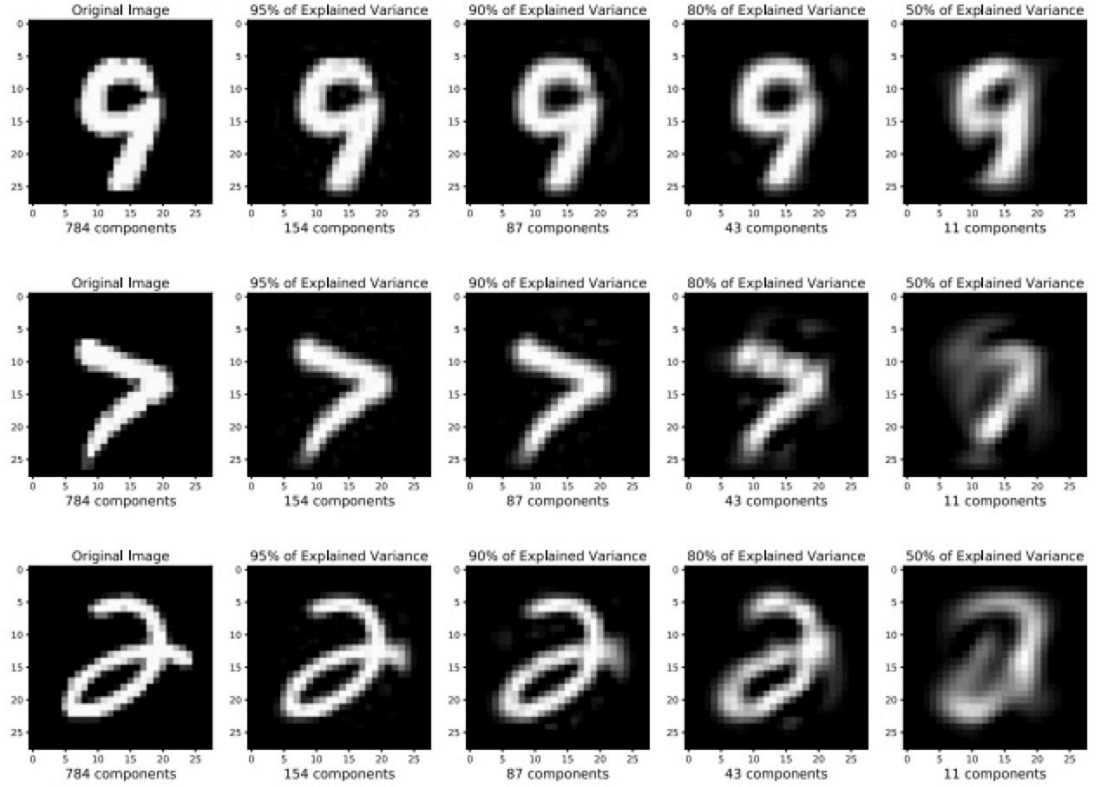
Final words on PCA

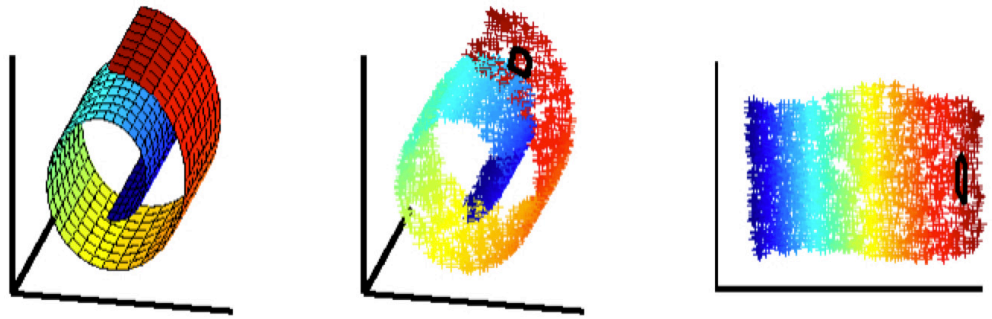
Advantages

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

Caveats

- Limited to **second-order** dependencies (variance is the limit)
- Limited to **linear** projections



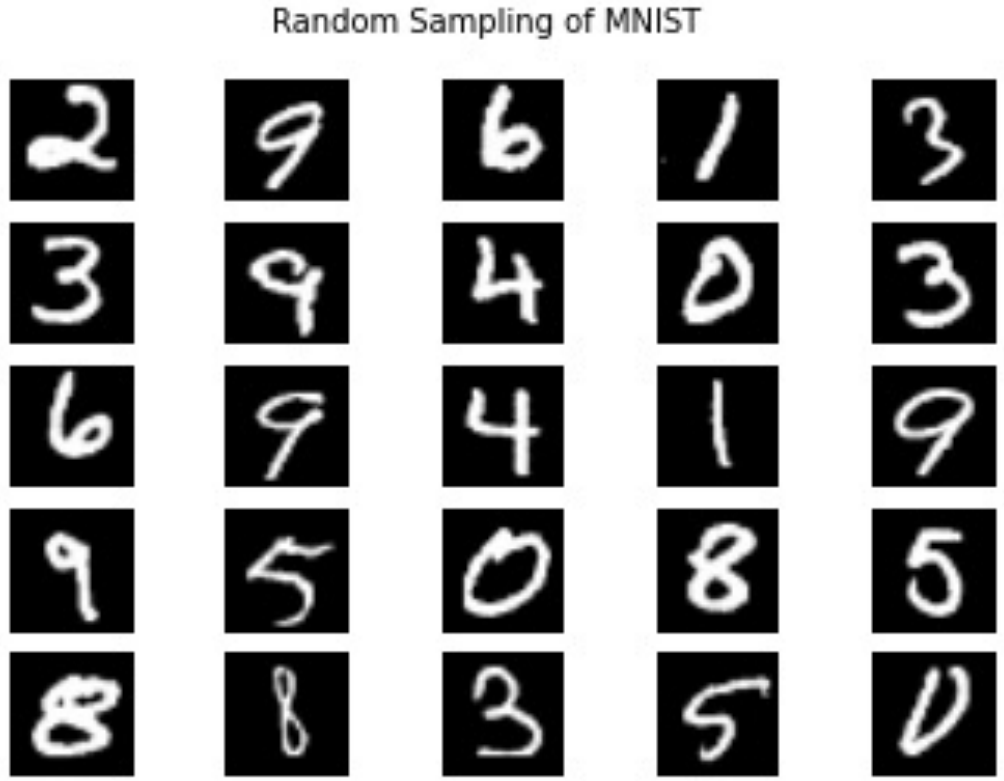


From Michael Guerzhoy's slides, UofT CSC320

t-SNE

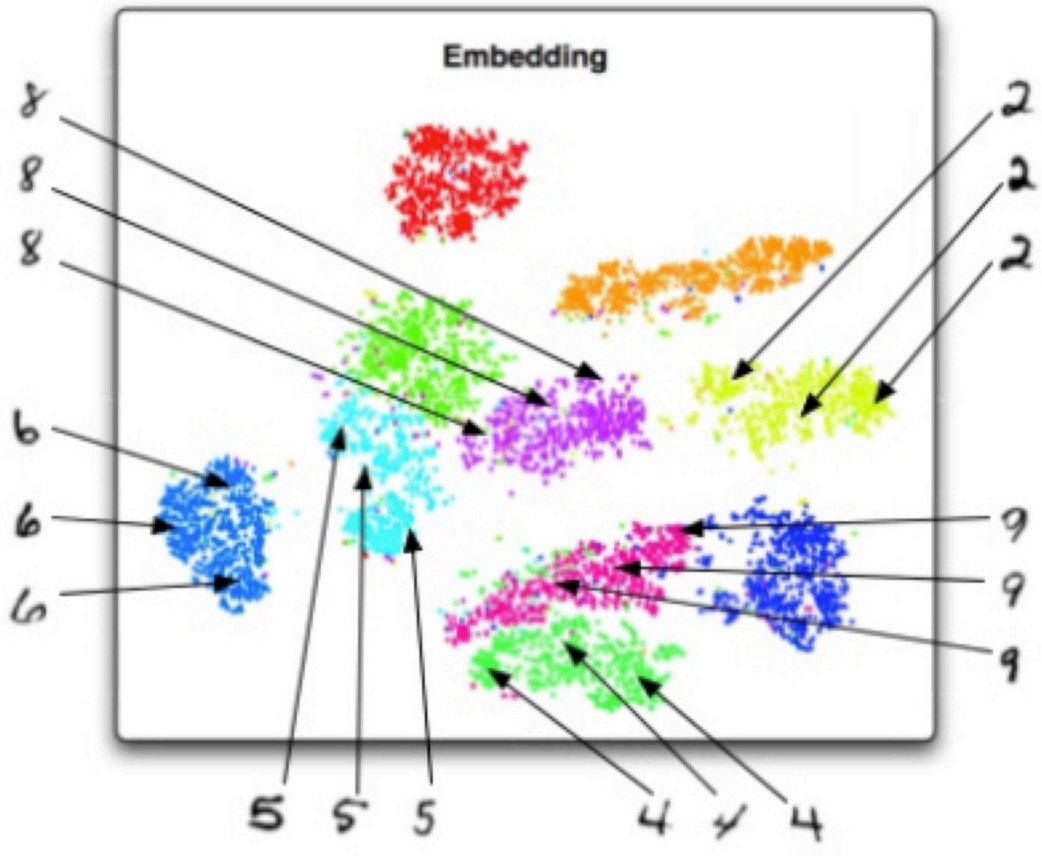
t-Distributed **S**tochastic **N**eighbor **E**mbedding

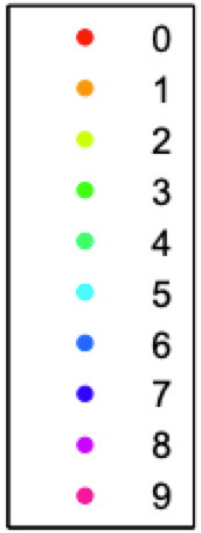
784 dimensions = 28x28 pixels



t-SNE

2 dimensions

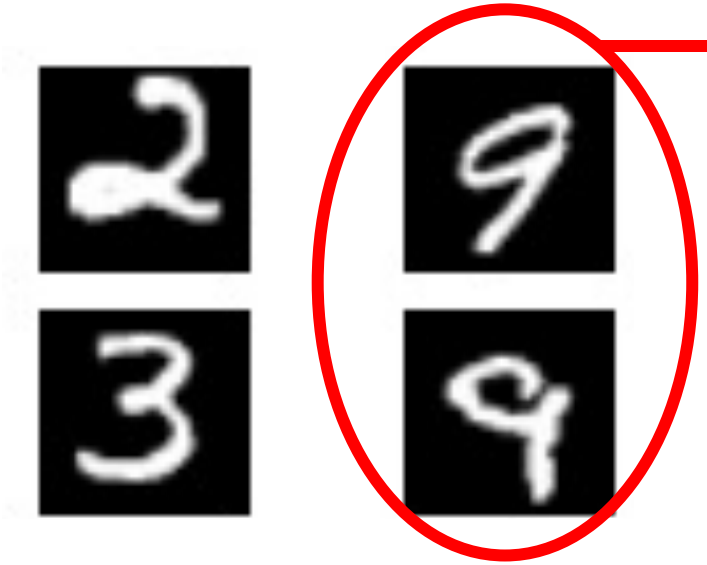




t-SNE

t-Distributed **S**tochastic **N**eighbor **E**mbedding

high probability



$$p_{j|i} = \frac{\exp\left(-\|x_i - x_j\|^2 / 2\sigma_i^2\right)}{\sum_{k \neq i} \exp\left(-\|x_i - x_k\|^2 / 2\sigma_i^2\right)}$$

Probability that point x_i "selects" x_j as "neighbor".
Based on transforming Euclidean distance to a probability via a Gaussian distribution.

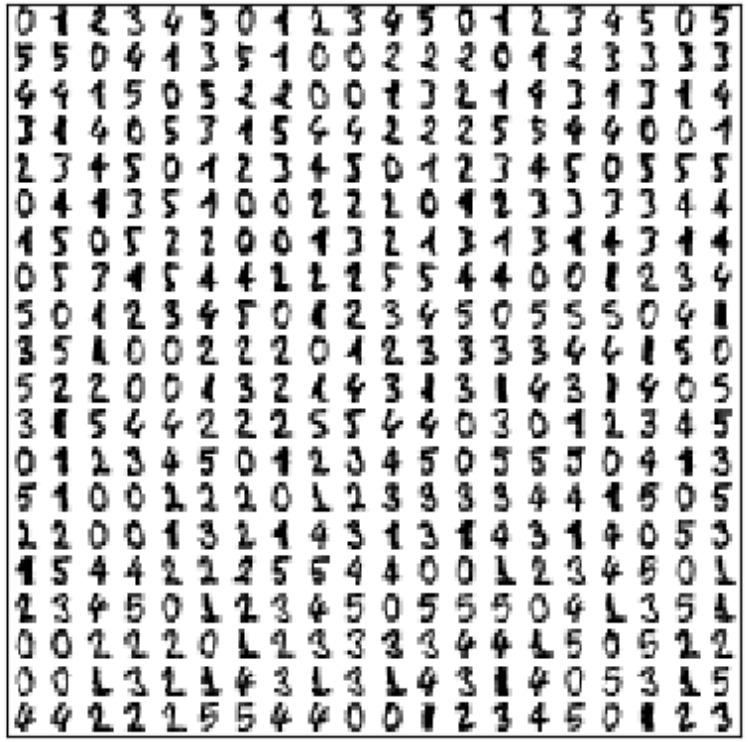
t-SNE finds a y_i for each x_i such that the two **probability distributions are similar**

$$q_{ij} = \frac{\left(1 + \|y_i - y_j\|^2\right)^{-1}}{\sum_{k \neq l} \left(1 + \|y_k - y_l\|^2\right)^{-1}}$$

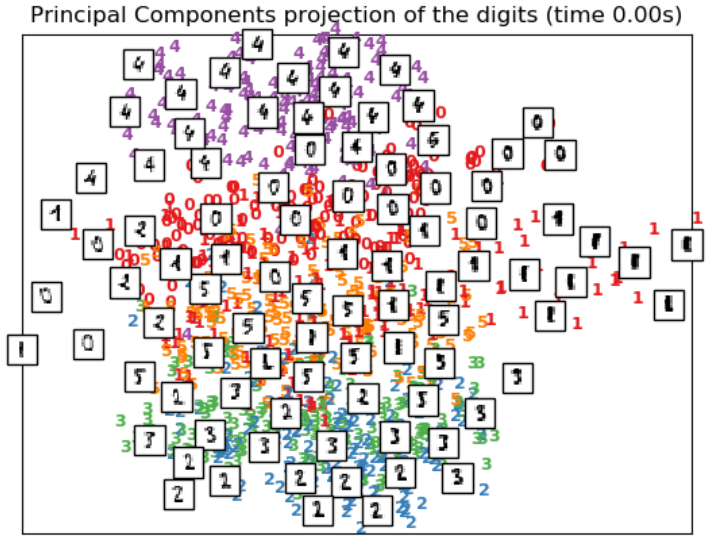
y_i is the low-dimensional mapping of x_i
q_{ij} is the probability that y_i "selects" y_j as "neighbor".

t-SNE
t-Distributed **S**tochastic **N**eighbor **E**mbedding

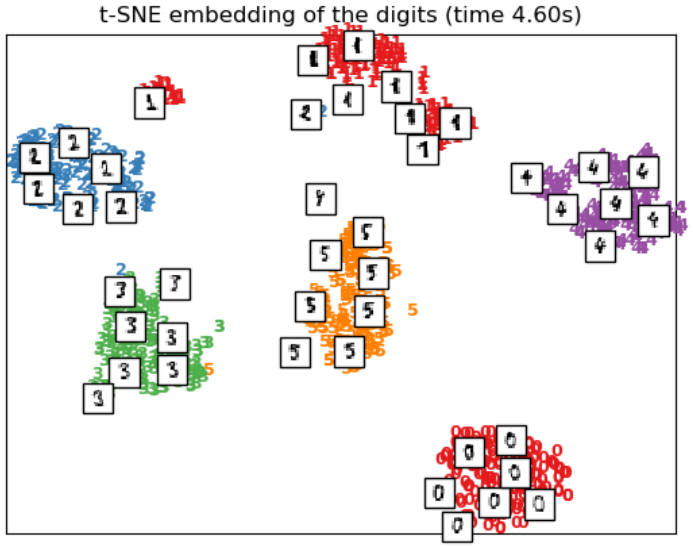
A selection from the 64-dimensional digits dataset



PCA



t-SNE



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

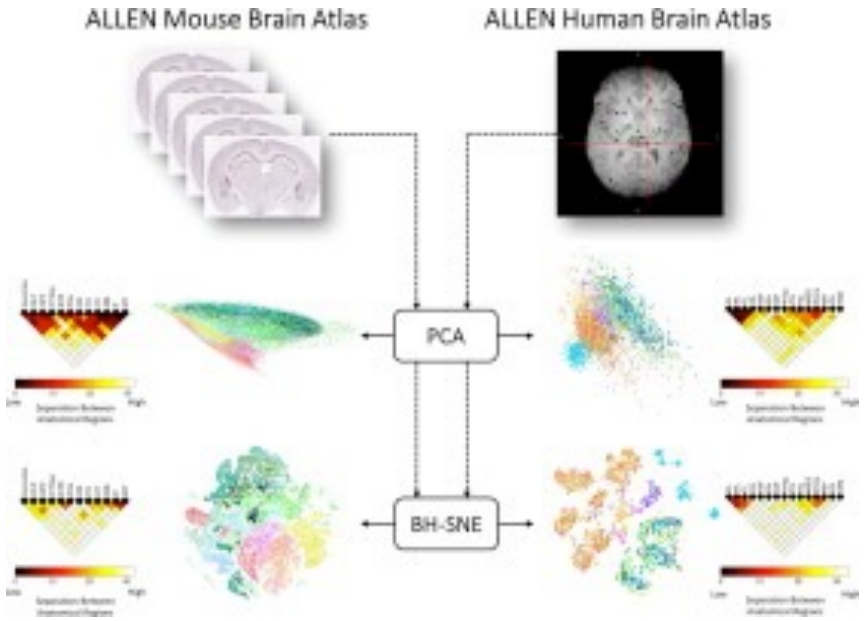
Final words on **t-SNE**

Advantages

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

Caveats

- **Slow** to compute, but **PCA** preprocessing speeds it up!
- 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