Clustering
Lecture 14

David Sontag

New York University

Slides adapted from Luke Zettlemoyer, Vibhav Gogate, Carlos Guestrin, Andrew Moore, Dan Klein

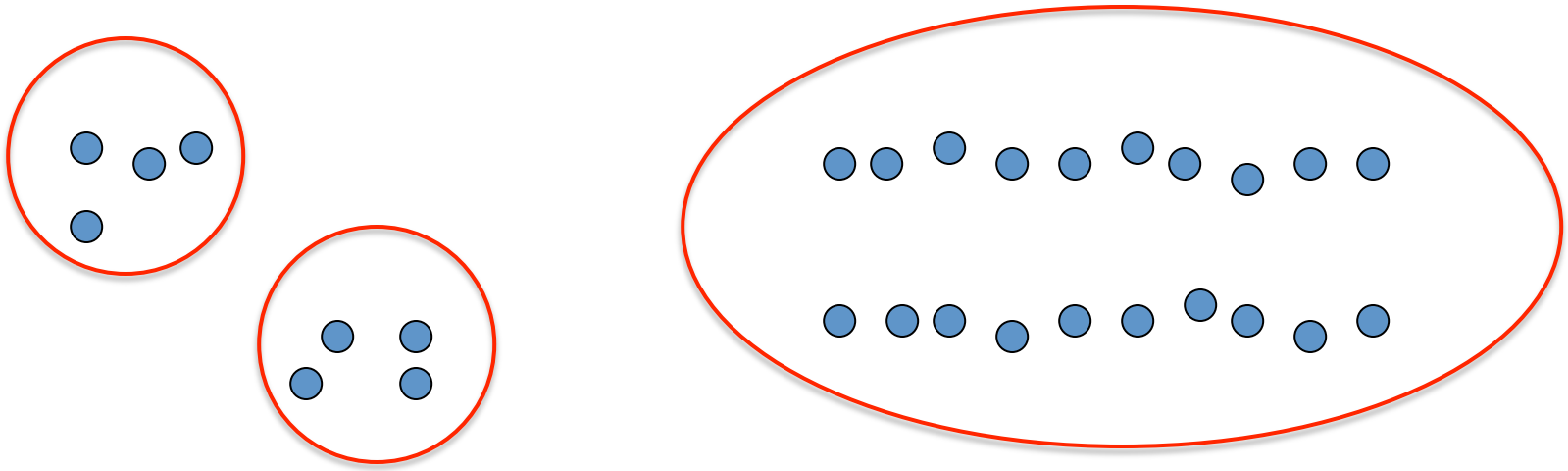
Clustering

Clustering:

- Unsupervised learning
- Requires data, but no labels
- Detect patterns e.g. in
  - Group emails or search results
  - Customer shopping patterns
  - Regions of images
- Useful when don't know what you're looking for
- But: can get gibberish

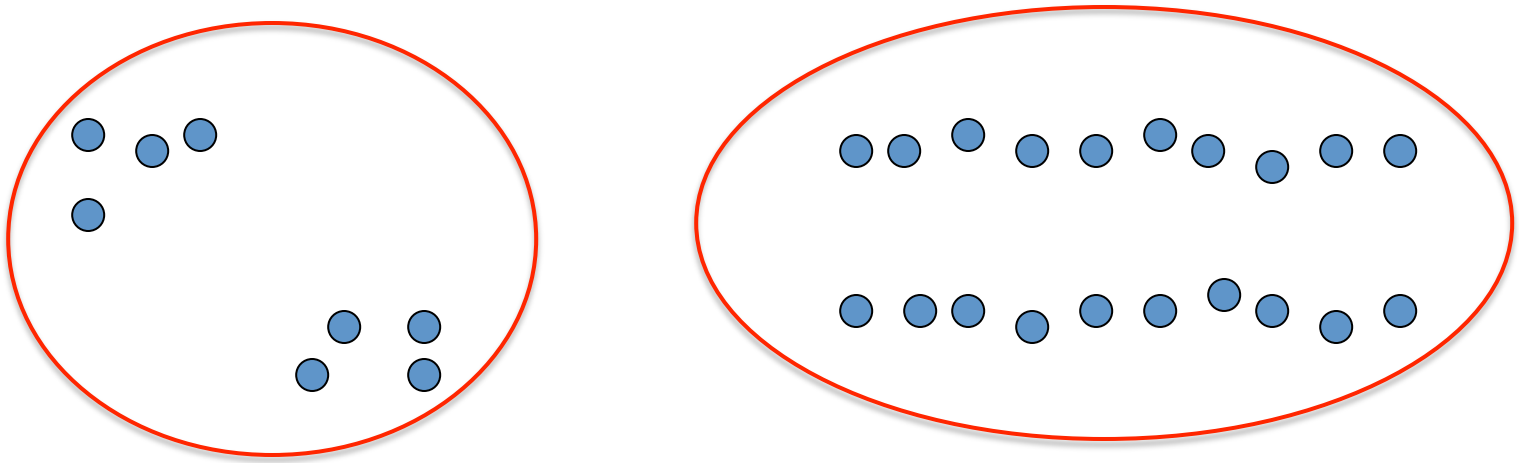
Clustering

- Basic idea: group together similar instances
- Example: 2D point patterns



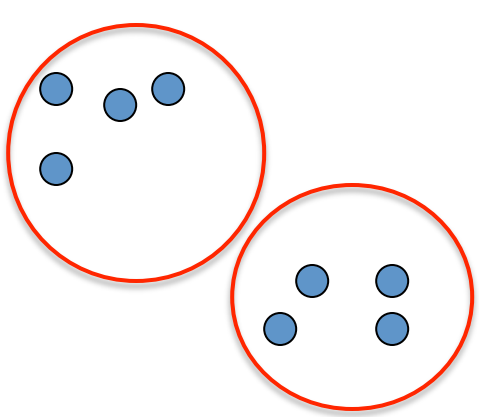
Clustering

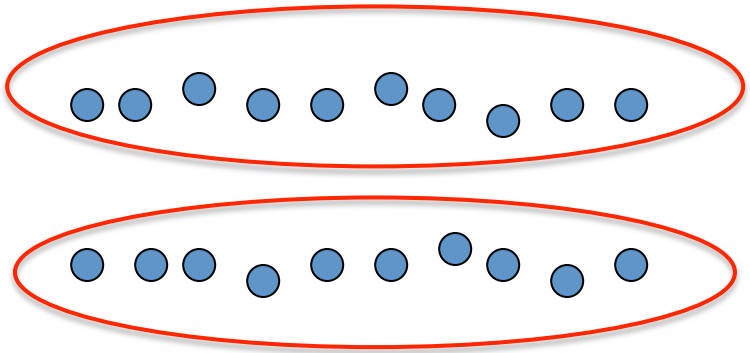
- Basic idea: group together similar instances
- Example: 2D point patterns



Clustering

- Basic idea: group together similar instances
- Example: 2D point patterns





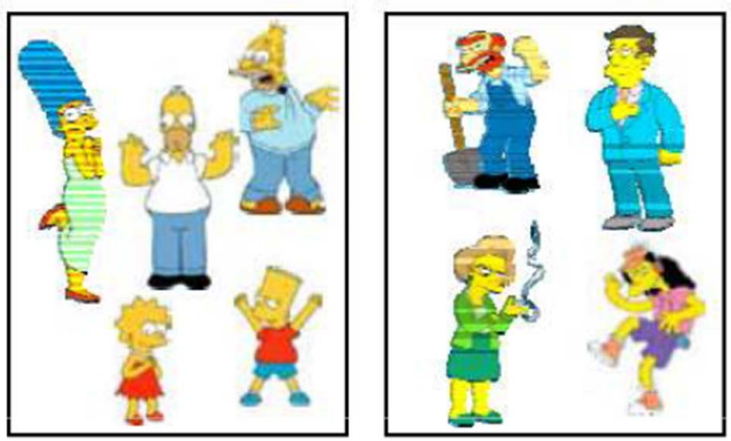
- What could "similar" mean?
  - One option: small Euclidean distance (squared)

$$\mathrm{dist}(\vec{x}, \vec{y}) = ||\vec{x} - \vec{y}||_2^2$$

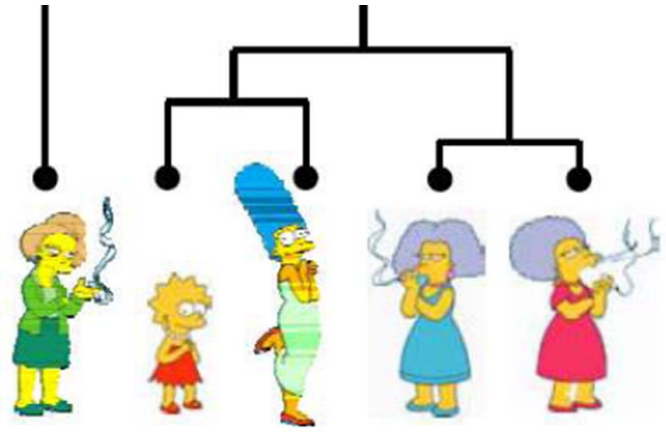
  - Clustering results are crucially dependent on the measure of similarity (or distance) between "points" to be clustered

Clustering algorithms

- Partition algorithms (Flat)
  - K-means
  - Mixture of Gaussian
  - Spectral Clustering



- Hierarchical algorithms
  - Bottom up – agglomerative
  - Top down – divisive



Clustering examples

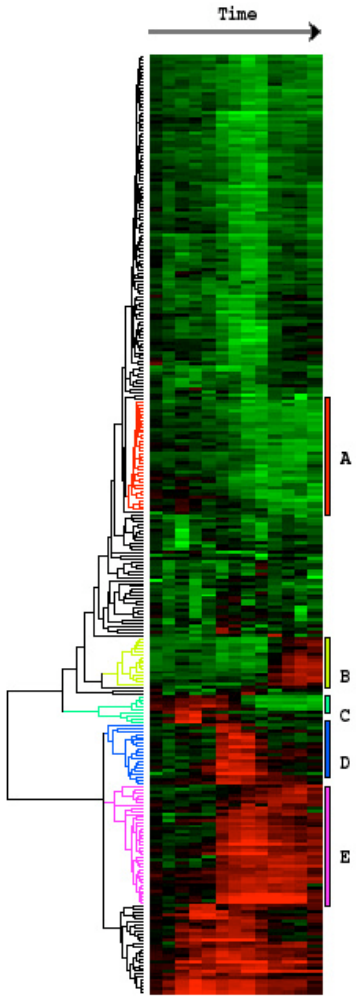
Image segmentation

Goal: Break up the image into meaningful or perceptually similar regions

[Slide from James Hayes]

Clustering examples

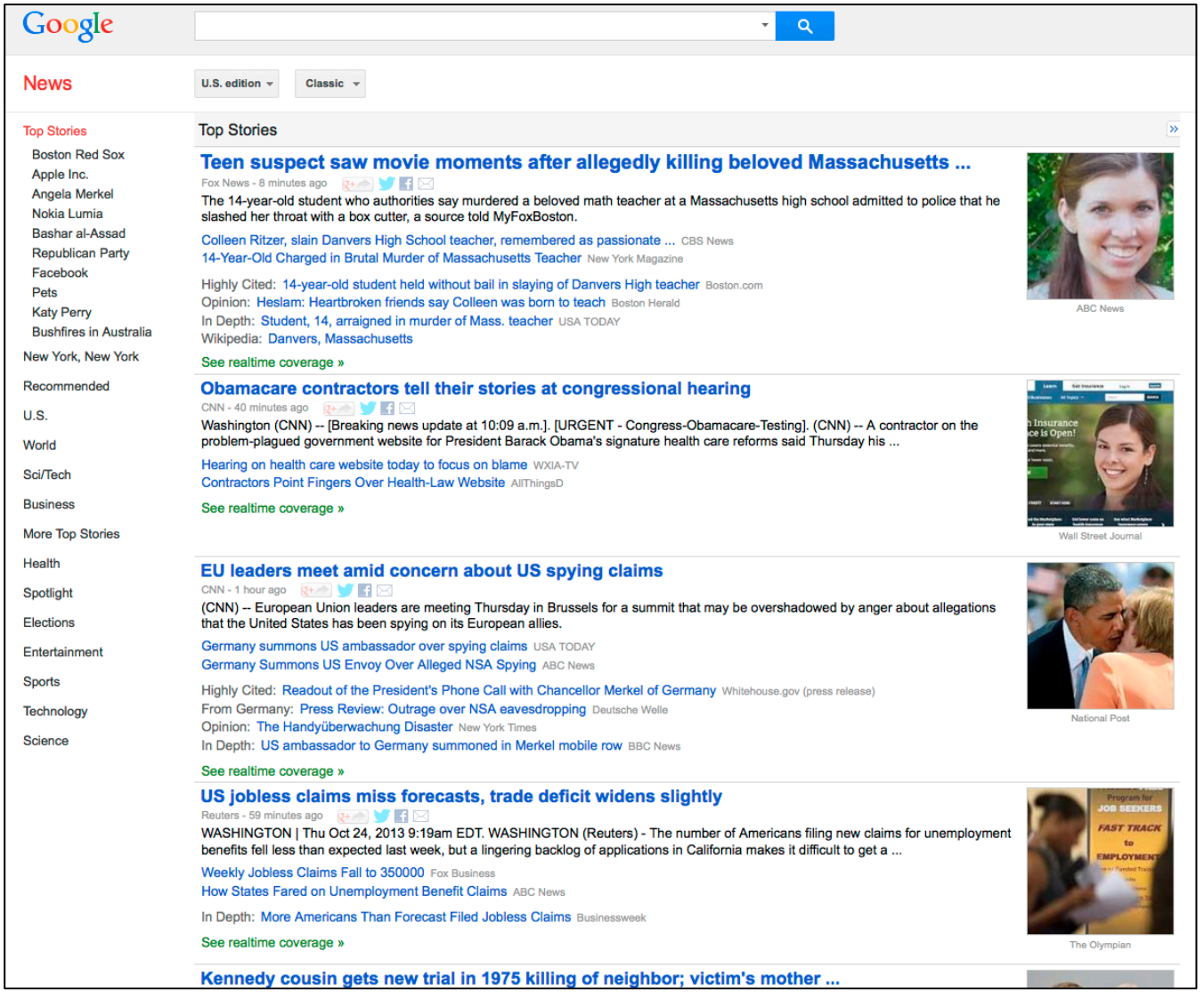
Clustering gene expression data



Eisen et al, PNAS 1998

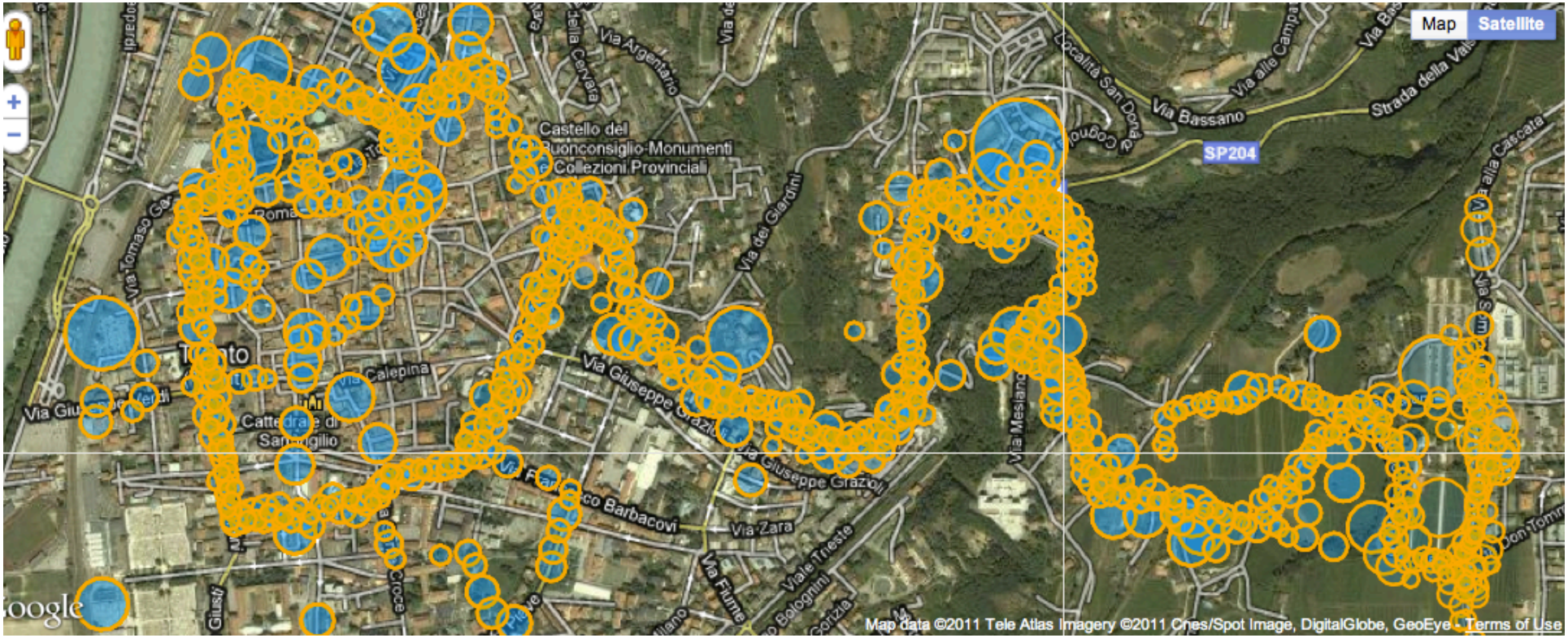
Clustering examples

Cluster news articles



Clustering examples

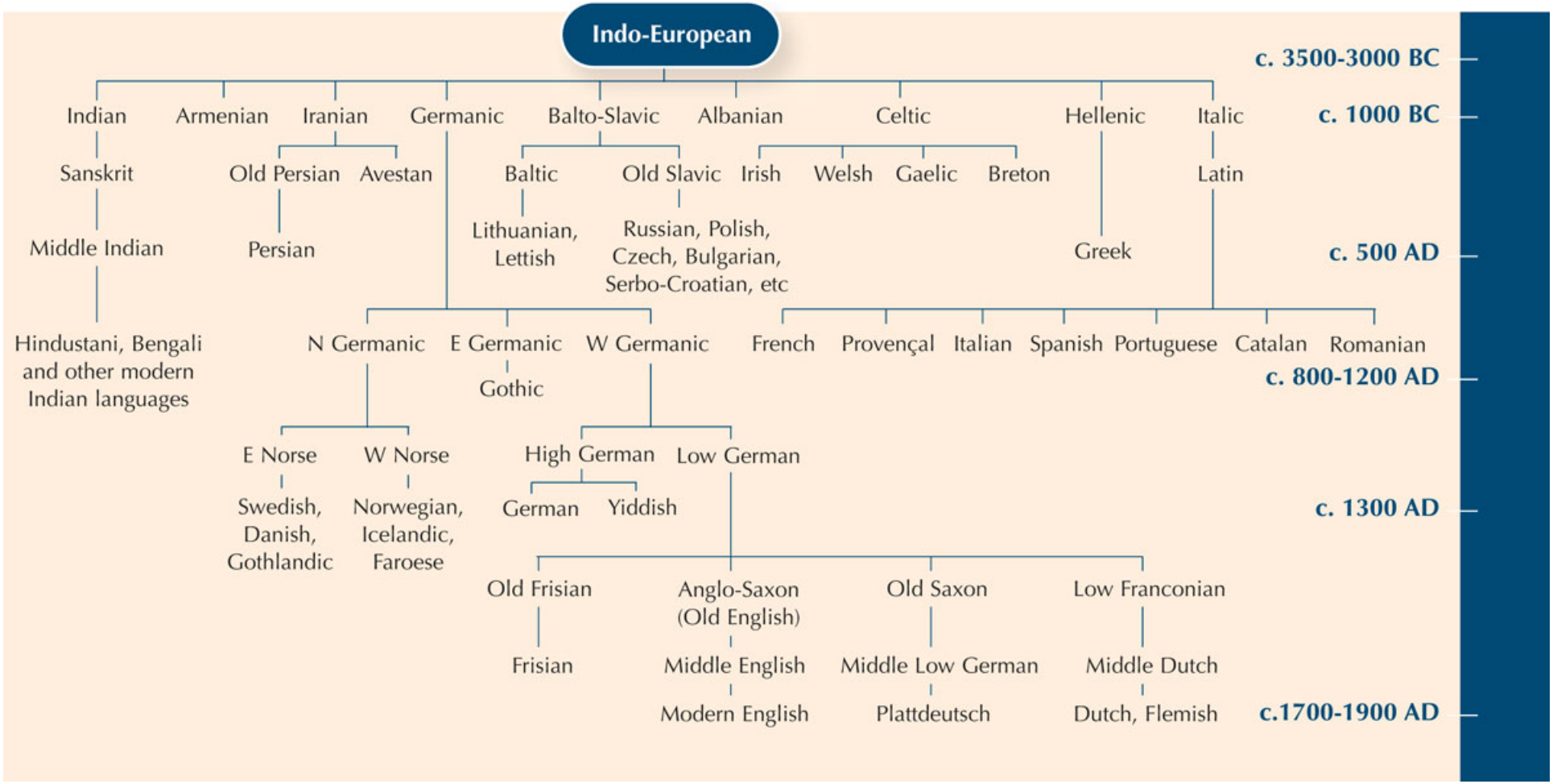
Cluster people by space and time



[Image from Pilho Kim]

Clustering examples

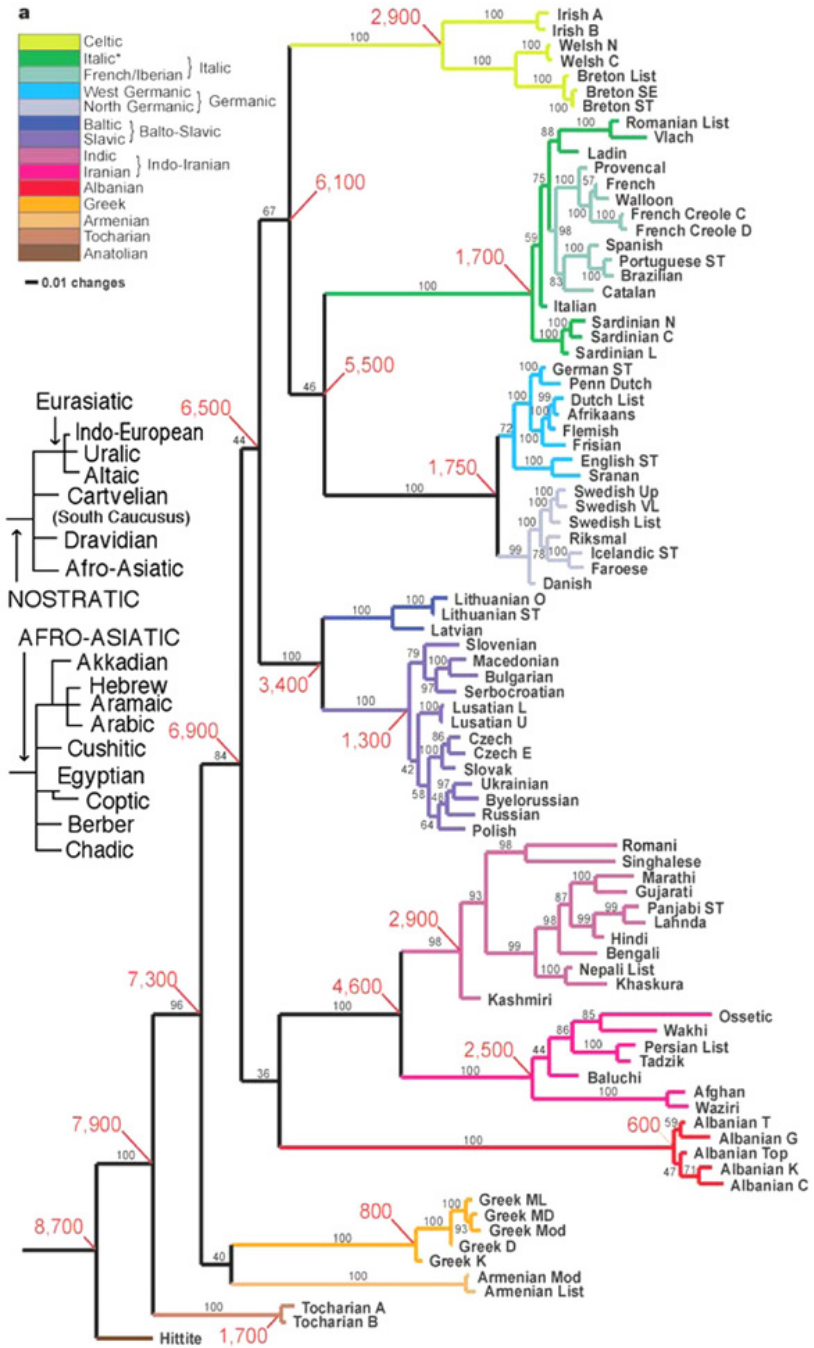
Clustering languages



[Image from scienceinschool.org]

Clustering examples

Clustering languages

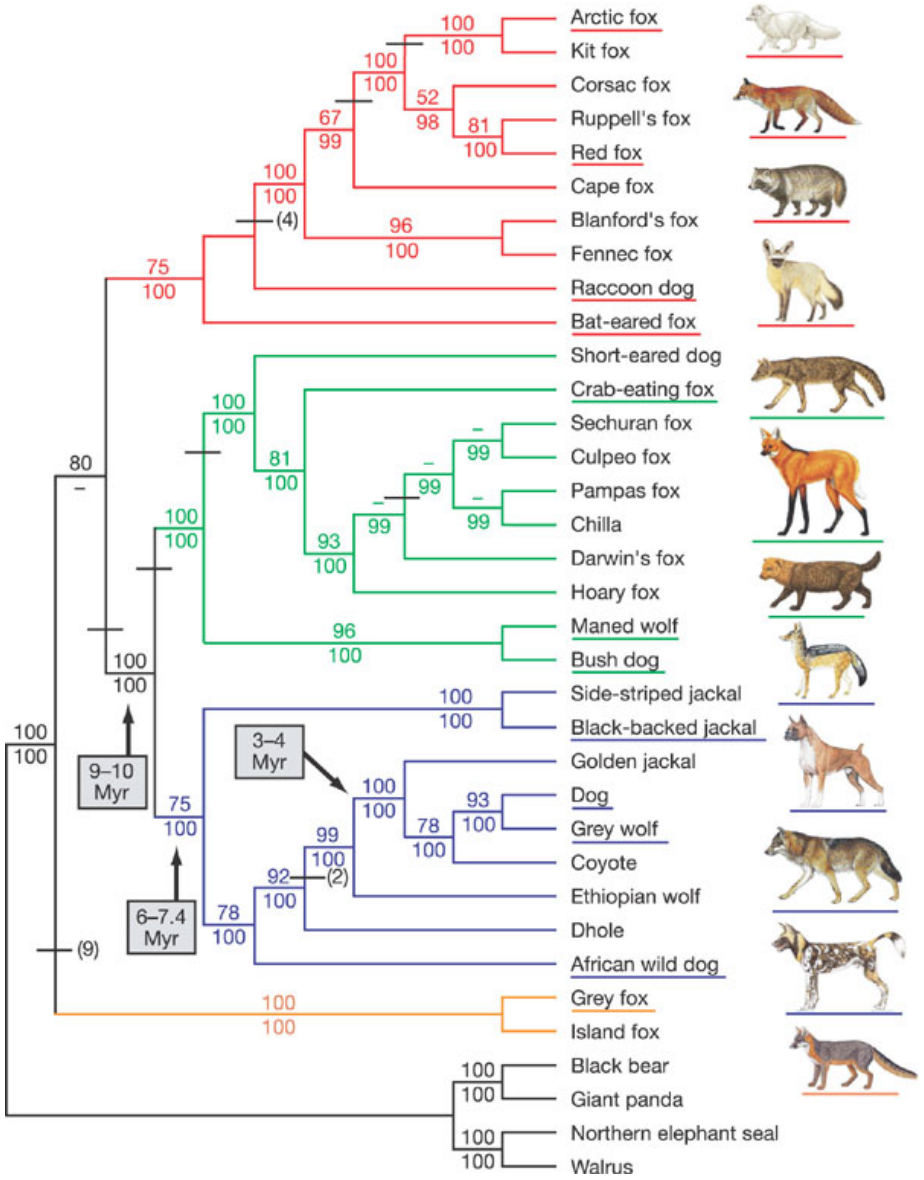


[Image from dhushara.com]

Clustering examples

Clustering species

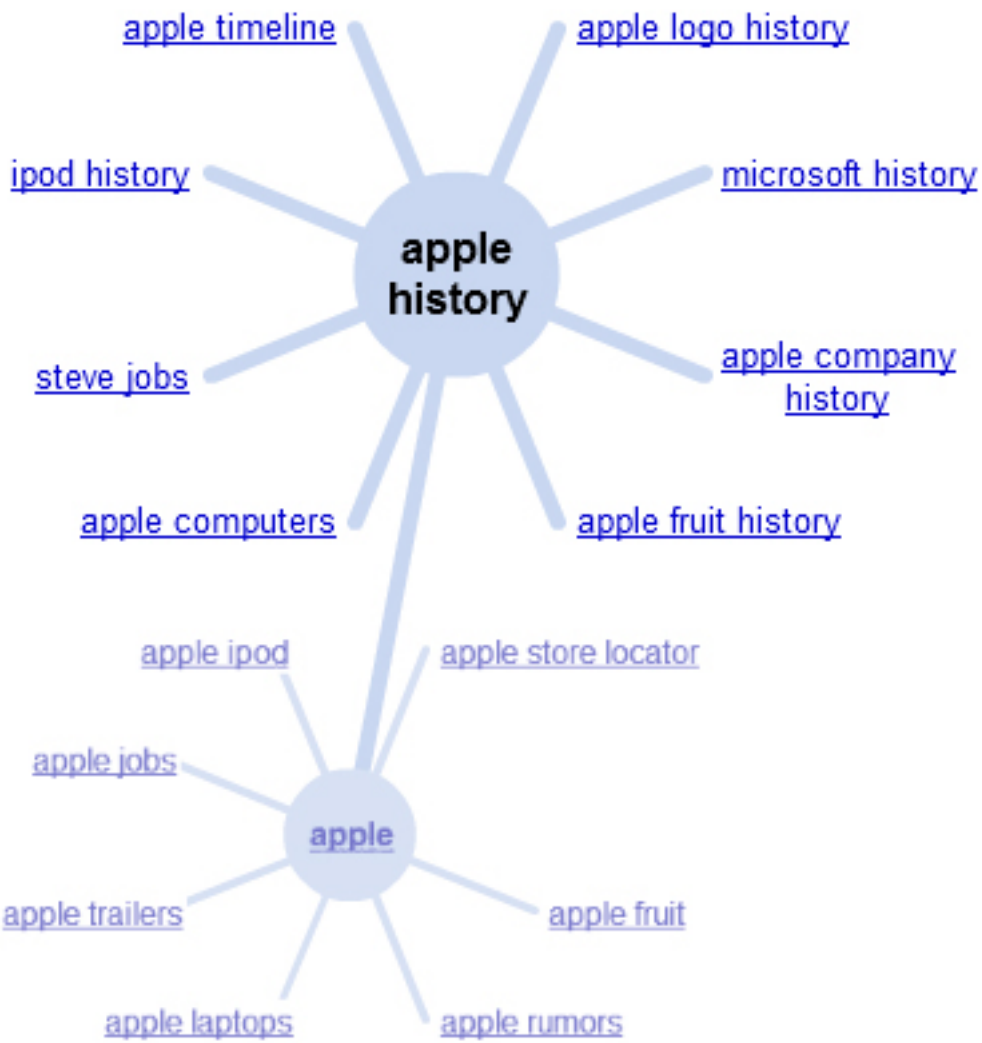
(“phylogeny”)



[Lindblad-Toh et al., Nature 2005]

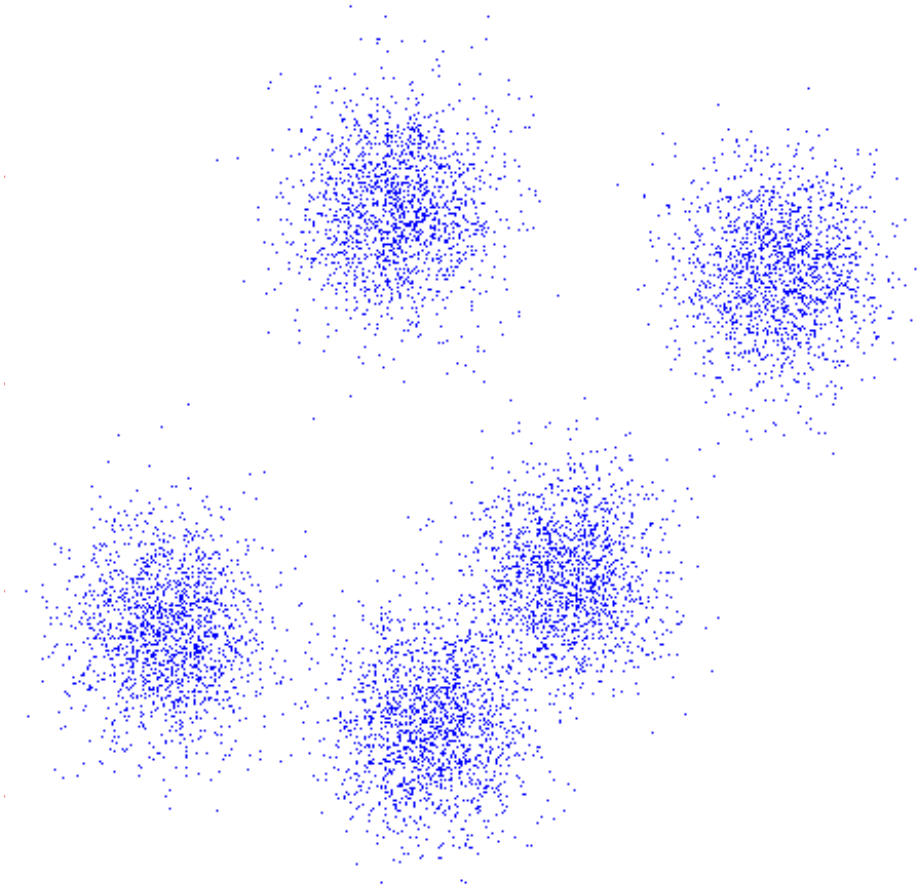
Clustering examples

Clustering search queries



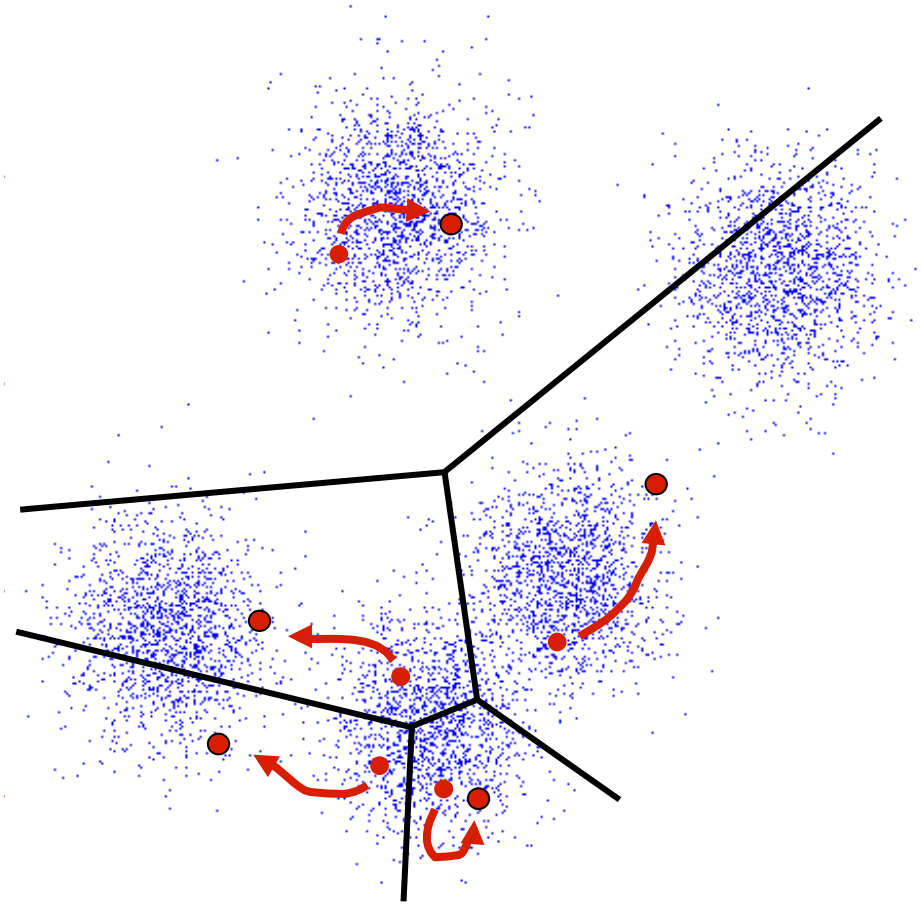
K-Means

- An iterative clustering algorithm
  - Initialize: Pick *K* random points as cluster centers
  - Alternate:
    1. Assign data points to closest cluster center
    2. Change the cluster center to the average of its assigned points
  - Stop when no points' assignments change

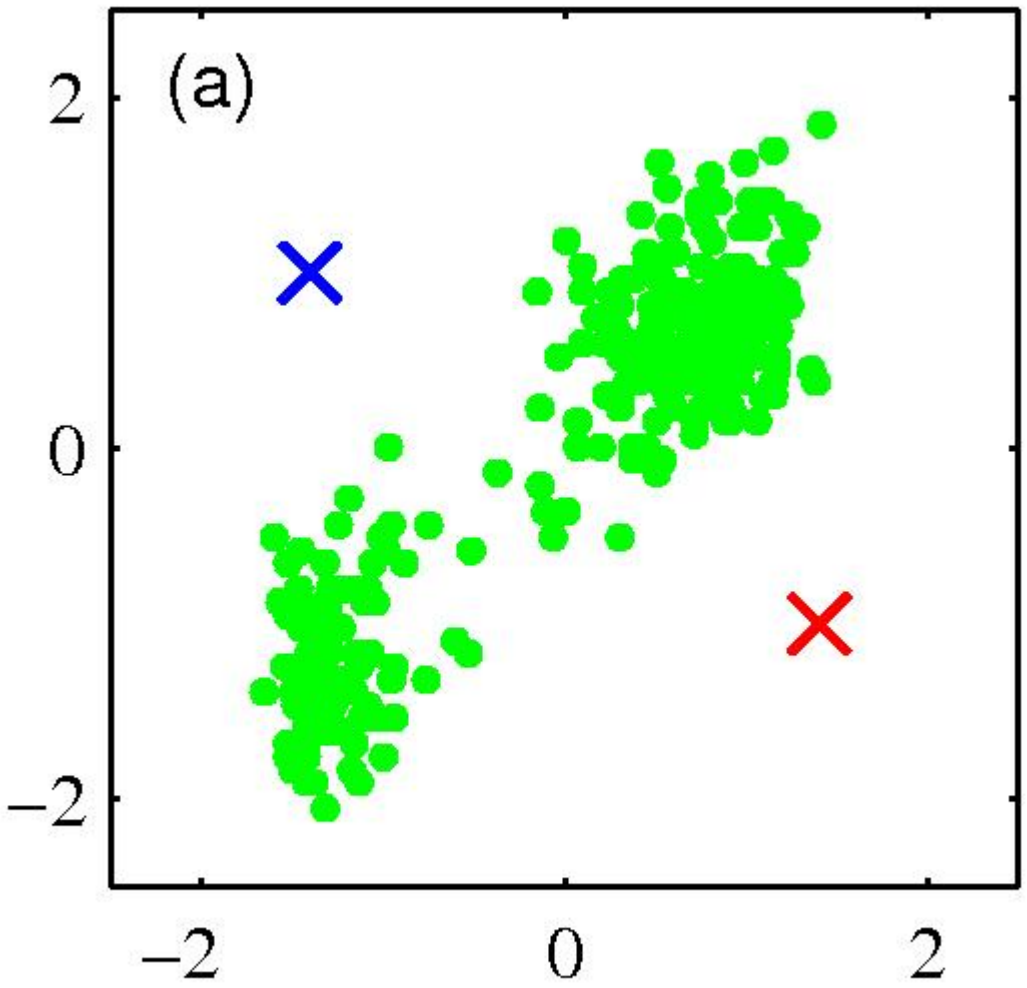


K-Means

- An iterative clustering algorithm
  - Initialize: Pick *K* random points as cluster centers
  - Alternate:
    1. Assign data points to closest cluster center
    2. Change the cluster center to the average of its assigned points
  - Stop when no points' assignments change



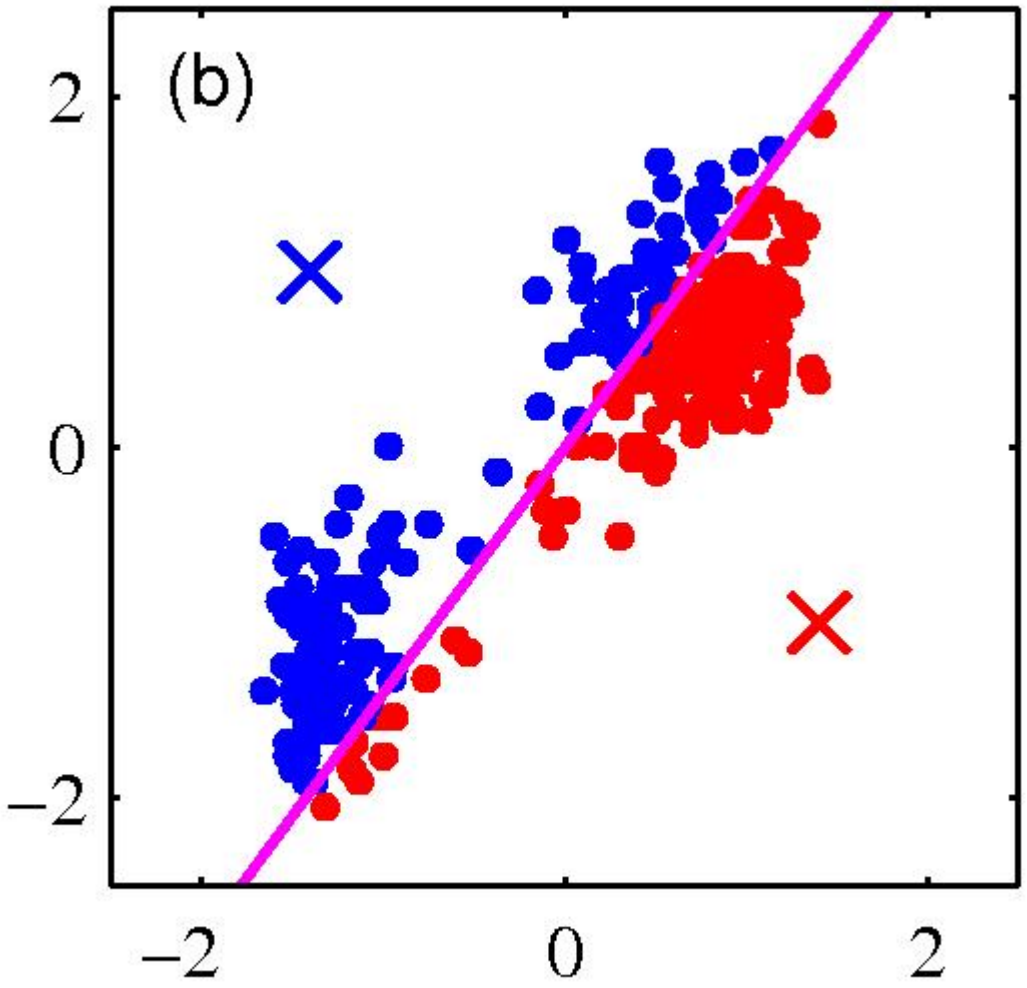
K-means clustering: Example



- Pick *K* random points as cluster centers (means)

Shown here for *K*=2

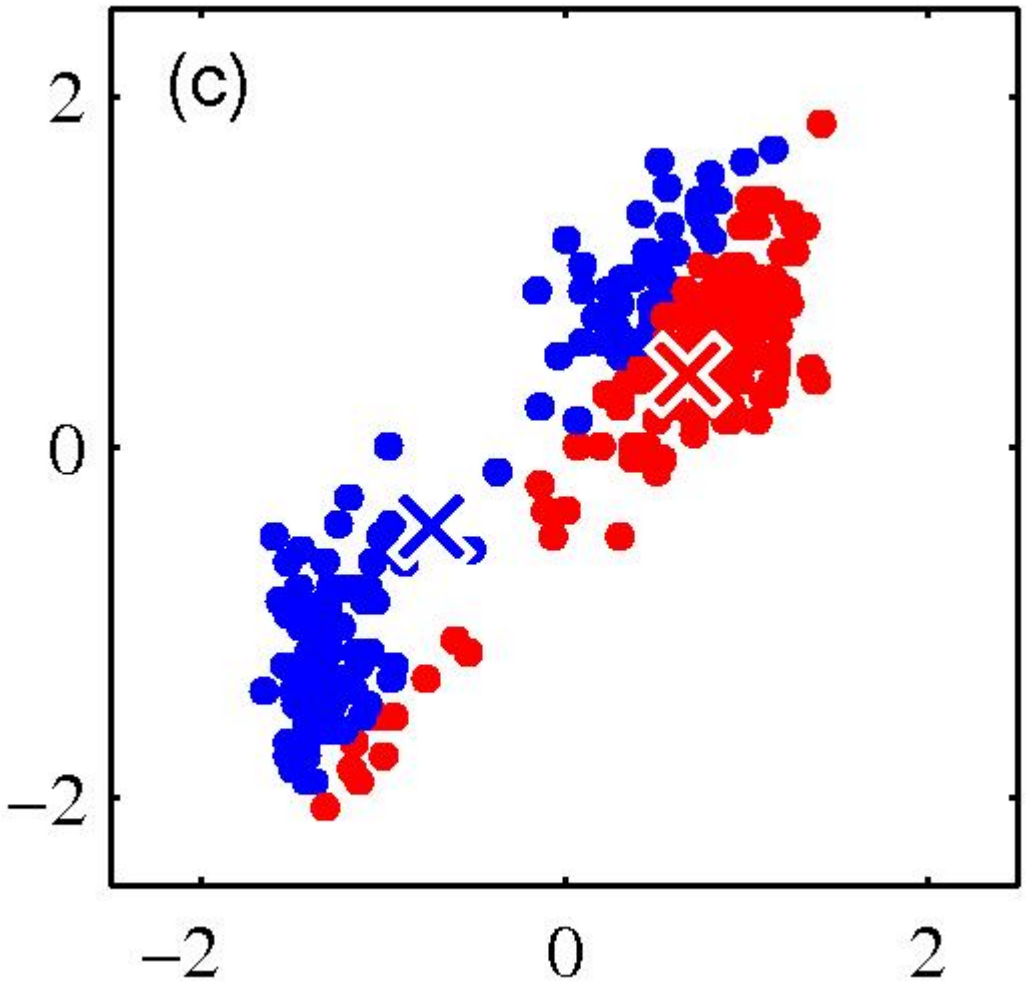
K-means clustering: Example



Iterative Step 1

- Assign data points to closest cluster center

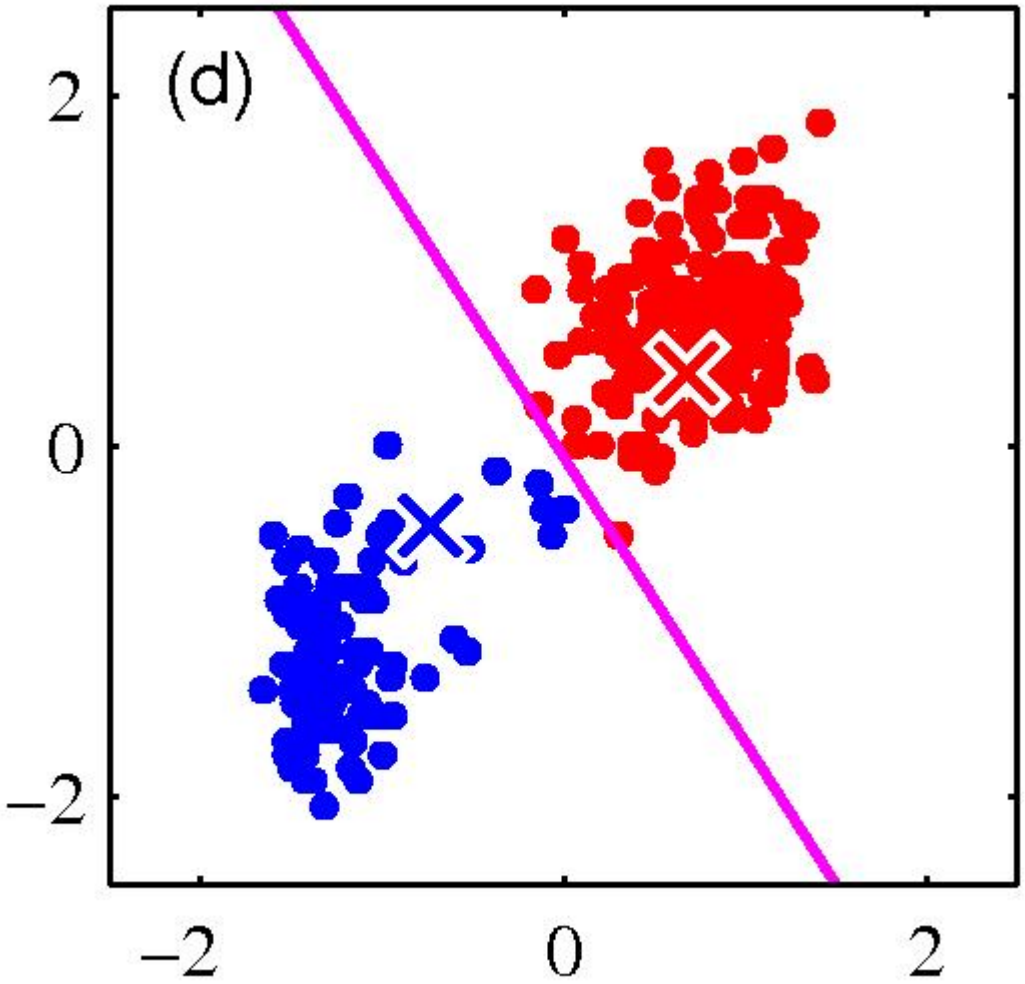
K-means clustering: Example



Iterative Step 2

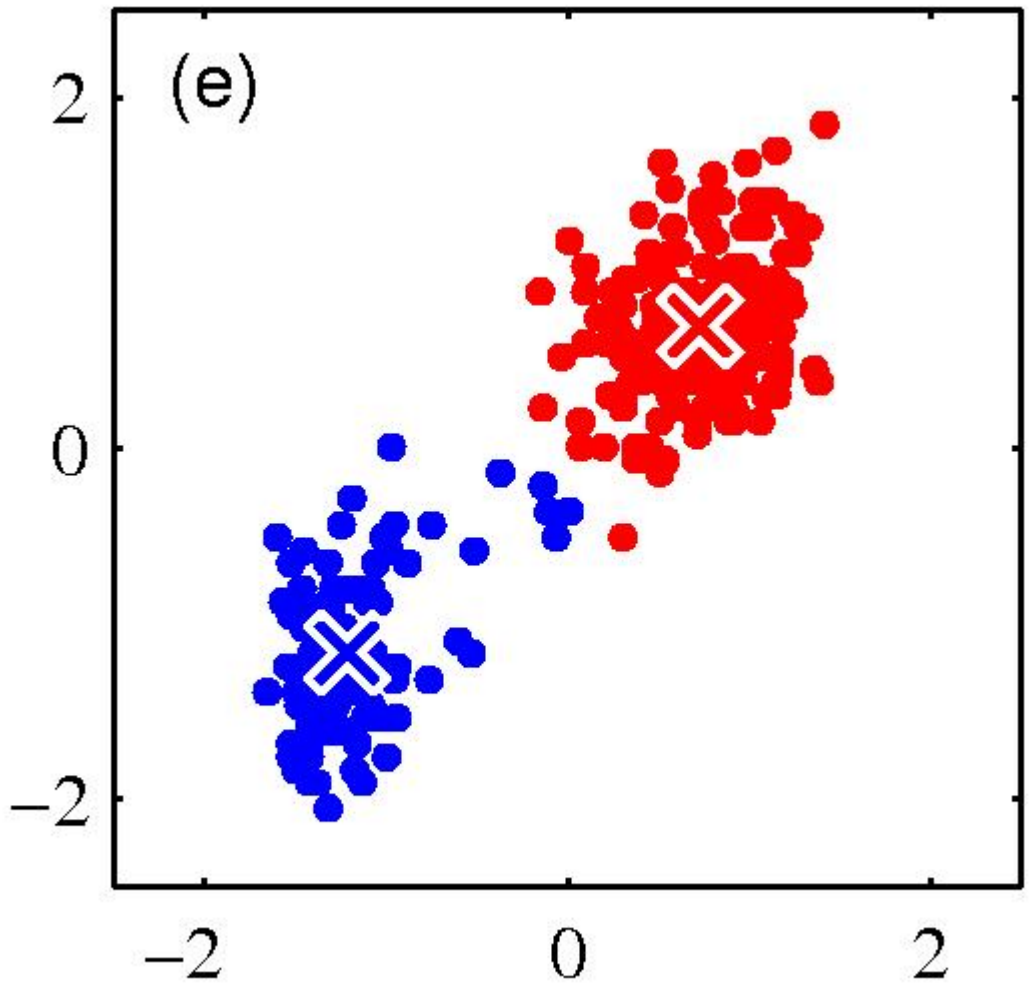
- Change the cluster center to the average of the assigned points

K-means clustering: Example

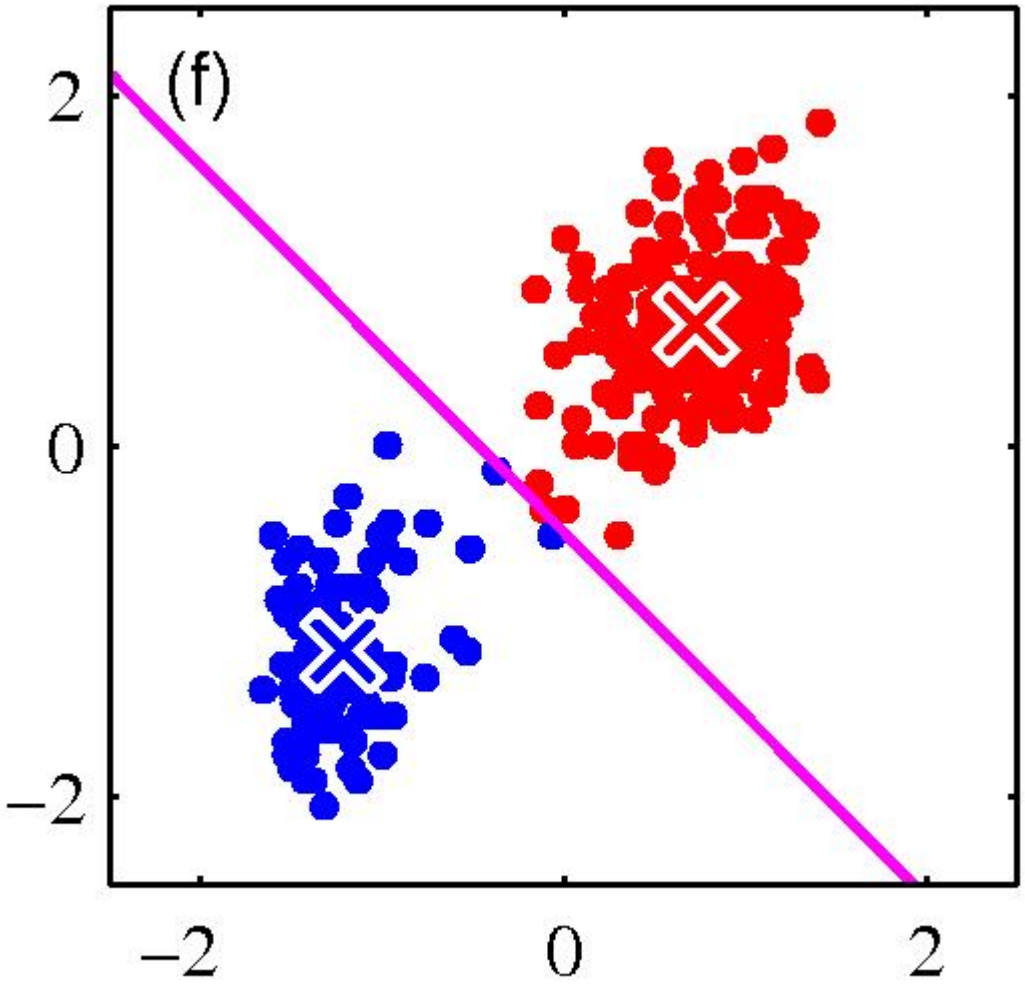


- Repeat until convergence

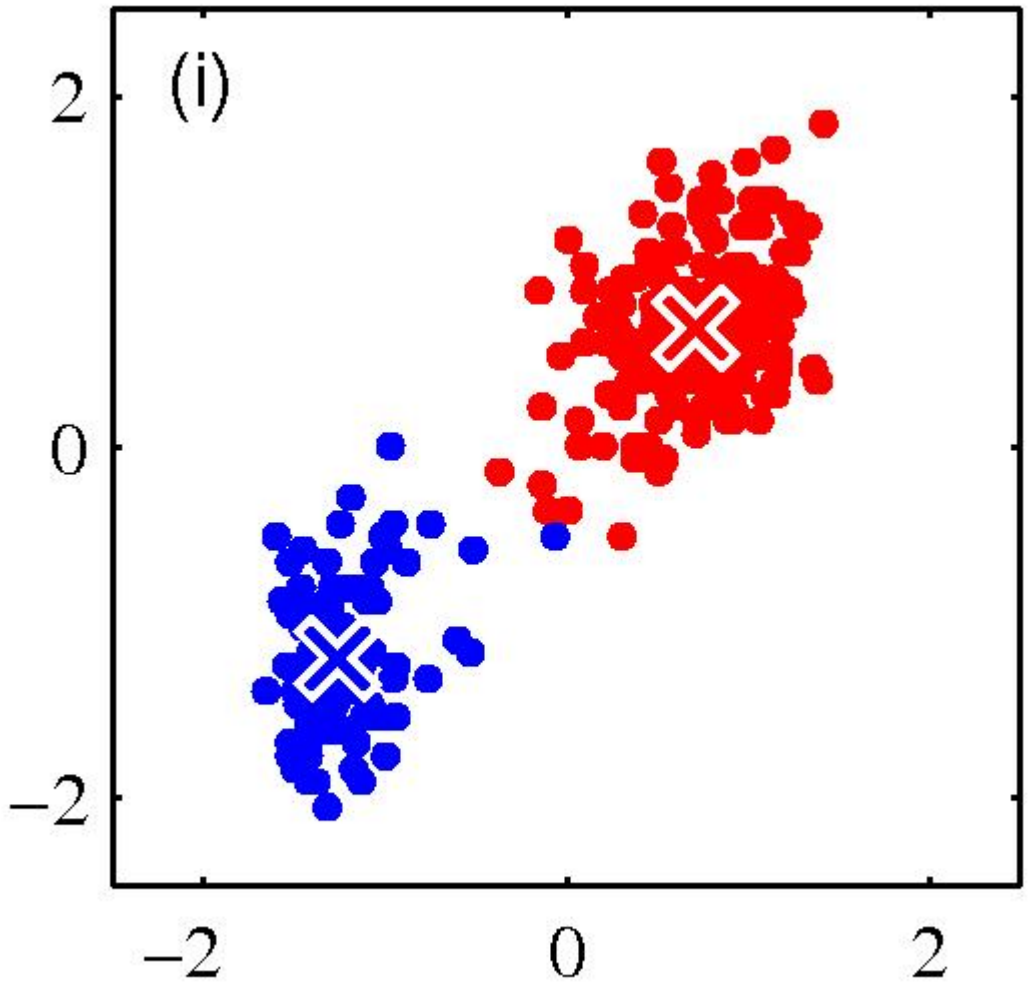
K-means clustering: Example



K-means clustering: Example



K-means clustering: Example



Properties of K-means **algorithm**

- Guaranteed to converge in a finite number of iterations

- Running time per iteration:
    1. Assign data points to closest cluster center

       O(KN) time

    2. Change the cluster center to the average of its assigned points

       O(N)

Kmeans Convergence

Objective

$$\min_{\mu}\min_{C}\sum_{i=1}^{k}\sum_{x\in C_i}|x-\mu_i|^2$$

1. Fix μ, optimize *C:*

Step 1 of kmeans

$$\min_{C}\sum_{i=1}^{k}\sum_{x\in C_i}|x-\mu_i|^2=\min_{c}\sum_{i}^{n}\left|x_i-\mu_{x_i}\right|^2$$

2. Fix *C,* optimize μ:

$$\min_{\mu}\sum_{i=1}^{k}\sum_{x\in C_i}|x-\mu_i|^2$$

   – Take partial derivative of μ_i and set to zero, we have

$$\mu_i=\frac{1}{|C_i|}\sum_{x\in C_i}x$$

Step 2 of kmeans

Kmeans takes an alternating optimization approach, each step is guaranteed to decrease the objective – thus guaranteed to converge

[Slide from Alan Fern]

Example: K-Means for Segmentation

K=2

Goal of Segmentation is to partition an image into regions each of which has reasonably homogenous visual appearance.

Original

Example: K-Means for Segmentation

K=2

K=3

Original

Example: K-Means for Segmentation

K=2

K=3

K=10

Original

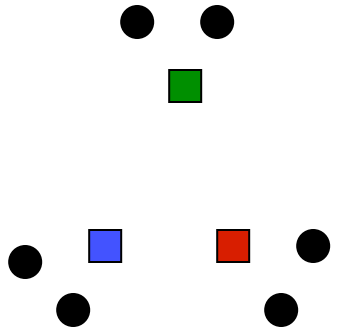
Example: Vector quantization

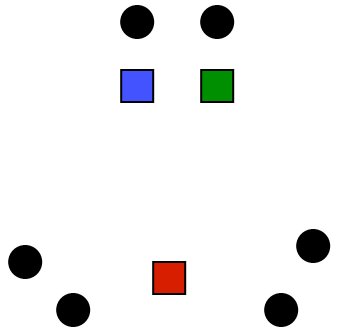
FIGURE 14.9. *Sir Ronald A. Fisher* $(1890 - 1962)$ *was one of the founders of modern day statistics, to whom we owe maximum-likelihood, sufficiency, and many other fundamental concepts. The image on the left is a* 1024×1024 *grayscale image at* 8 *bits per pixel. The center image is the result of* 2×2 *block VQ, using* 200 *code vectors, with a compression rate of* 1.9 *bits/pixel. The right image uses only four code vectors, with a compression rate of* 0.50 *bits/pixel*

[Figure from Hastie *et al.* book]

Initialization

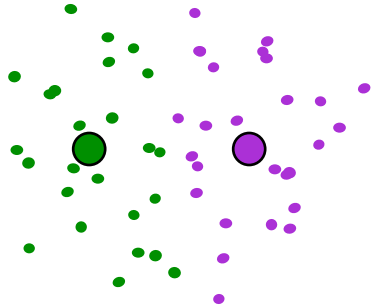
- K-means **algorithm** is a heuristic
  - Requires initial means
  - It does matter what you pick!
  - What can go wrong?
  - Various schemes for preventing this kind of thing: variance-based split / merge, initialization heuristics



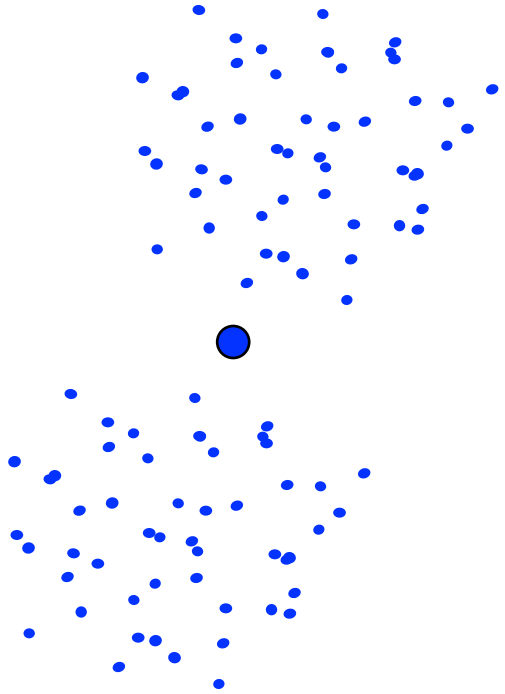


K-Means Getting Stuck

A local optimum:

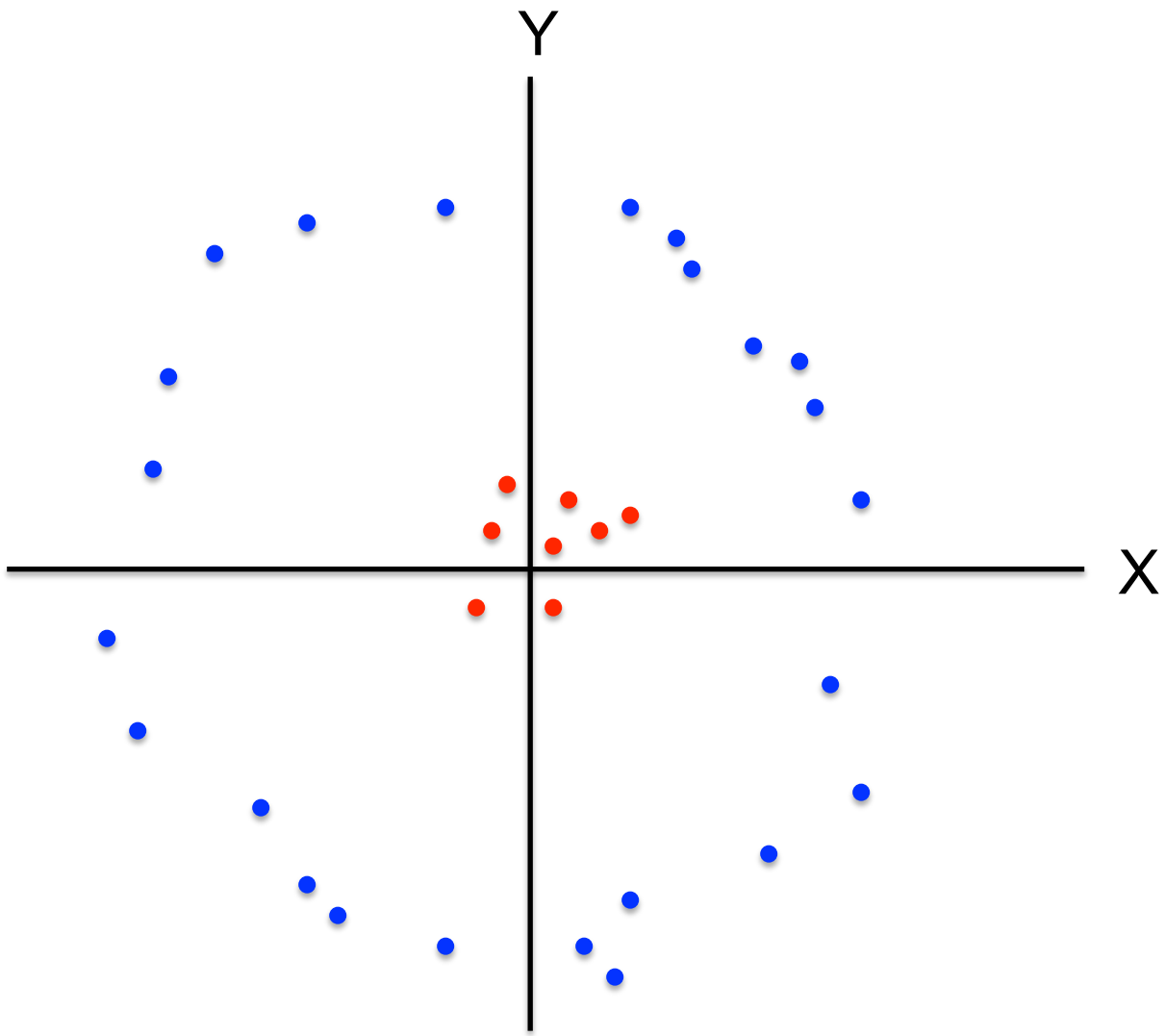


Would be better to have
one cluster here



… and two clusters here

K-means not able to properly cluster



Changing the features (distance function) can help