Clustering

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WiDS Austin, Jan 23, 2017

Slides adapted from David Blei, David Sontag, Piyush Rai, Jure Leskove, Anand Rajaraman, Shimon Ullman and Elena Marchiori

What is clustering?

- Given a set of data points, group them into clusters so that:
  - points within each cluster are similar to each other
  - points from different clusters are dissimilar

- Requires data, but no labels

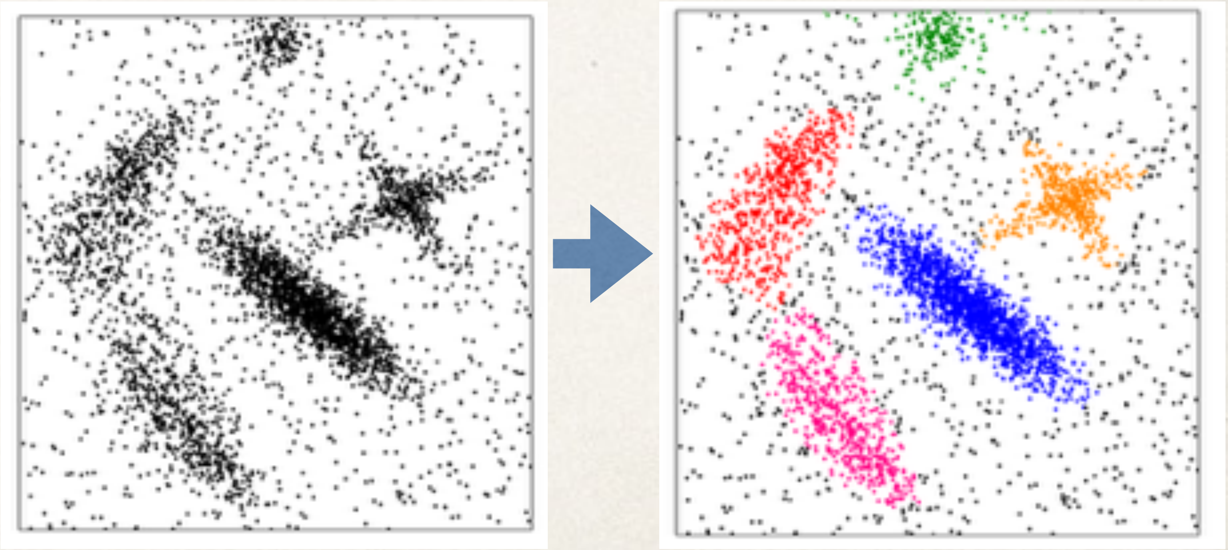

Image credit: http://people.sissa.it/~laio/Research/Res_clustering.php

Why would we want to do this?

- Group customers according to purchase histories
- Group search results according to topics
- Detect regions of images
- Clustering gene expression data

K=2	K=3	K=10	Original

4%	8%	17%	

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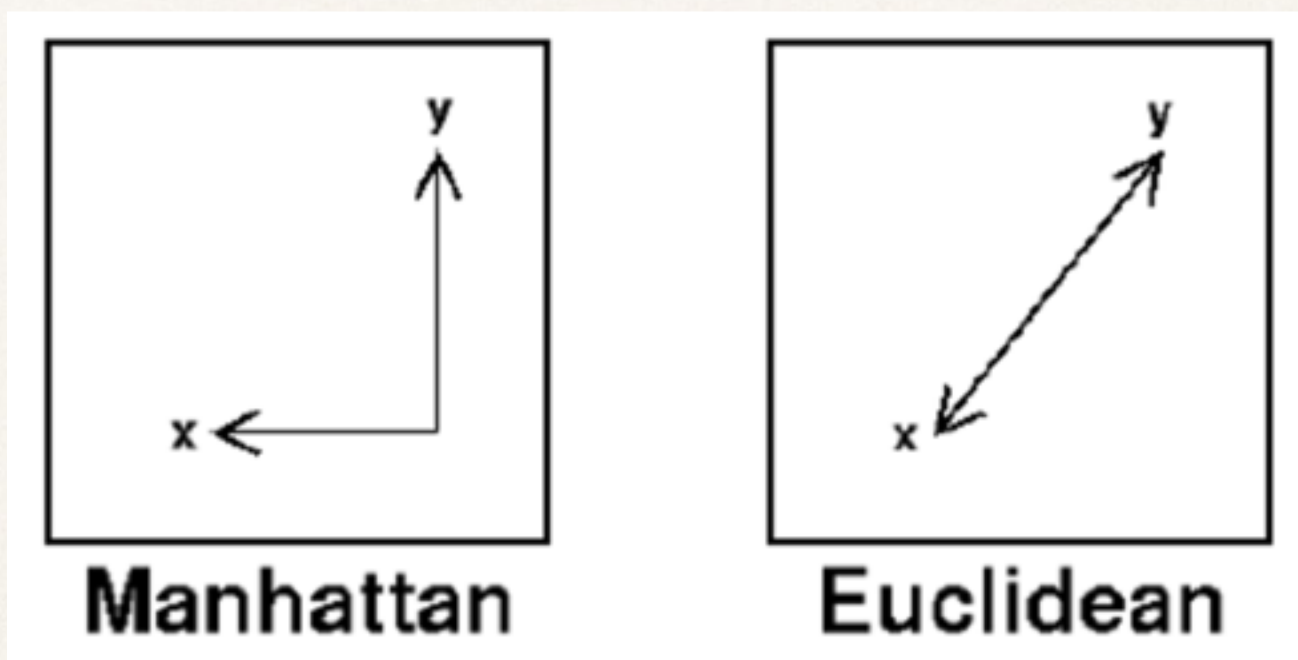
- It depends on how we define the distance/similarity
- Euclidean distance, Manhattan (L1) distance



$$\sum_{i=1} |a_i - b_i|.$$

$$\sqrt{\sum_{i=1}^{d} (a_i - b_i)^2}.$$

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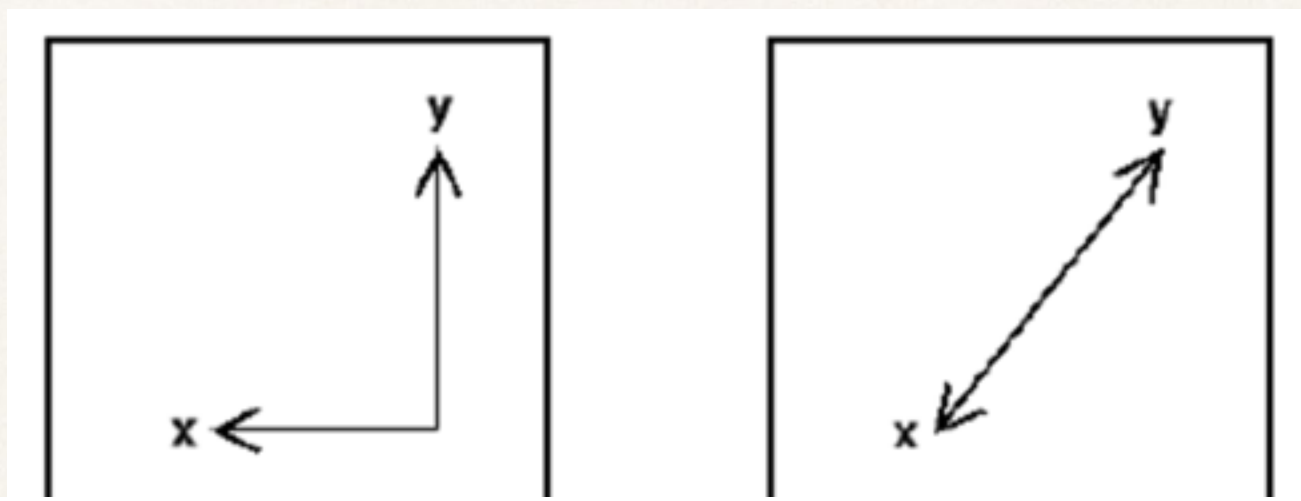

They are special cases of **Minkowski distance:**

$$d_p(\mathbf{x}_i, \mathbf{x}_j) = \left(\sum_{k=1}^{m} \left| x_{ik} - x_{jk} \right|^p \right)^{\frac{1}{p}}$$

- Jaccard distance

$$\mathbf{d}_J(A,B) = 1 - \mathsf{JS}(A,B) = 1 - \frac{|A \cap B|}{|A \cup B|}.$$

- Cosine distance

$$\mathbf{d}_{\cos}(a,b) = 1 - \frac{\langle a, b \rangle}{\|a\| \, \|b\|} = 1 - \frac{\sum_{i=1}^{d} a_i b_i}{\|a\| \, \|b\|}$$

How do we do it?

- Partition algorithms: determine all clusters at once.
- Hierarchical algorithms (agglomerative): find successive clusters using previously established clusters.
  - Do not need the number of clusters as an input, and can be viewed at different levels of granularities with different k

K-means

- A partition algorithm
- Basic idea: to describe each cluster by its mean value
- Goal: find the assignment of k clusters that minimizes the sum of square distance of cluster members to their cluster centers.

1. Initialization
   - Data are $\mathbf{x}_{1:N}$
   - Choose initial cluster means $\mathbf{m}_{1:k}$ (same dimension as data).

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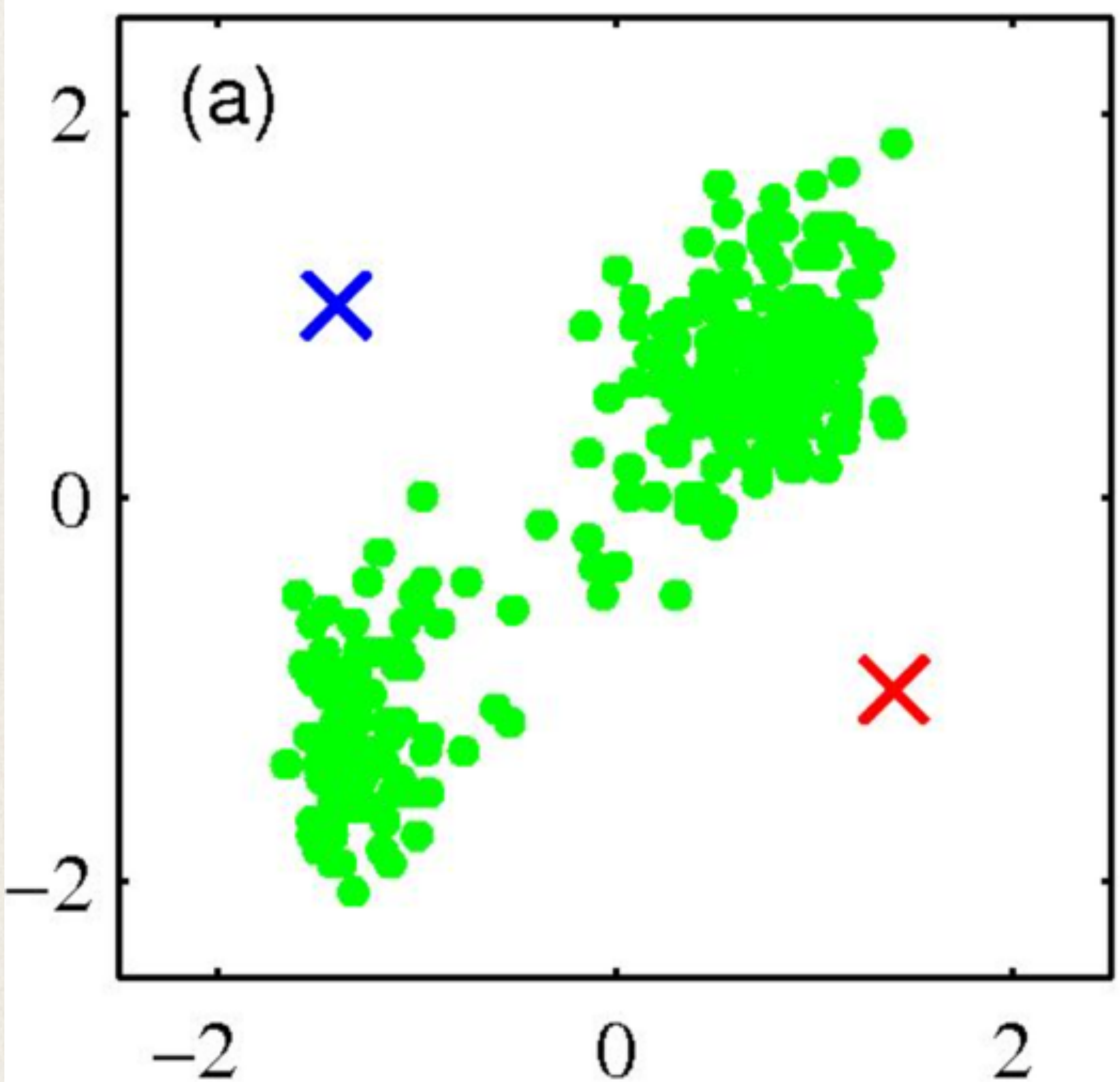
3. Until assignments $\mathbf{z}_{1:N}$ do not change

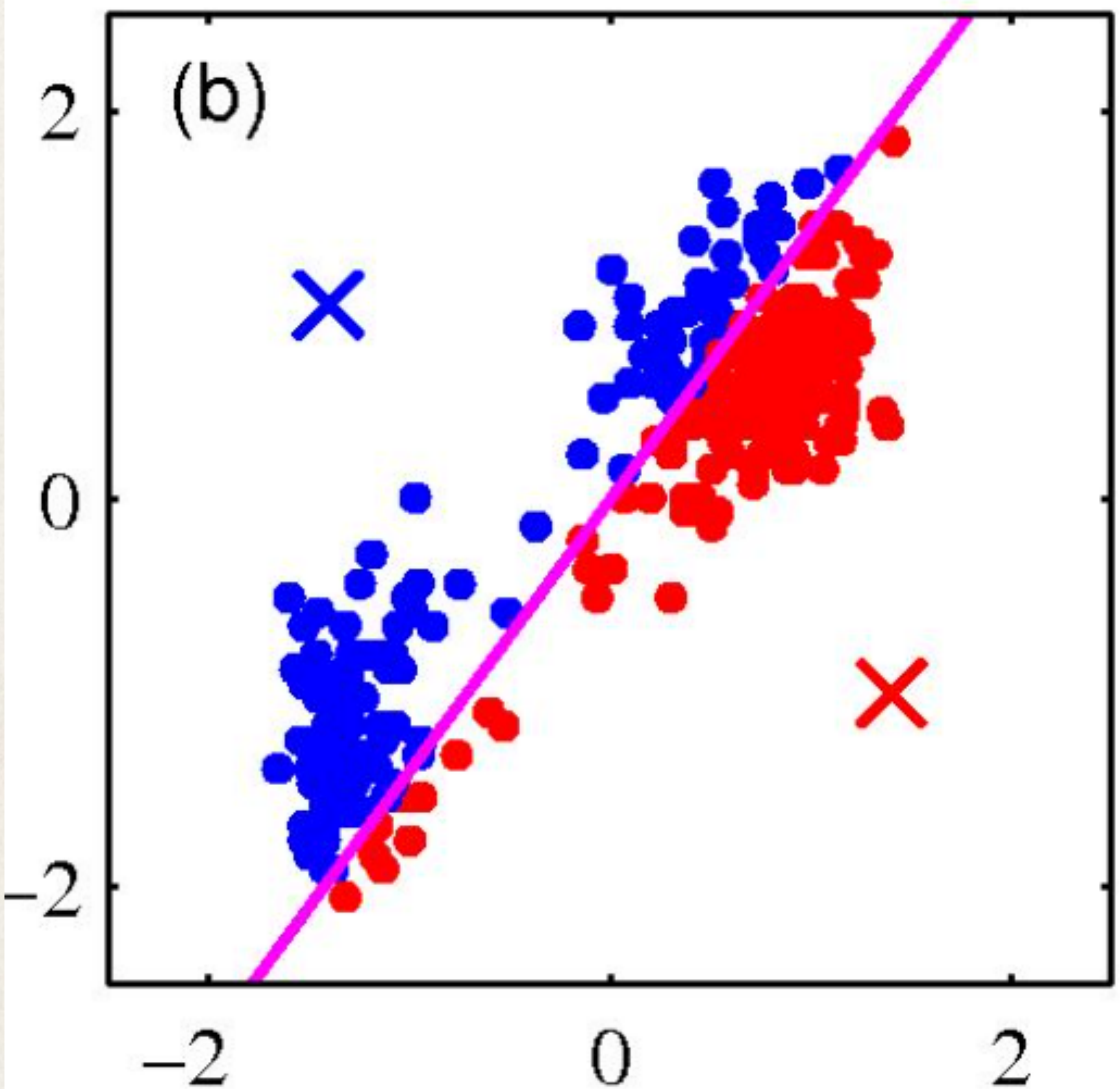
K-means — an example



- Pick K random points as cluster centers (means)

Shown here for K=2

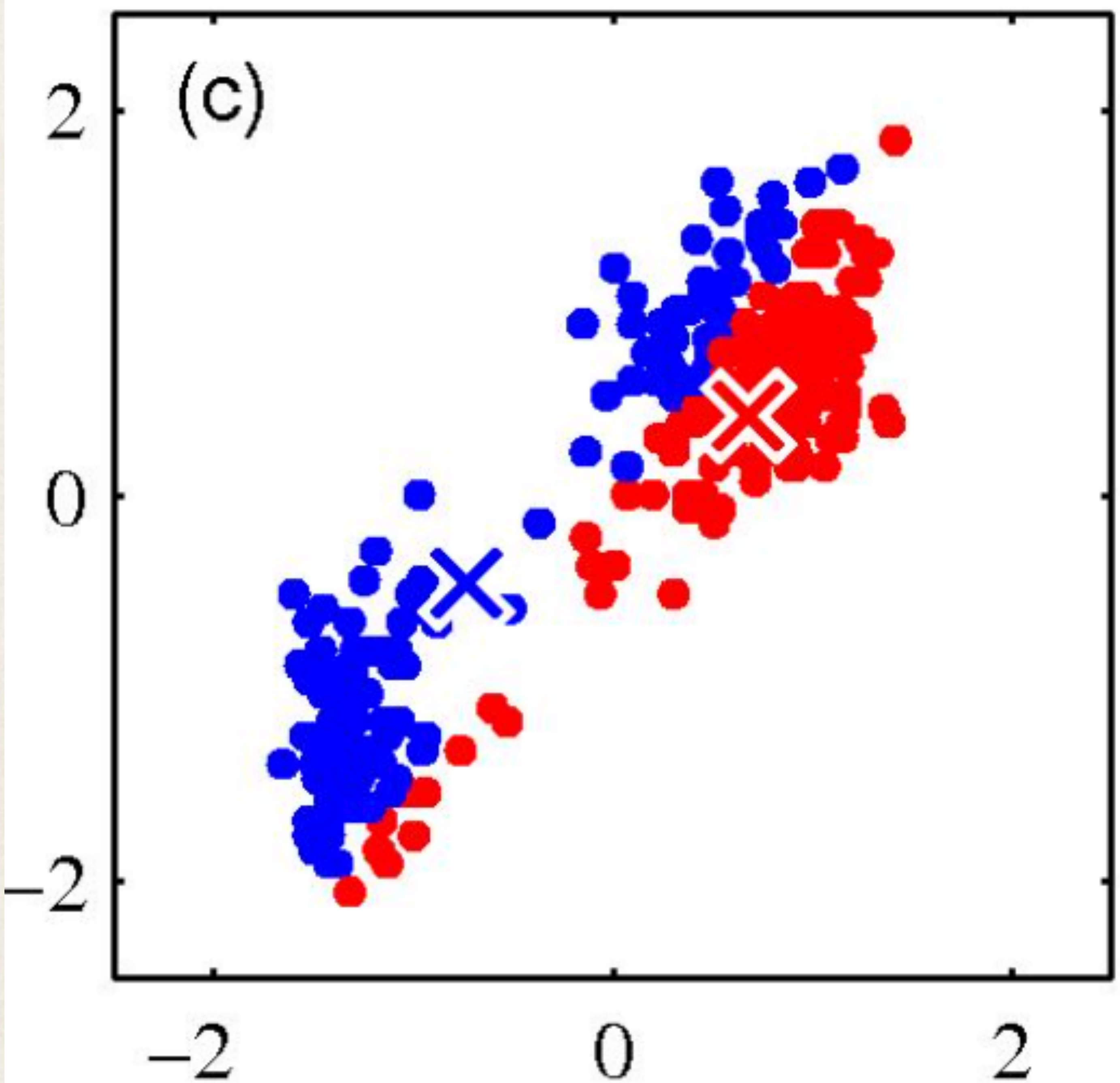
K-means — an example



Iterative Step 1

- Assign data points to closest cluster center

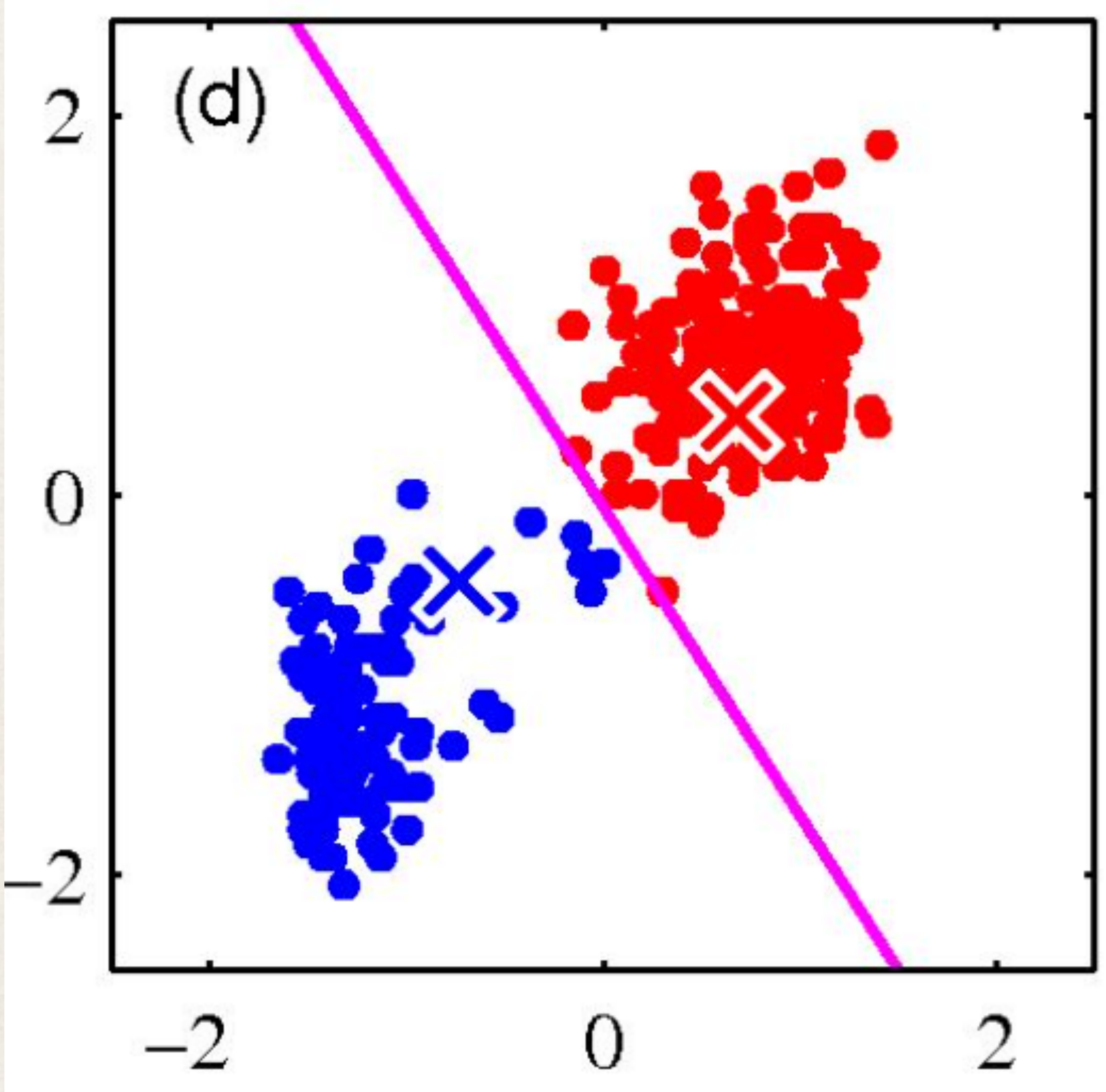
K-means — an example



Iterative Step 2

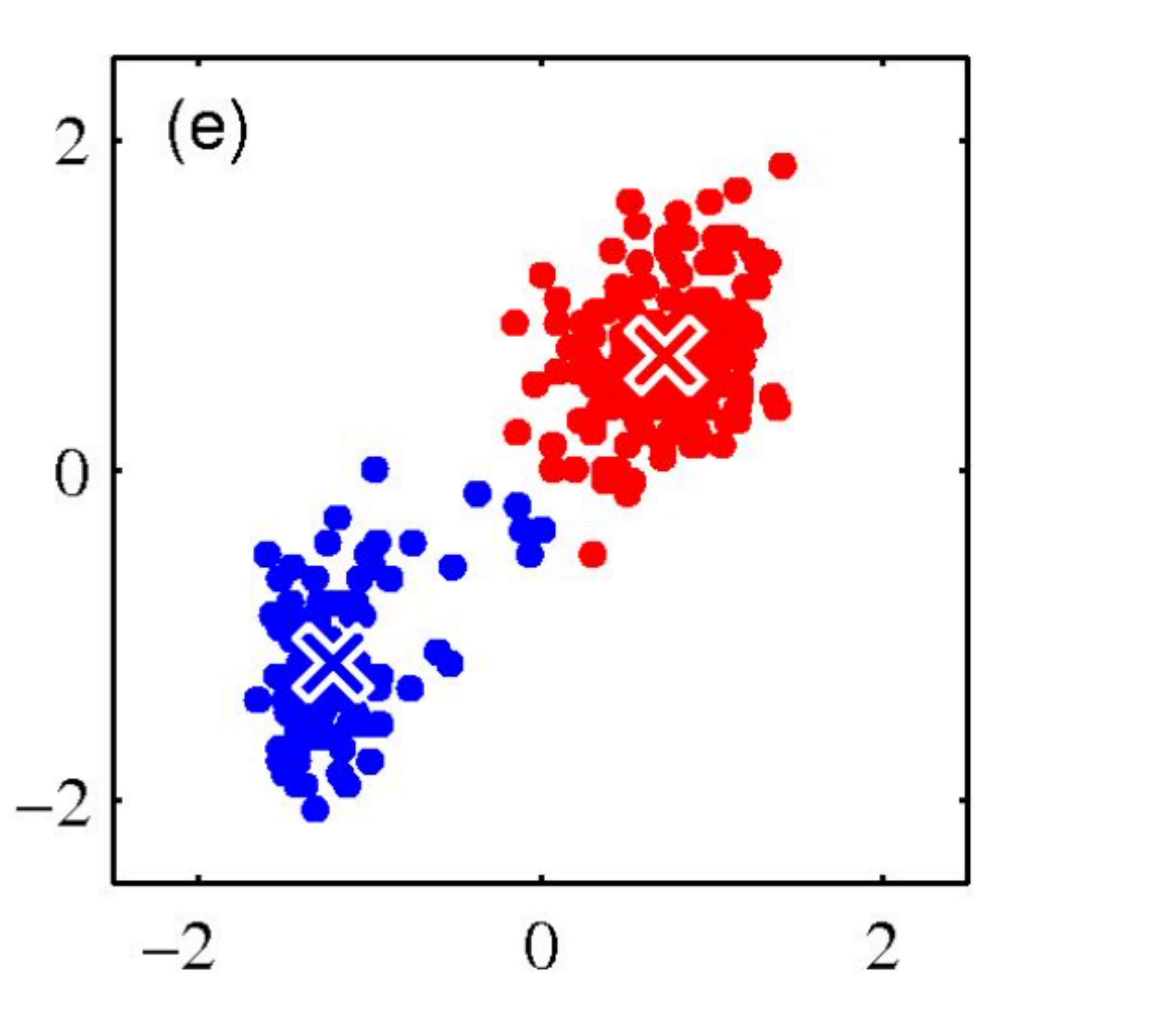
- Change the cluster center to the average of the assigned points

K-means — an example



- Repeat until convergence

K-means — an example



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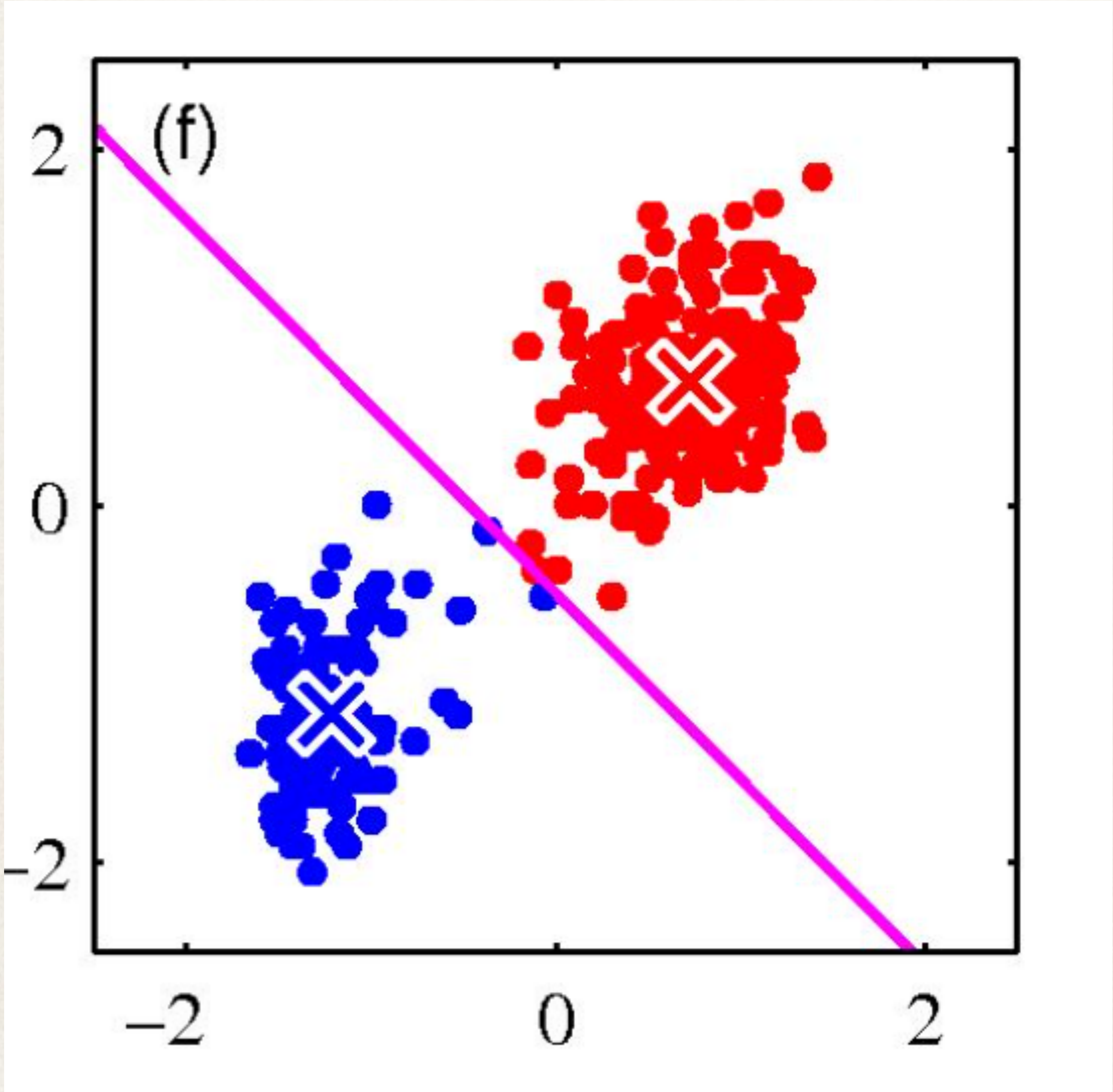

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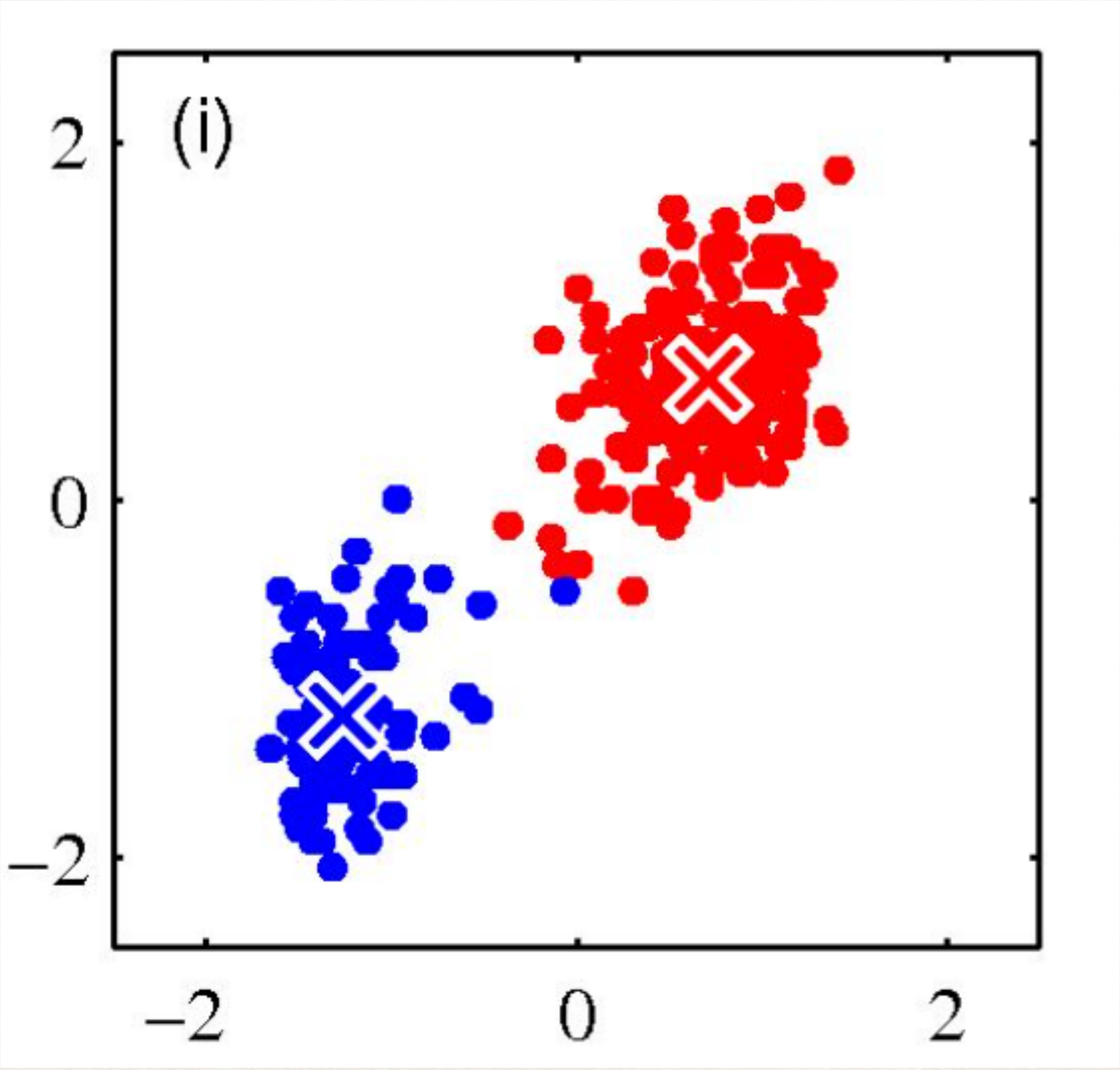


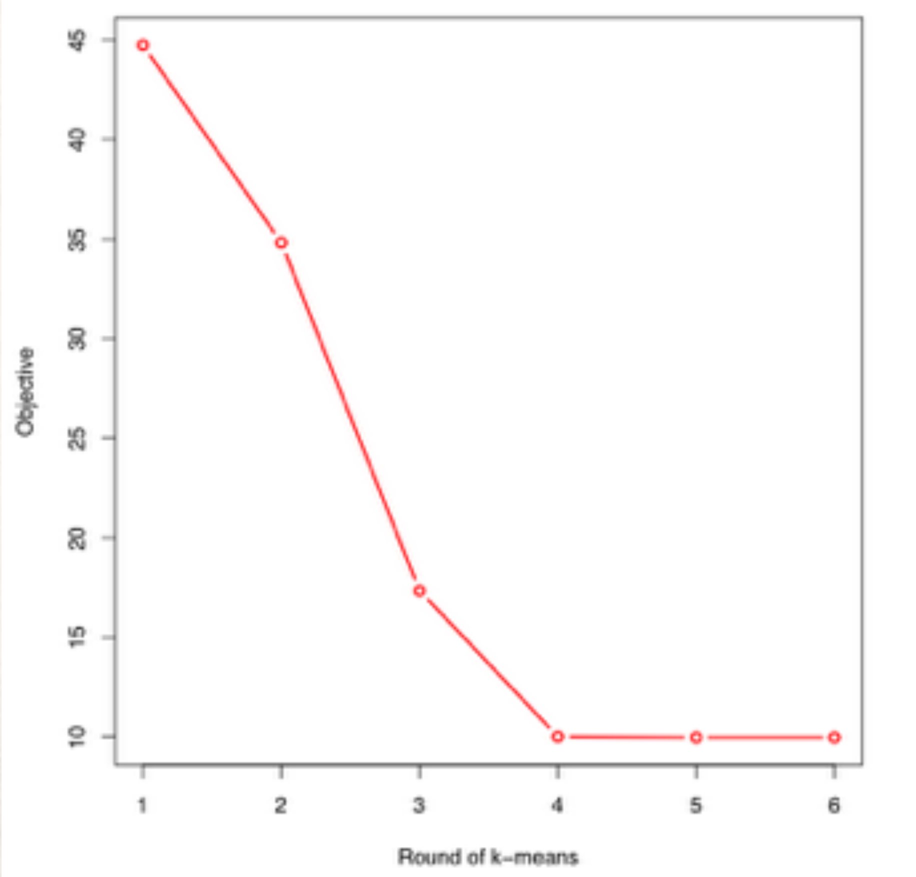
Coordinate descent

$$F(z_{1:N}, \mathbf{m}_{1:k}) = \frac{1}{2} \sum_{n=1}^{N} ||\mathbf{x}_n - \mathbf{m}_{z_n}||^2$$

- Holding the means fixed, assigning each point to its closest mean minimizes F with respect to $z_{1:N}$.
- Holding the assignments fixed, computing the centroids of each cluster minimizes F with respect to $\mathbf{m}_{1:k}$.

When to stop?

- No (or minimum) re-assignment of data points to different clusters, or
- no (or minimum) change of centroids, or
- minimum decrease in the sum of squared error

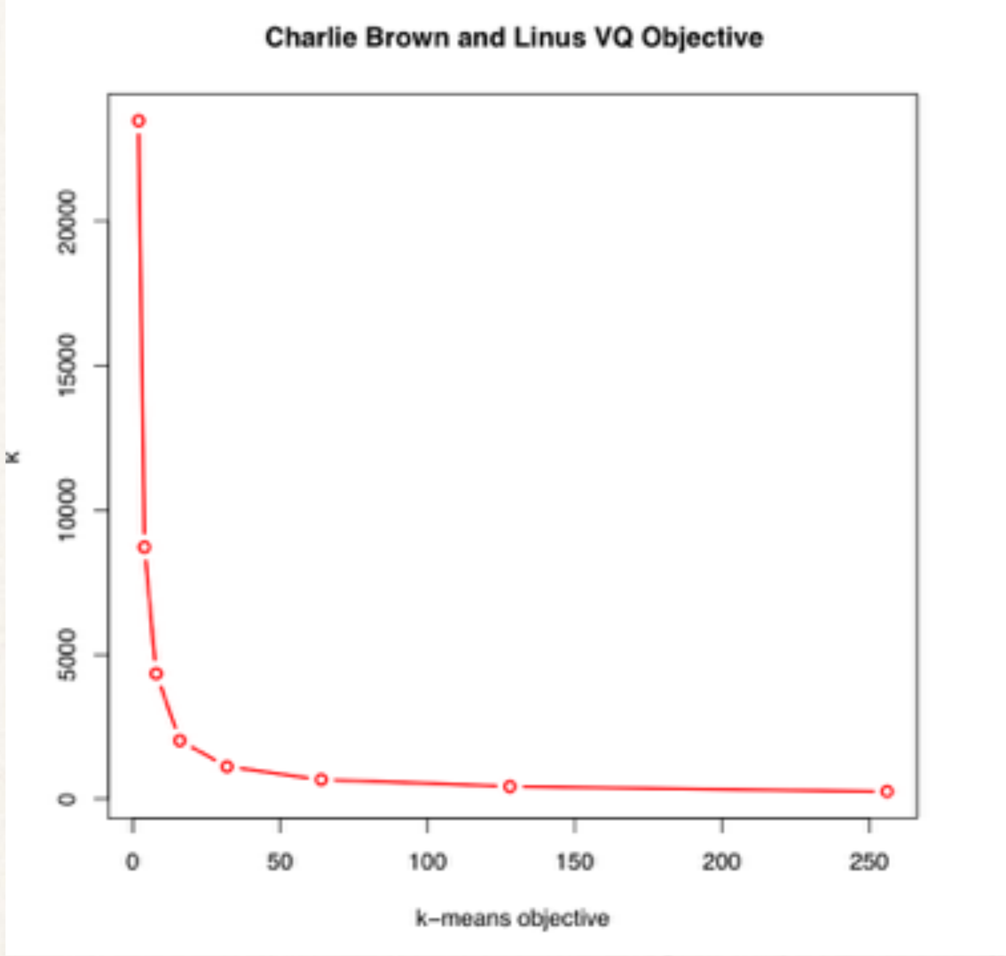


Knobs to turn:

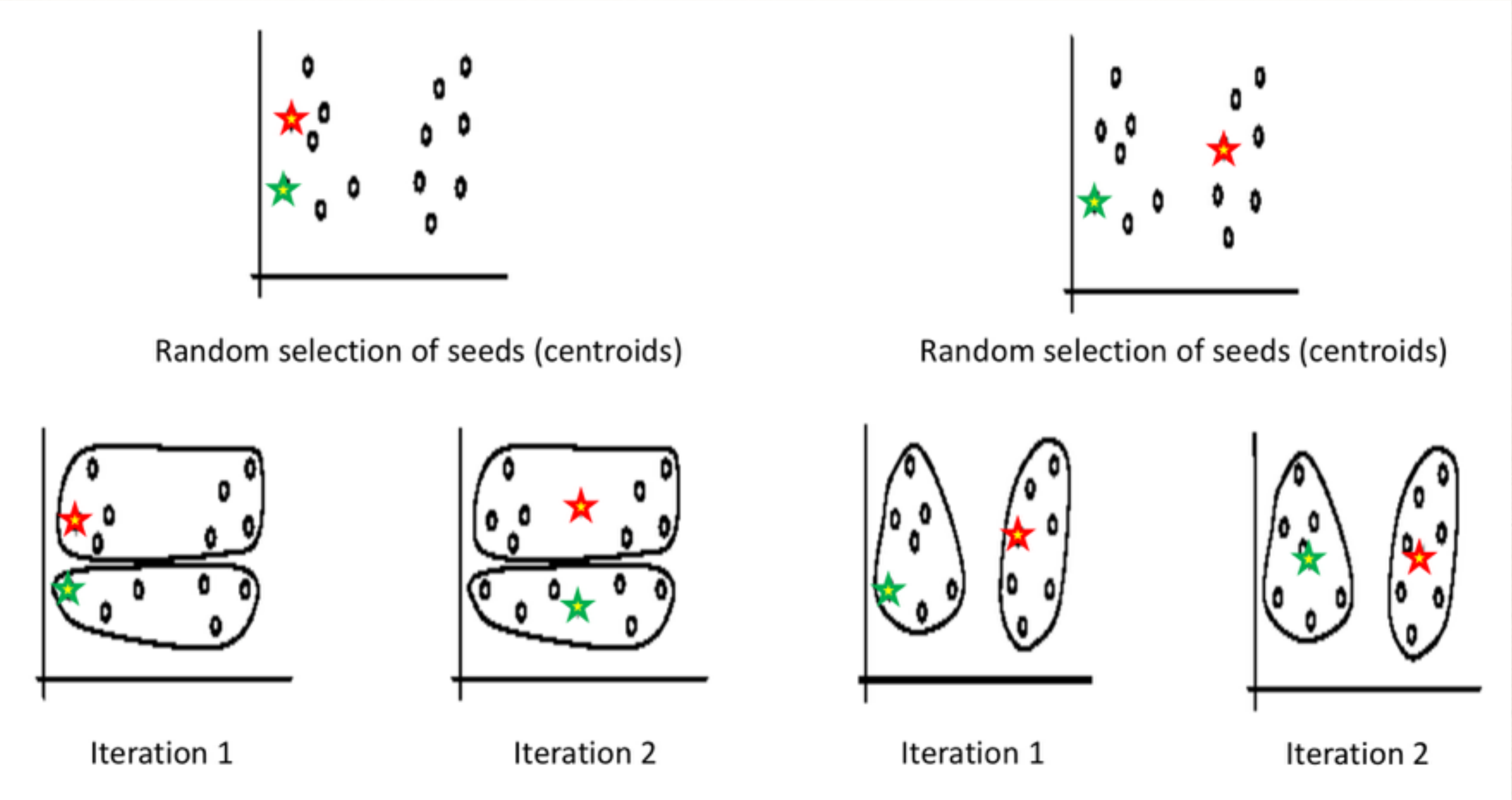
- a distance measure between data points
- number of clusters k
- initial assignment of data to clusters

How to choose K?

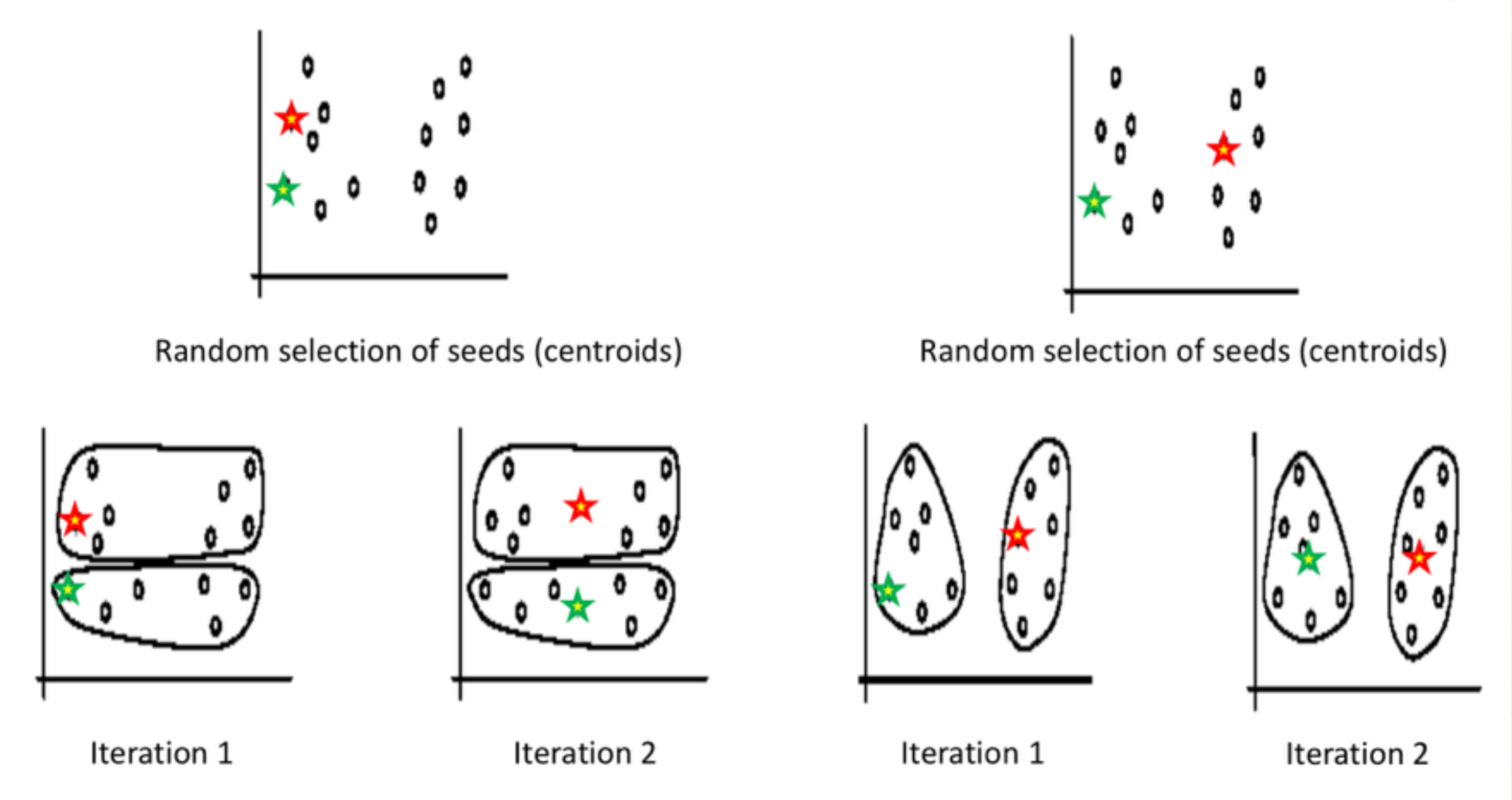
- Base on the required quality in the image compressing case
- Base on limits in real life applications
- Heuristic: a kink in the objective function



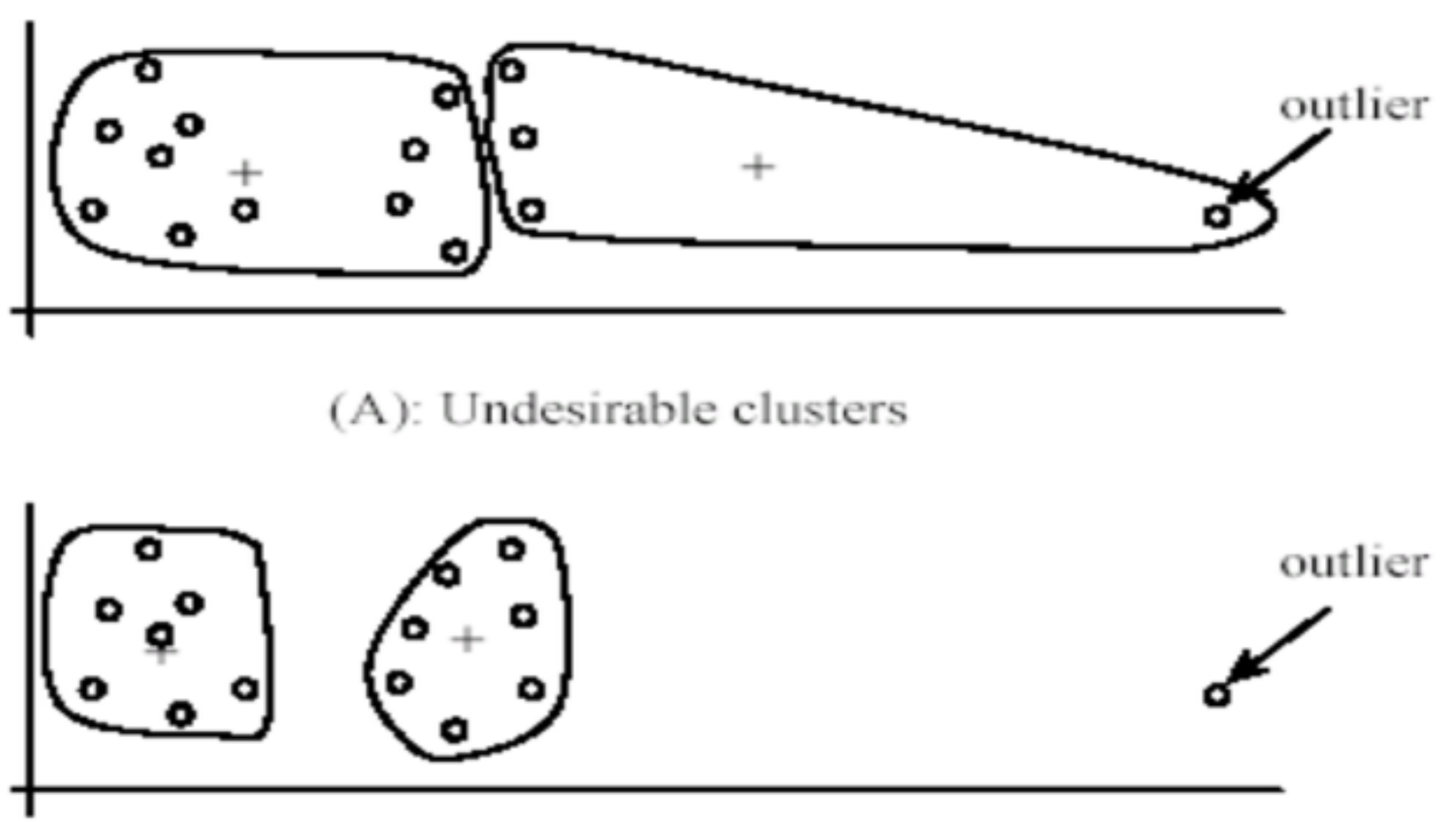
- K-mean algorithm finds the local minimum and is sensitive to initialization



- K-mean algorithm finds the local minimum and is sensitive to initialization
    - Try multiple initiations and choose the best result



- k-mean algorithm is sensitive to outliers

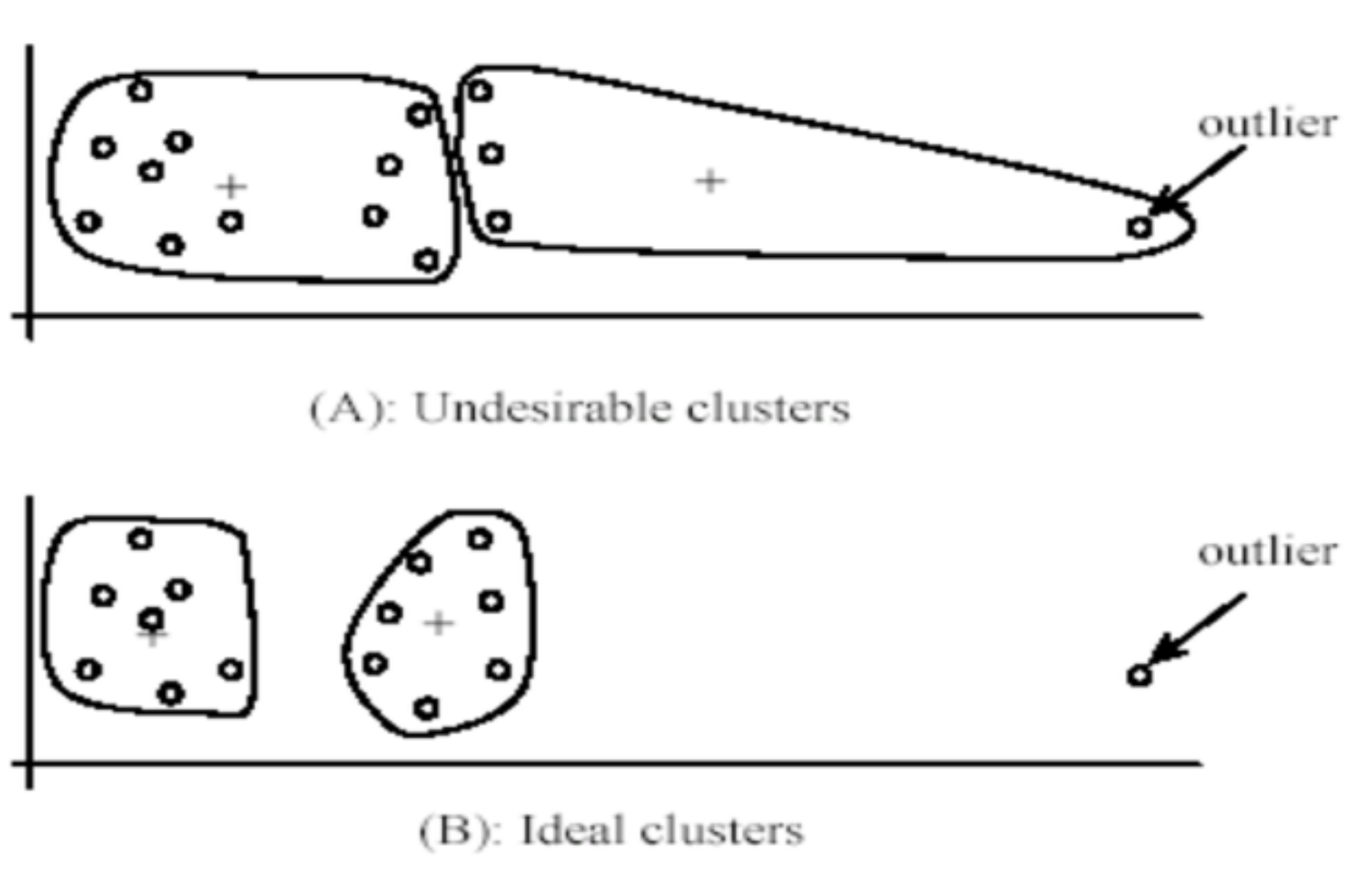


(A): Undesirable clusters

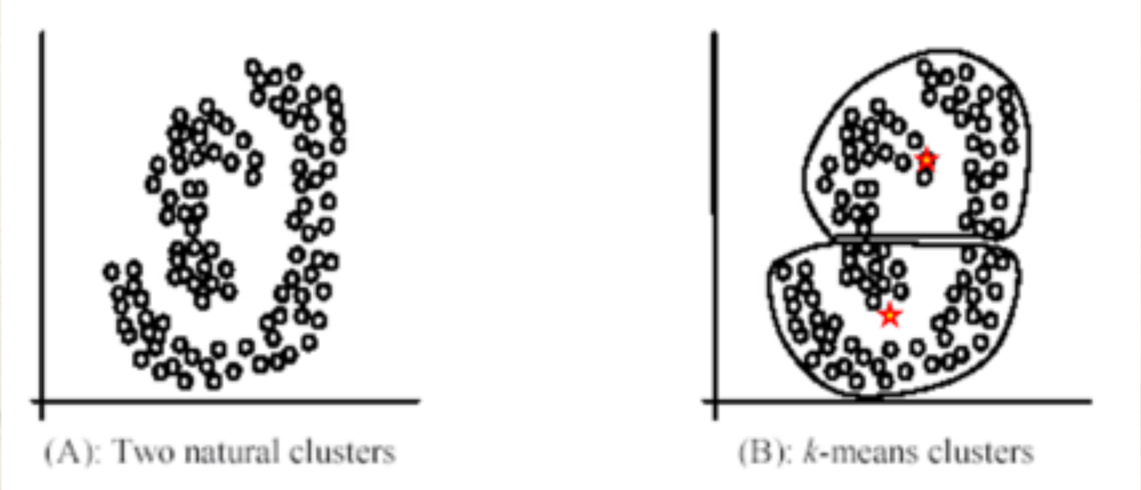
(B): Ideal clusters

- k-mean algorithm is sensitive to outliers

  - Remove outliers, resample, or use medians



- K-means is efficient to compute - O(tkn) (t is the number of iteration)
- K-means requires hard assignment - a point either belongs to a cluster or not. Other methods such as gaussian mixture models and fuzzy k-means allow one to assign a point to multiple clusters with certain probabilities
- K-means works well with round shaped clusters of roughly equal sizes and densities



Hierarchical clustering

- Basic idea: Initially, each point is a cluster by itself. Repeatedly combine the two "nearest" clusters into one.
- It only requires a measure of similarity between groups of data points
- It's up to the user to choose a "natural" clustering from the merging sequence

How to define “closest” for clusters?

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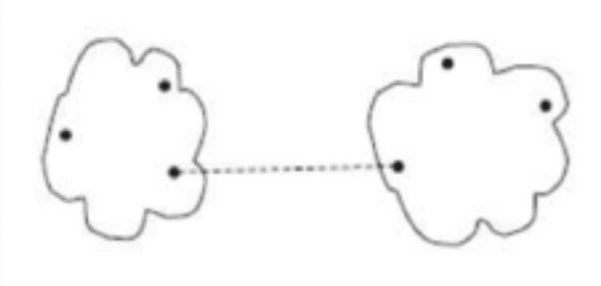
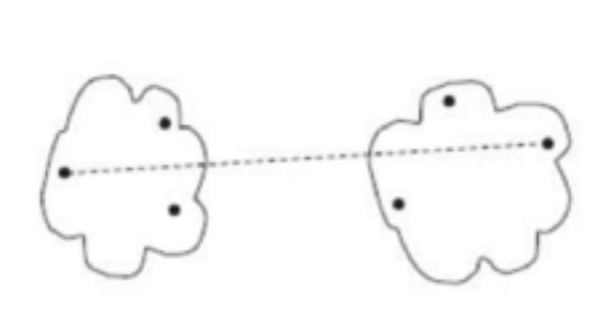
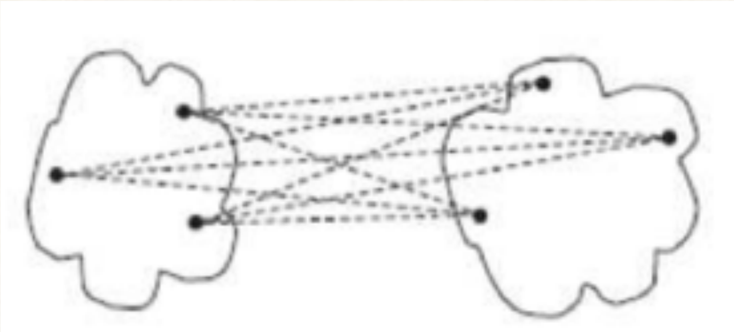
- Closest pair: single - link clustering



- Farthest pair: complete-link clustering



- Average similarity between groups: group average clustering

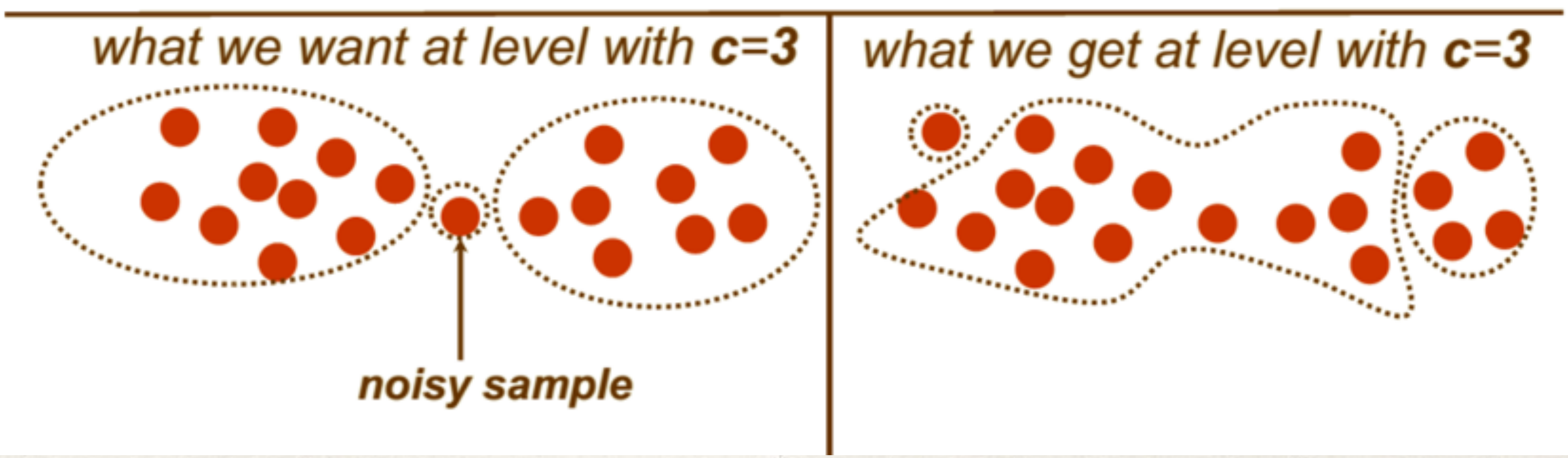


Single linkage

- Agglomerative clustering with minimum distance

$$d_{\min}(D_i, D_j) = \min_{x \in D_i, y \in D_j} \| x - y \|$$

- generates minimum spanning tree
- encourages growth of elongated clusters
- disadvantage: very sensitive to noise

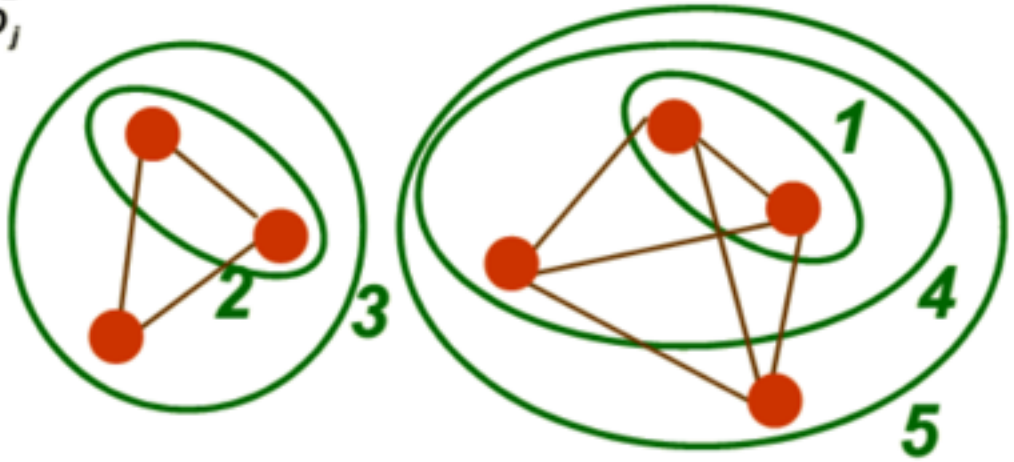


Complete linkage

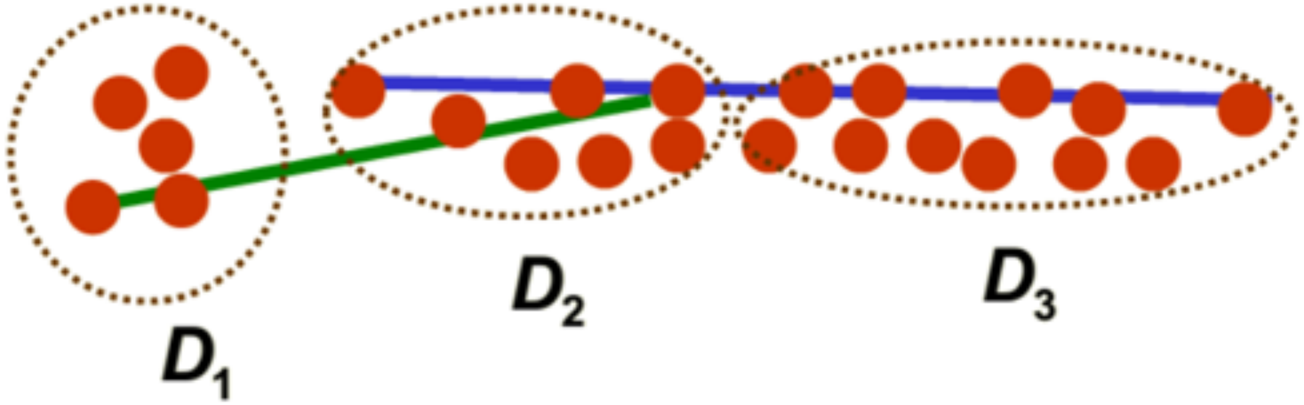
- Agglomerative clustering with maximum distance

$$d_{\max}(D_i, D_j) = \max_{x \in D_i, y \in D_j} \| x - y \|$$

- encourages compact clusters



- Does not work well if elongated clusters present

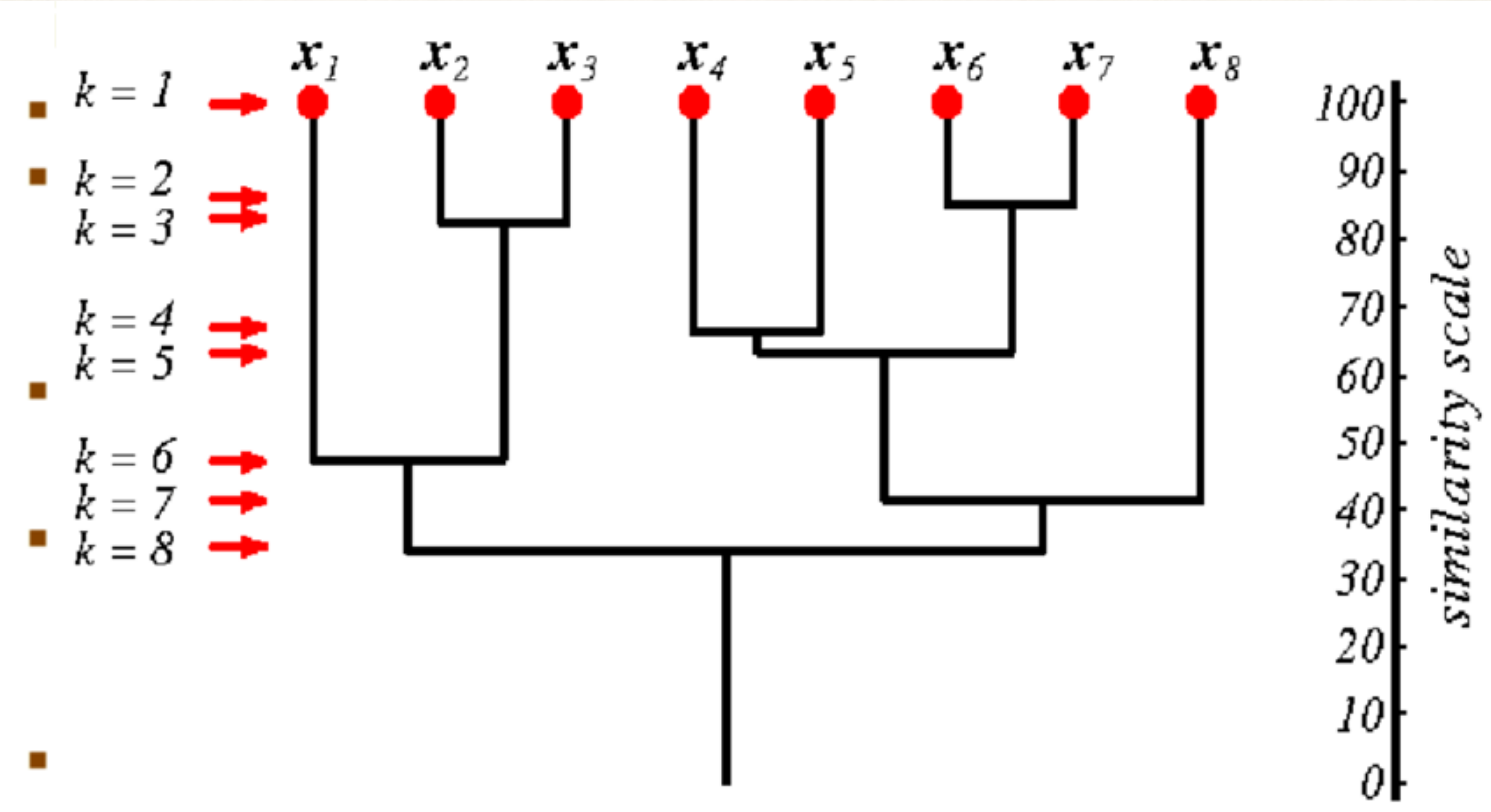


  - $d_{\max}(D_1, D_2) < d_{\max}(D_2, D_3)$
  - thus D_1 and D_2 are merged instead of D_2 and D_3

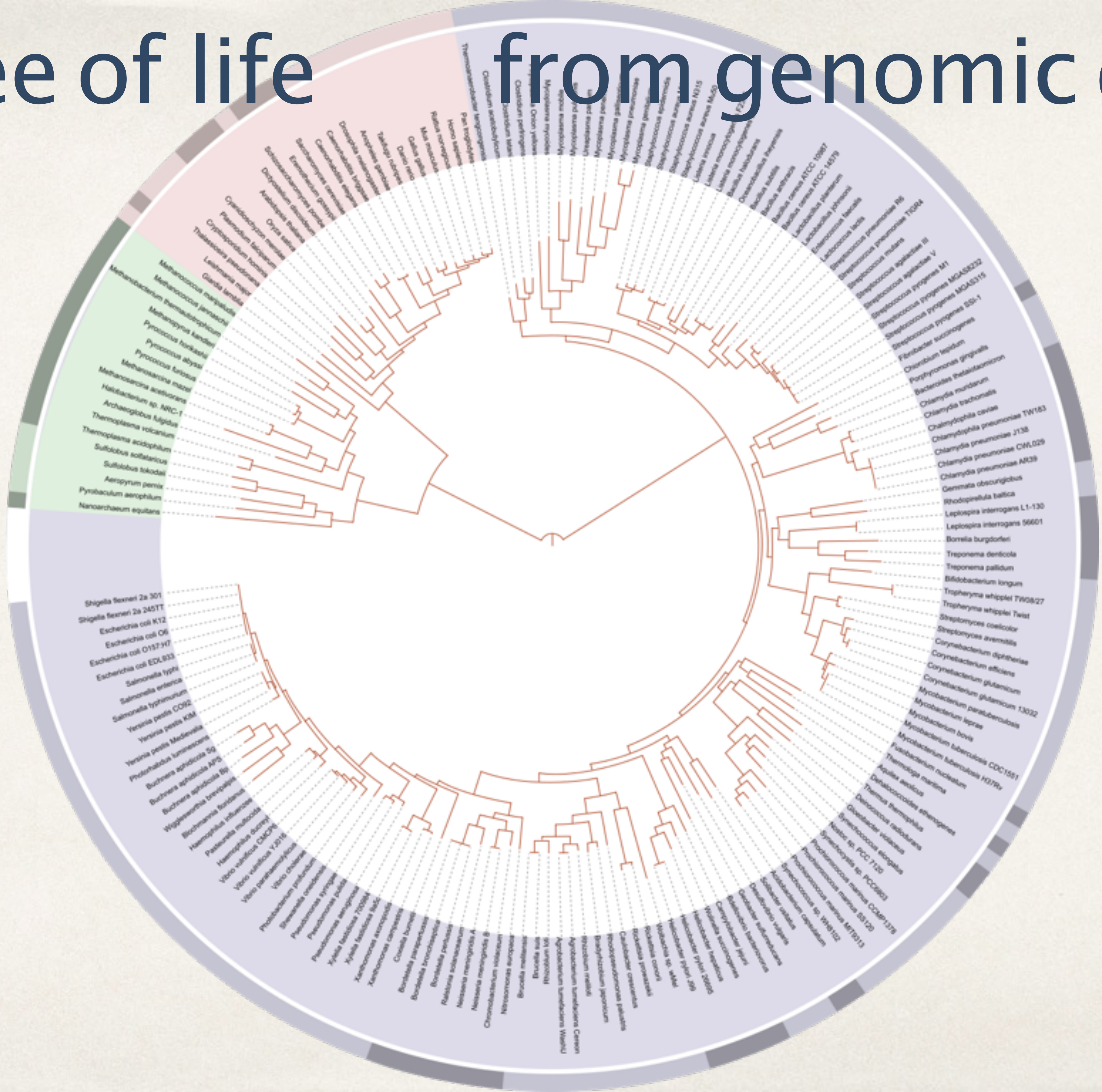
When to stop?

- Stop when we have k clusters
- Stop when cohesion of the cluster resulting from the best merger falls below a threshold
- Stop when there is a sudden jump in the cohesion value

Visualizing with a dendrogram

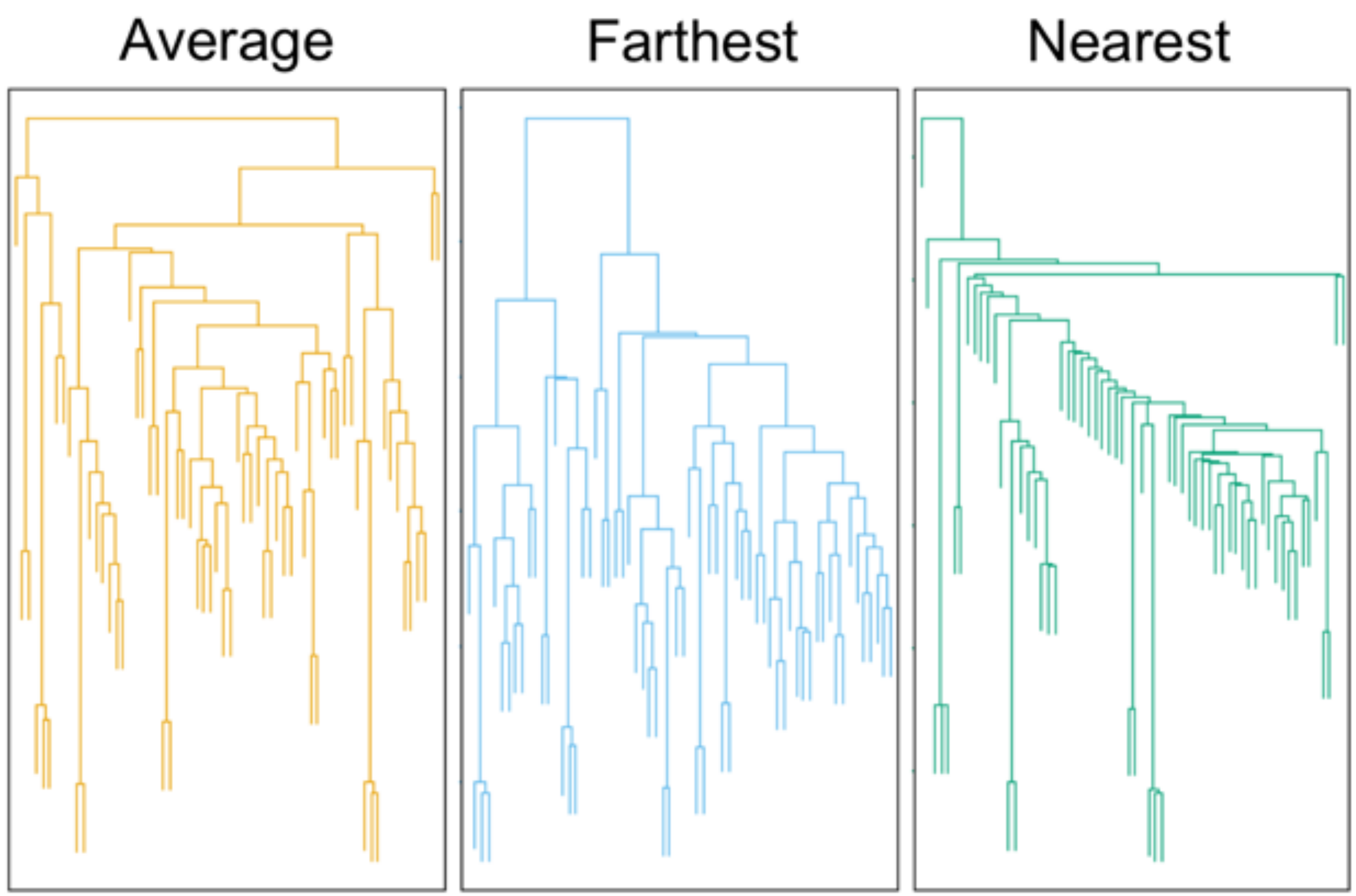


Tree of life from genomic data



Caveats

- Different decisions about group similarities can lead to vastly different dendrograms



Mouse tumor data from [Hastie *et al.*]

- Be cautious! The algorithm imposes a hierarchical structure on the data, even when it's not appropriate
- It's quite expensive to compute pairwise distances between each pair of cluster (naive implementation $O(N^3)$, with a priority queue $O(N^2 \log N)$)

Demo time!

Useful materials

- Distance metrics:

- http://www.improvedoutcomes.com/docs/WebSiteDocs/Clustering/Clustering_Parameters/Distance_Metrics_Overview.htm

- http://scikit-learn.org/stable/modules/generated/sklearn.neighbors.DistanceMetric.html

- https://www.cs.utah.edu/~jeffp/teaching/cs5955/L7-Distances.pdf