Lecture 12 – Clustering

Bulat Ibragimov

bulat@di.ku.dk

Department of Computer Science
University of Copenhagen

UNIVERSITY OF COPENHAGEN

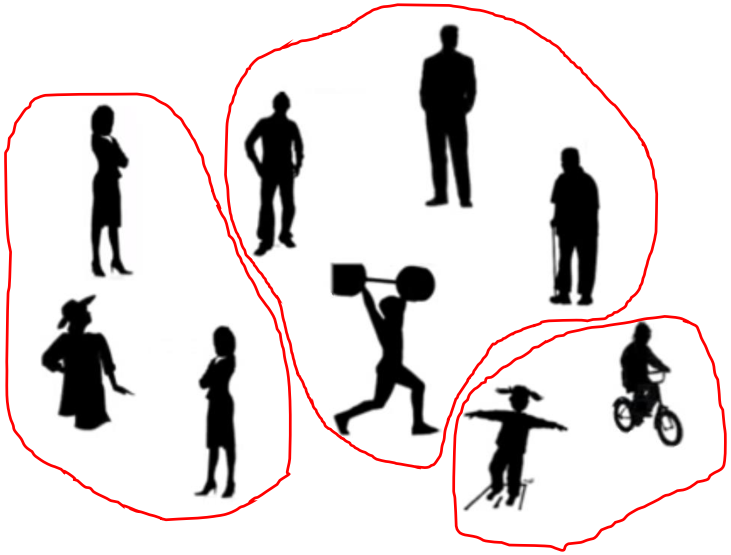
Week X - today

9.00 – 10.30	What is segmentation
	How can we use segmentation in medical imaging
	Simple segmentation techniques
	break
	Must-have tools in medical image analysis
10:30 -	Study group work

Classification

- Unsupervised
  - Try to understand underlying structure of the data and nothing specific

- What sub-populations exist in the data?
  - How many clusters?
  - How big?
  - Outliers?



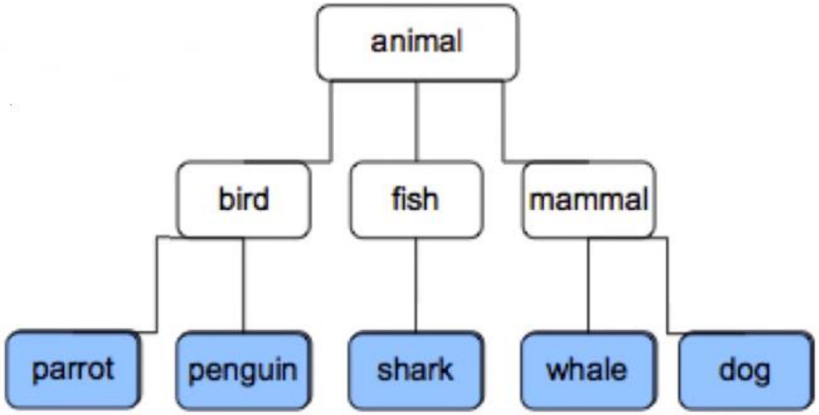
http://homepages.inf.ed.ac.uk/vlavrenk

Clustering types

- Goal
  - Monothetic: looking for specific properties for cluster members
    - e. g. all people younger than 15 – cluster of kids
  - Polythetic: cluster members are similar to each other
    - We compute distance between elements for clustering

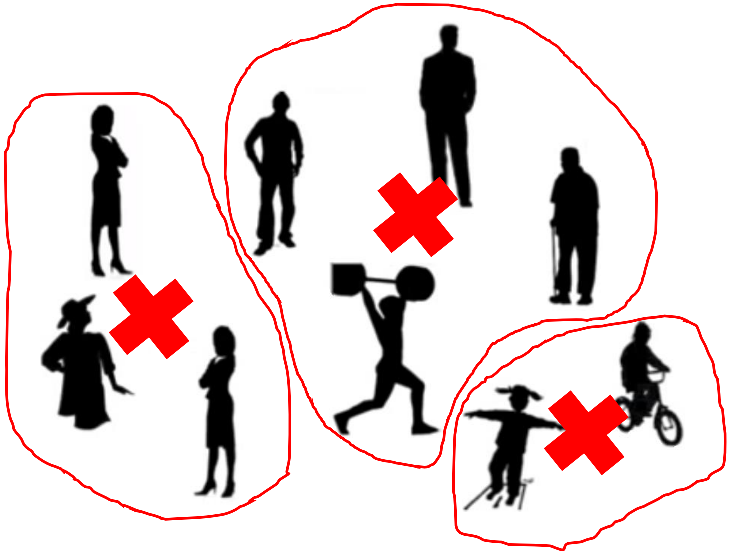
- Overlap
  - Hard clustering – no overlap is allowed
  - Soft clustering – estimate "membership strength" for datapoints

- Depth
  - Flat
  - Hierarchy

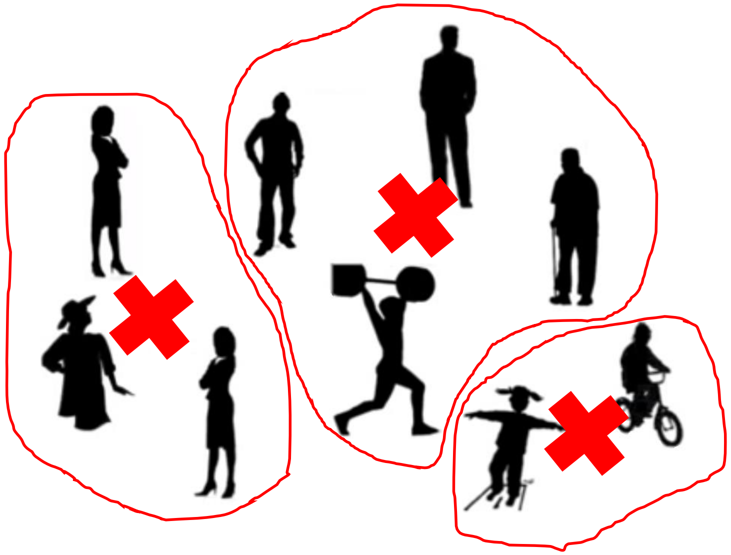


k-mean clustering

- Properties
  - Polythetic clustering
  - Data partitioned into k sub-populations (k must be specified)
  - Datapoints in sub-population are similar to its "centroid"
  - Clusters are hard
  - Clusters form flat structure

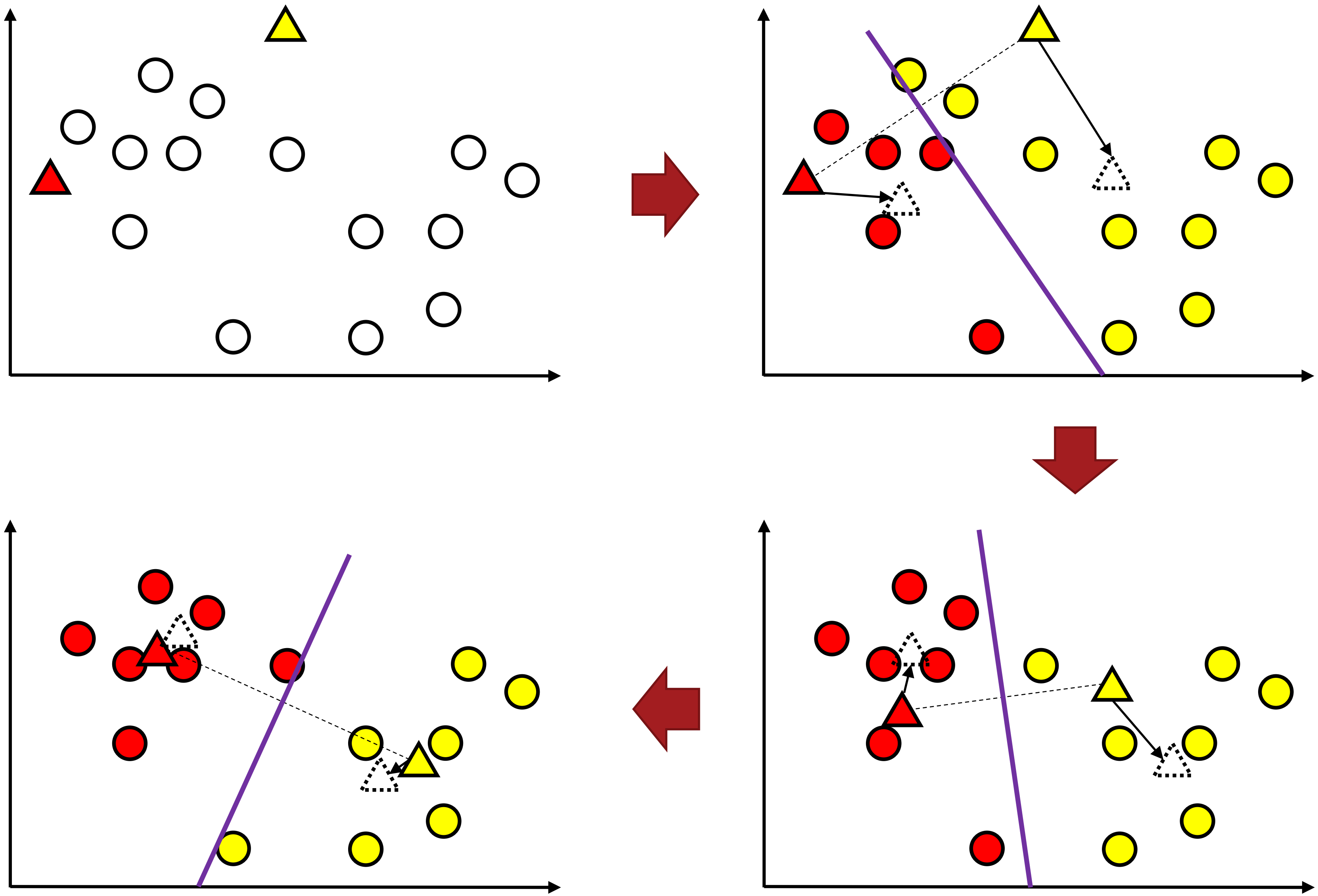


k-mean clustering



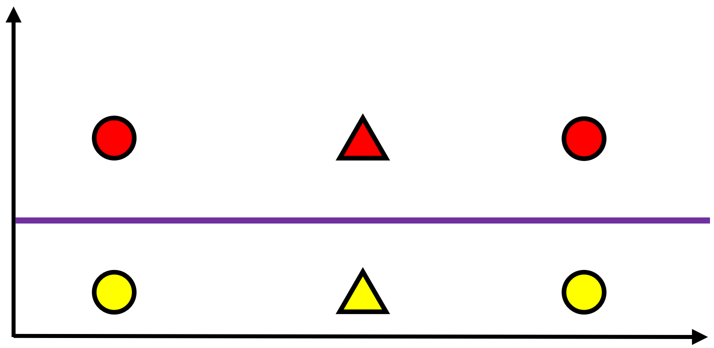
- Input: K, set of points $x_1, \dots, x_n$
- Generate random $c_1, \dots, c_k$ centroids
- Repeat:
  - Assign each x_i to the nearest centroid c_j $\underset{j}{\mathbf{argmin}}\, \boldsymbol{D}(\boldsymbol{x}_i, \boldsymbol{c}_j)$
  - Compute new centroids $\boldsymbol{c}_j \leftarrow \frac{\mathbf{1}}{\boldsymbol{n}_j} \sum_{\boldsymbol{x}_i \in \boldsymbol{c}_j} \boldsymbol{x}_i$
- Stop when assignment of x_i does not change

k-mean clustering: visualization



k-mean clustering

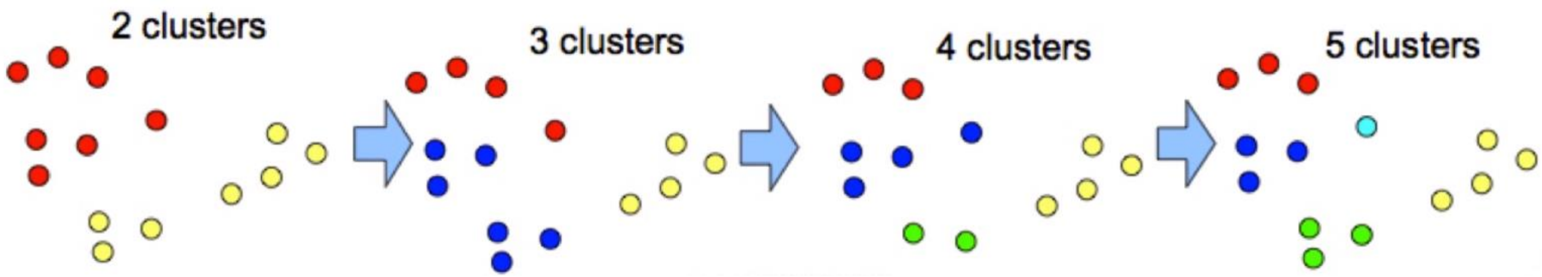
- Solution:
  - Minimized intra-cluster distance $\sum_j \sum_{x_i \in c_j} D(c_j, x_i)^2$
  - Converges to local minimum.
    - Different seed centroids -> different results
    - Run several times and select solution with lowest cost, i.e. intra-cluster distance
  - Nearby points may be assigned to different clusters



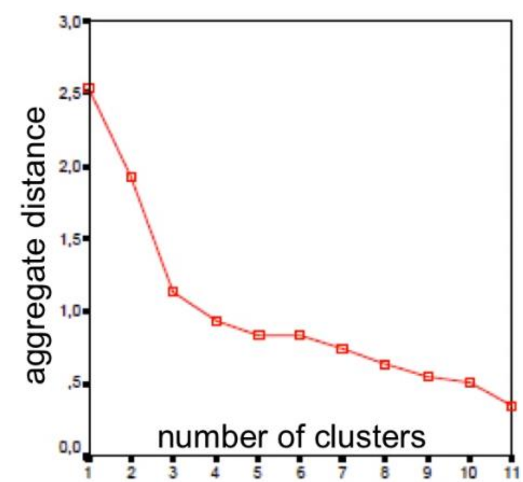
k-mean clustering: optimal k

- How many cluster are in the data:
  - Prior knowledge, e.g. for clustering of digits $k = 10$
  - Try different Ks
    - Record the behavior of cost function

What is the problem with this idea?

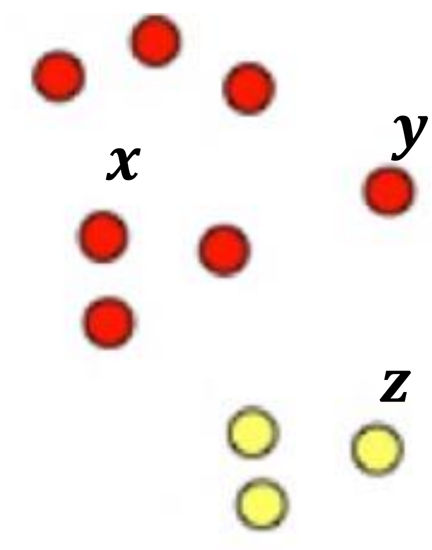


- The cost will always go down. The optimal $k = n$.
- Elbow method



k-mean clustering: silhouette score

- Intra-cluster distance $\boldsymbol{x} \in \boldsymbol{c_j}$:
  - $a(\boldsymbol{x}) = \frac{1}{|\boldsymbol{c_i}|-1} \sum_{\boldsymbol{y} \in \boldsymbol{c_i}} \boldsymbol{D}(\boldsymbol{x}, \boldsymbol{y})$
- Inter-cluster distance $\boldsymbol{x} \in \boldsymbol{c_j}$:
  - $b(\boldsymbol{x}) = \min_{i \neq j} \frac{1}{|\boldsymbol{c_j}|-1} \sum_{\boldsymbol{z} \in \boldsymbol{c_j}} \boldsymbol{D}(\boldsymbol{x}, \boldsymbol{z})$
- Silhouette:
  - $s(\boldsymbol{x}) = \begin{cases} 1 - a(\boldsymbol{x})/b(\boldsymbol{x}) & if\ a(\boldsymbol{x}) < b(\boldsymbol{x}) \\ 0 & if\ a(\boldsymbol{x}) = b(\boldsymbol{x}), or\ |\boldsymbol{c_i}| = 1 \\ b(\boldsymbol{x})/a(\boldsymbol{x}) - 1 & if\ a(\boldsymbol{x}) > b(\boldsymbol{x}) \end{cases}$
- Score = $\operatorname{mean}_{x} s(\boldsymbol{x})$



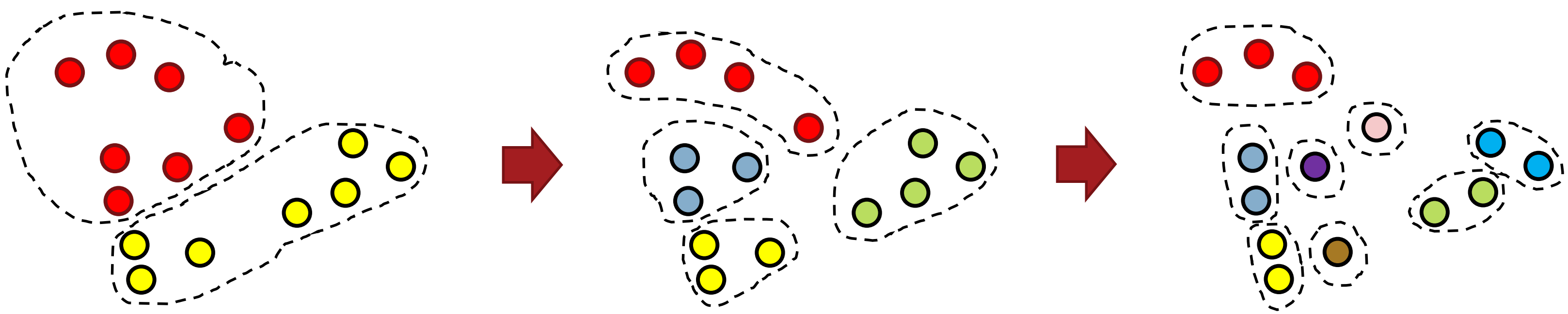
Hierarchical clustering

- Selecting k is difficult, even for a human
- Alternative is to create hierarchy of clusters:
  - Top-down approach: start with one cluster, and recursively split clusters
  - Bottom-up approach: start with individual datapoints, iteratively merge by some criterion

How many clusters?

Hierarchical k-means

- Top-down approach
- Select a relatively low k, e.g. 2.
- Run k-mean clustering on original data $x_1, \dots, x_n$
- For each of the resulting clusters $c_i : i = 1, \dots, k$:
  - Recursively run k-means on centroids in c_i

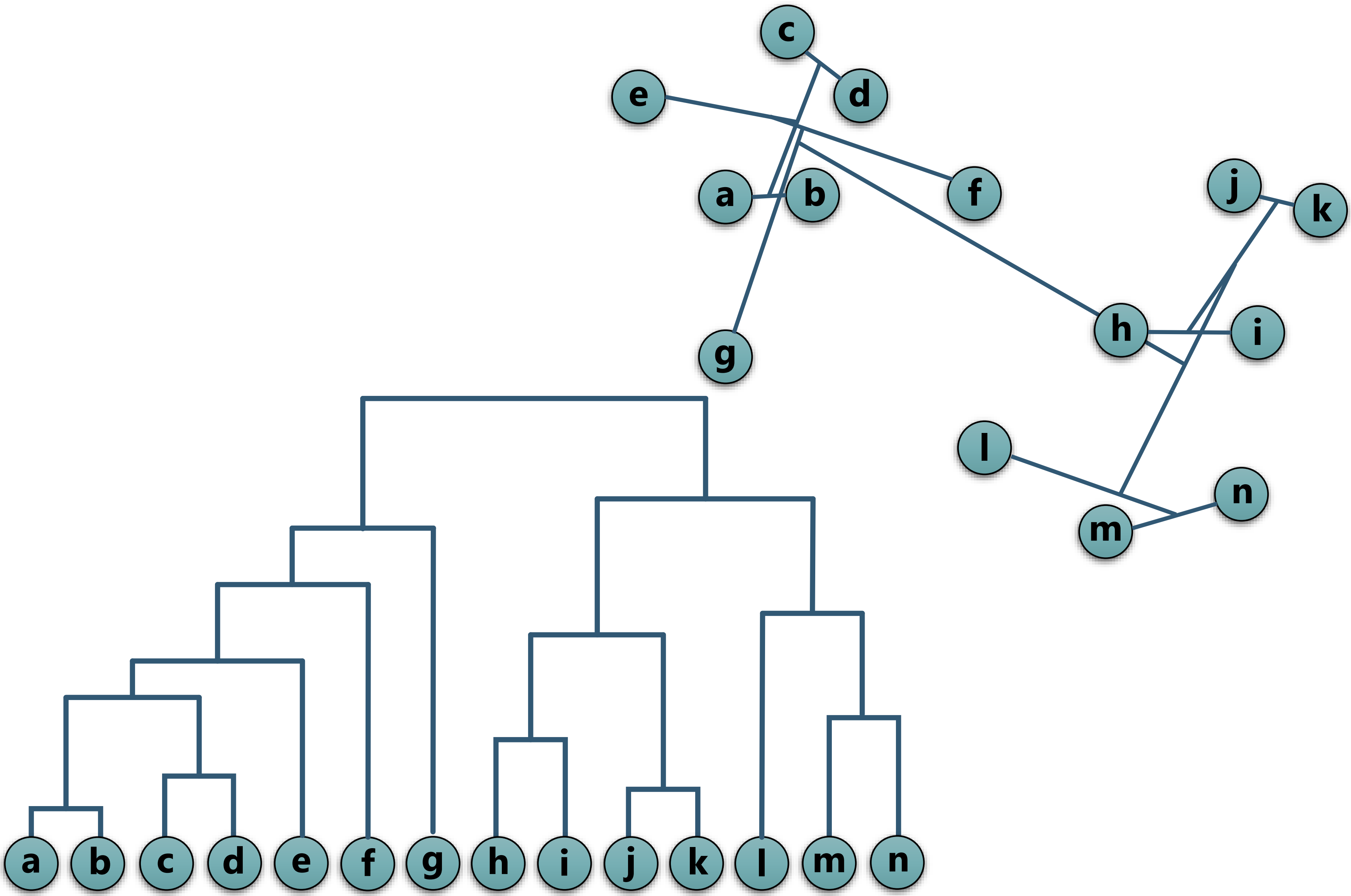


- There is still a problem of close points being assigned to different clusters

Agglomerative clustering

- Bottom-up approach
- Start with a collection C of n single-datapoint clusters
  - Each cluster contains one single point: $c_i = \{x_i\}$
- Repeat until only one cluster left:
  - Find a pair of clusters that is closest using some **distance** metric
  - Merge clusters c_i, c_j into a new cluster c_r
  - Remove c_i, c_j from the collection C, add c_r
- Slow: $\mathrm{O}(n^2 d + n^3)$, because need to recompute distance matrices multiple times
- There is still a problem of close points being assigned to different clusters

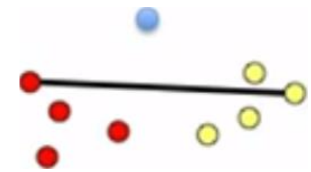
Agglomerative clustering: example



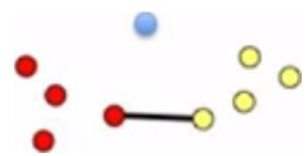
Agglomerative clustering: distance metric

What kind of distance metrics are possible?

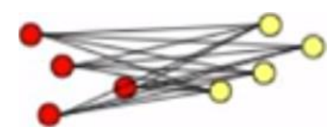
- Maximum distance (complete-linkage): $D = \max\{d(a,b): a \in c_i, b \in c_j\}$



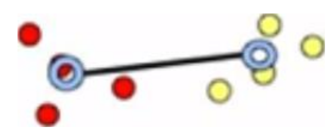
- Minimum distance (single-linkage): $D = \min\{d(a,b): a \in c_i, b \in c_j\}$



- Average linkage distance: $D = \frac{1}{|c_i||c_j|} \sum_{a \in c_i} \sum_{b \in c_j} d(a,b)$



- Centroid distance: $D = \left\| \bar{c}_i - \bar{c}_j \right\|$



- Minimum energy distance:

$$D = \frac{2}{|c_i||c_j|} \sum_{a \in c_i} \sum_{b \in c_j} d(a,b) - \frac{1}{|c_i|^2} \sum_{a \in c_i} \sum_{a' \in c_i} d(a,a') - \frac{1}{|c_j|^2} \sum_{b \in c_j} \sum_{b' \in c_j} d(b,b')$$

Minimal energy distance: example

Minimal energy distance:

$$D = \frac{2}{|c_i||c_j|} \sum_{a \in c_i} \sum_{b \in c_j} d(a,b) - \frac{1}{|c_i|^2} \sum_{a \in c_i} \sum_{a' \in c_i} d(a,a') - \frac{1}{|c_j|^2} \sum_{b \in c_j} \sum_{b' \in c_j} d(b,b')$$

- Let's define:
  - $d(a,a') = 1, \qquad d(b,b') = 1, \qquad d(a,b) = 3$
- Scenario $|c_i| = 3$, $|c_j| = 3$:

$$D = \frac{2}{3 \cdot 3} 9 \cdot 2 - \frac{1}{3^2} 6 \cdot 1 - \frac{1}{3^2} 6 \cdot 1 = 4 - \frac{2}{3} - \frac{2}{3} = \frac{8}{3}$$

- Scenario $|c_i| = 3$, $|c_j| = 1$:

$$D = \frac{2}{3 \cdot 1} 3 \cdot 2 - \frac{1}{3^2} 6 \cdot 1 - \frac{1}{1^2} 1 \cdot 1 = 4 - \frac{2}{3} - 1 = \frac{7}{3}$$

- Scenario $|c_i| = 1$, $|c_j| = 1$:

$$D = \frac{2}{1 \cdot 1} 1 \cdot 2 - \frac{1}{1^2} 1 \cdot 1 - \frac{1}{1^2} 1 \cdot 1 = 4 - 1 - 1 = \frac{6}{3}$$

Clustering: summary

- Clustering discover underlying sub-populations in the data
- K-means:
  - Fast, iterative. Leads to a local minimum
  - K is the key parameter of the algorithm
- Hierarchical clustering:
  - Top-down k-means clustering
    - Slow, iterative
  - Bottom-up approach. Agglomerative clustering
    - Fast, iterative
    - Requires specific distance metric

Questions?