Machine Learning

Lecture Notes on Clustering (II)
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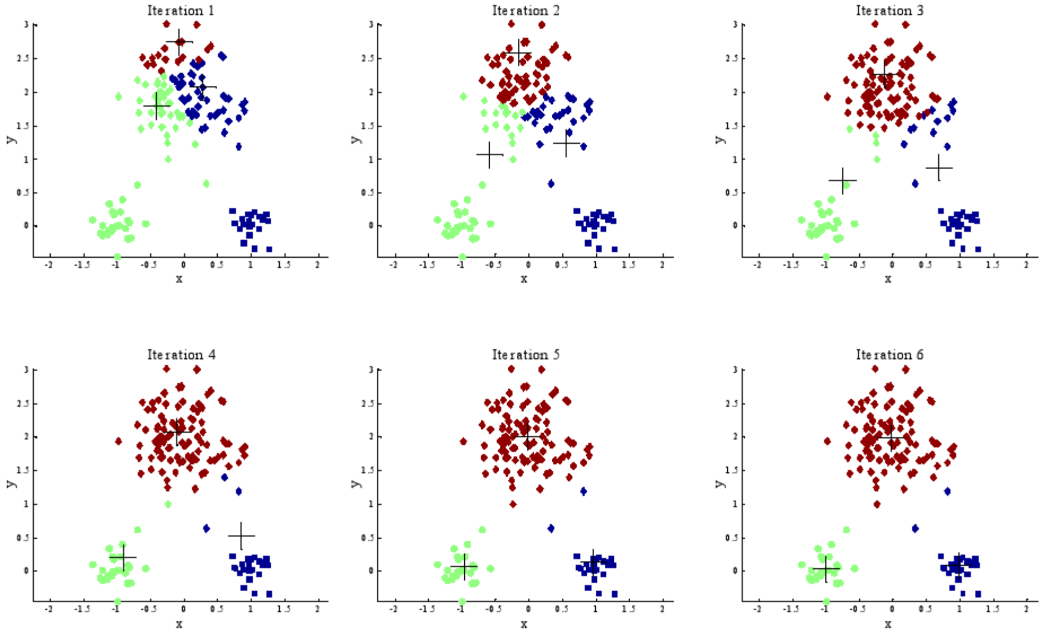
Today's Outline

- K-Means limits
- K-Means extensions: K-Medoids and Fuzzy C-Means
- Hierarchical Clustering

K-Means limits

Importance of choosing initial centroids



K-Means limits

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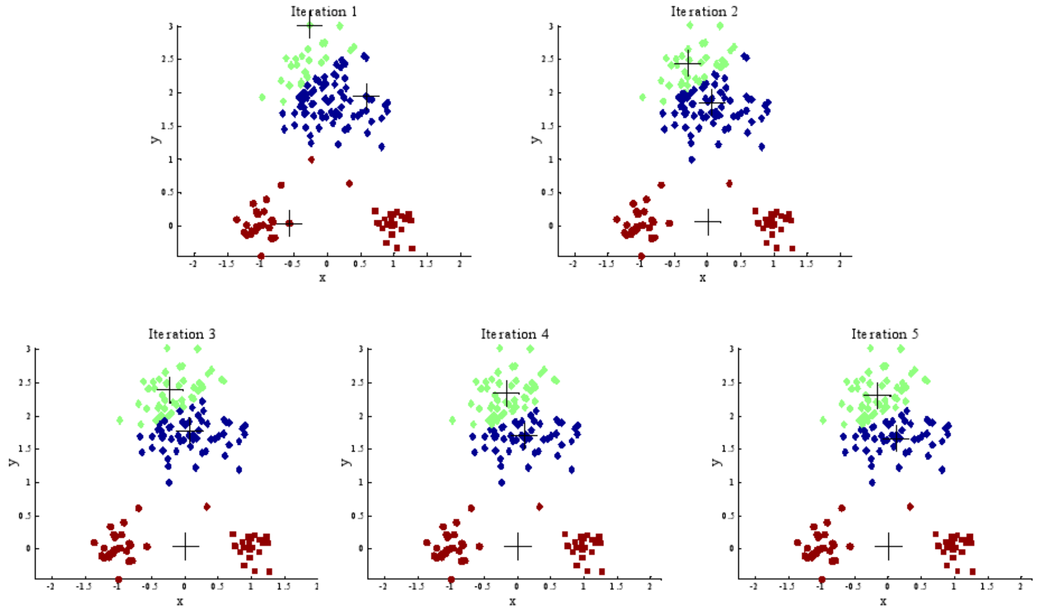
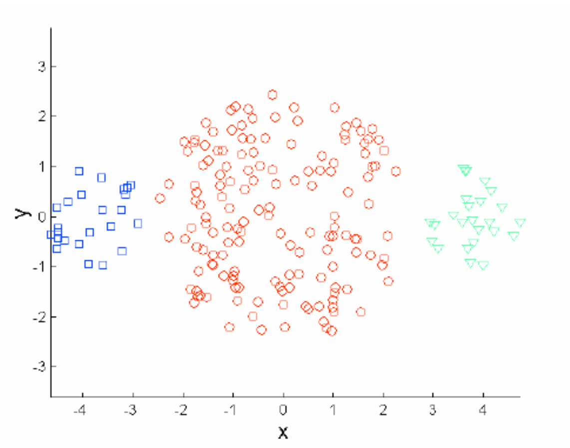
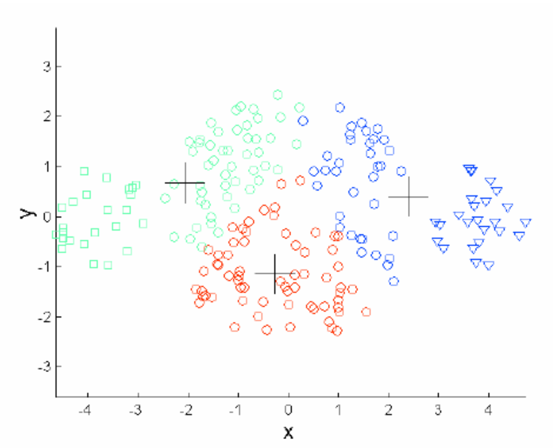


K-Means limits

Differing sizes

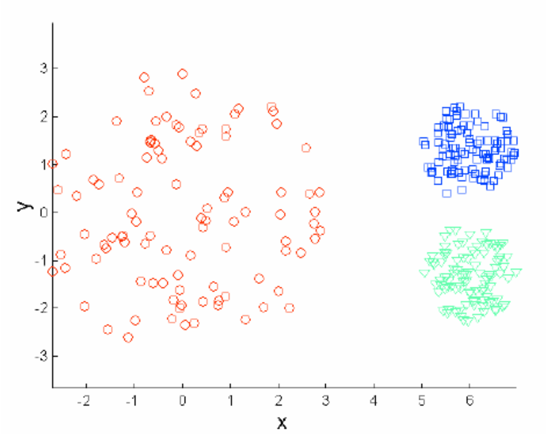


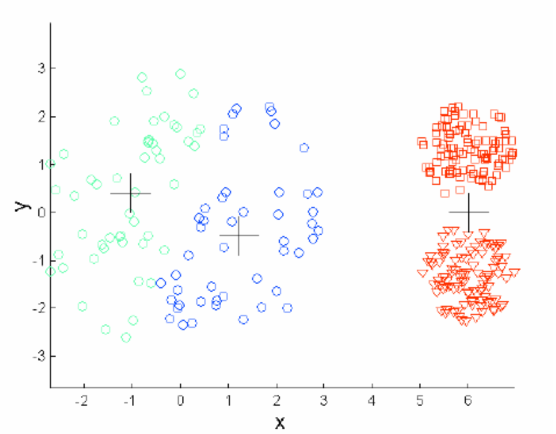


Original Points **K-means Clusters**

K-Means limits

Differing density

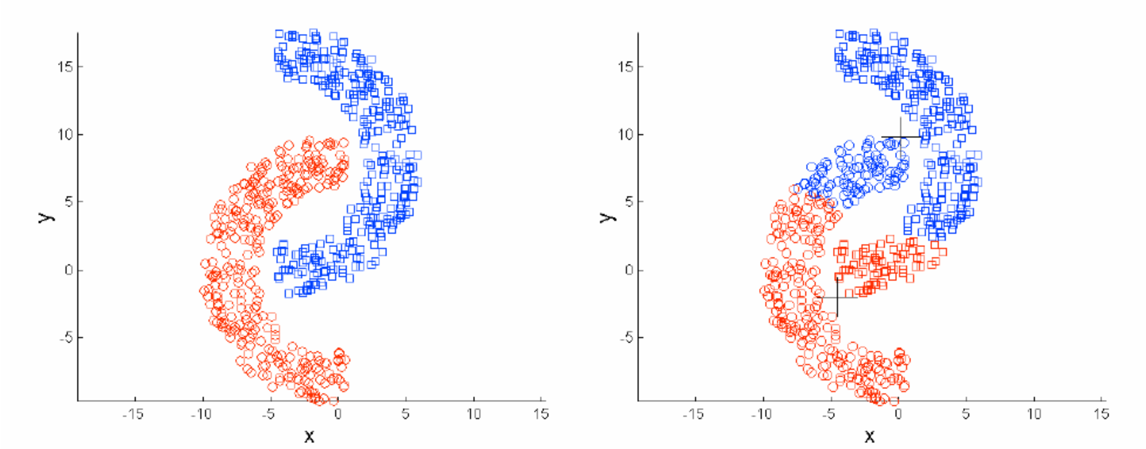




Original Points **K-means Clusters**

K-Means limits

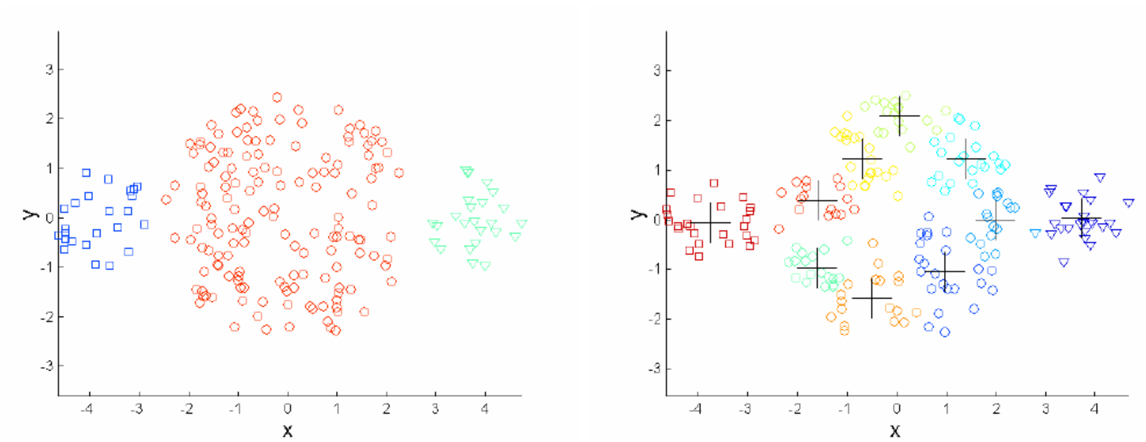
Non-globular shapes



Original Points **K-means Clusters**

K-Means: higher K

What if we tried to increase K to solve K-Means problems?



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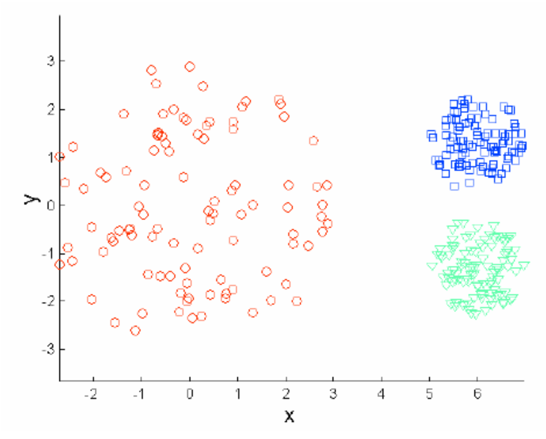
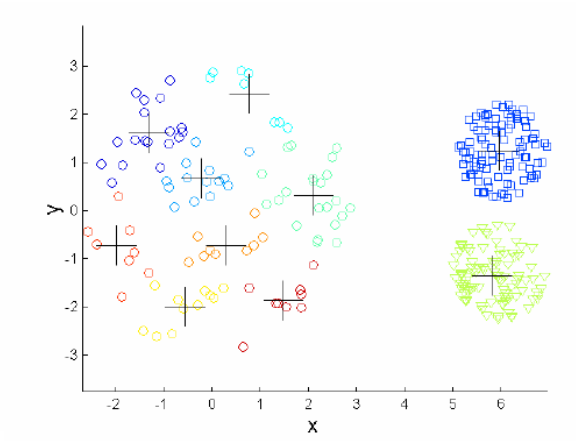


Original Points



K-means Clusters

K-Means: higher K

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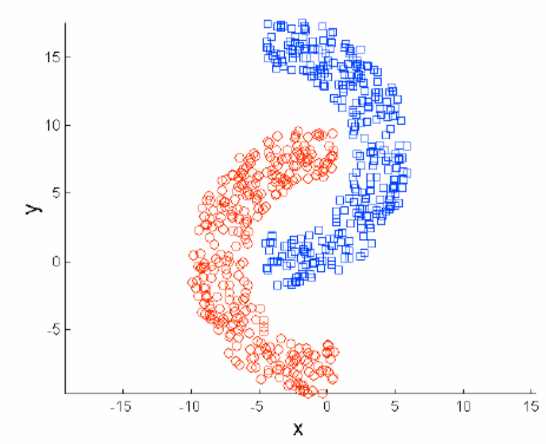
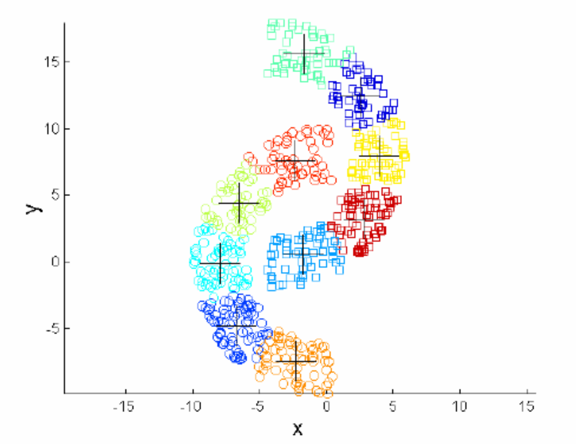


Original Points



K-means Clusters

K-Medoids

- K-Means algorithm is too sensitive to outliers
  - An object with an extremely large value may substantially distort the distribution of the data
- **Medoid**: the most centrally located point in a cluster, as a representative point of the cluster
- Note: while a medoid is always a point inside a cluster too, a centroid could be not part of the cluster
- Analogy to using *medians*, instead of *means*, to describe the representative point of a set
  - Mean of 1, 3, 5, 7, 9 is 5
  - Mean of 1, 3, 5, 7, 1009 is 205
  - Median of 1, 3, 5, 7, 1009 is 5

PAM

PAM means **P**artitioning **A**round **M**edoids. The algorithm follows:

1. Given k
2. Randomly pick k instances as initial medoids
3. Assign each data point to the nearest medoid x
4. Calculate the objective function
   - the sum of dissimilarities of all points to their nearest medoids. (squared-error criterion)
5. For each non-medoid point y
   - swap x and y and calculate the objective function
6. Select the configuration with the lowest cost
7. Repeat (3-6) until no change

PAM

- Pam is more robust than k-means in the presence of noise and outliers
  - A medoid is less influenced by outliers or other extreme values than a mean (can you tell why?)
- Pam works well for small data sets but does not scale well for large data sets
  - $O(k(n-k)^2)$ for each change where n is # of data objects, k is # of clusters
- NOTE: not having to calculate a *mean*, we do not need actual *positions* of points but just their *distances*!

Fuzzy C-Means

Fuzzy C-Means (FCM, developed by Dunn in 1973 and improved by Bezdek in 1981) is a method of clustering which allows one piece of data to belong to two or more clusters.

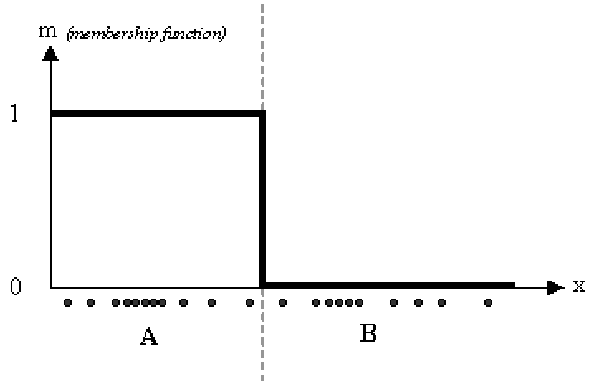
- frequently used in pattern recognition
- based on minimization of the following objective function:

$$J_m = \sum_{i=1}^{N} \sum_{j=1}^{C} u_{ij}^m \|x_i - c_j\|^2, 1 \leq m < \infty$$

where:
m is any real number greater than 1 (*fuzziness coefficient*),
u_{ij} is the degree of membership of x_i in the cluster j,
x_i is the i-th of d-dimensional measured data,
c_j is the d-dimension center of the cluster,
$\|\cdot\|$ is any norm expressing the similarity between measured data and the center.

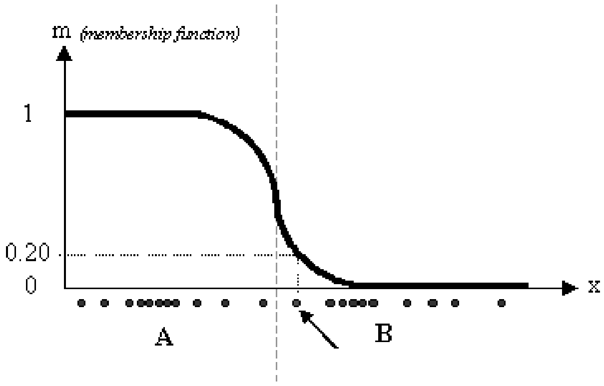
K-Means vs. FCM

- With K-Means, every piece of data either belongs to centroid A or to centroid B



K-Means vs. FCM

- With FCM, data elements do not belong exclusively to one cluster, but they may belong to several clusters (with different membership values)



Data representation

$$(KM)U_{N\times C} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \\ 1 & 0 \\ \dots & \dots \\ 0 & 1 \end{bmatrix}$$

$$(FCM)U_{N\times C} = \begin{bmatrix} 0.8 & 0.2 \\ 0.3 & 0.7 \\ 0.6 & 0.4 \\ \dots & \dots \\ 0.9 & 0.1 \end{bmatrix}$$

FCM Algorithm

The algorithm is composed of the following steps:

1. Initialize $U = [u_{ij}]$ matrix, $U^{(0)}$
2. At t-step: calculate the centers vectors $C^{(t)} = [c_j]$ with $U^{(t)}$:

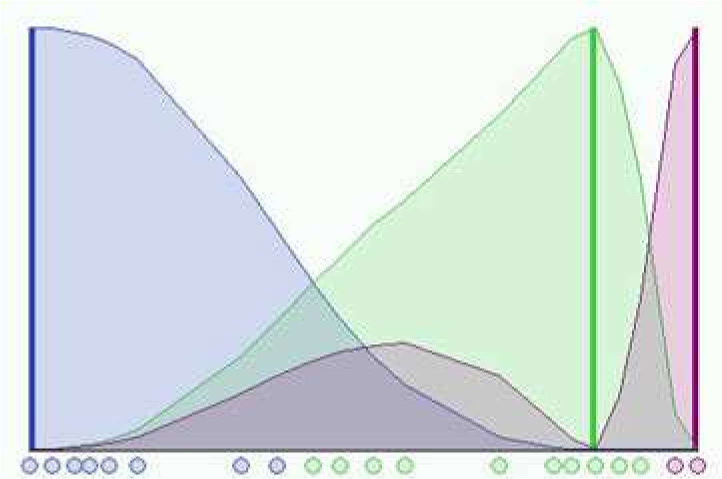
$$c_j = \frac{\sum_{i=1}^{N} u_{ij}^m \cdot x_i}{\sum_{i=1}^{N} u_{ij}^m}$$

3. Update $U^{(t)}$, $U^{(t+1)}$:

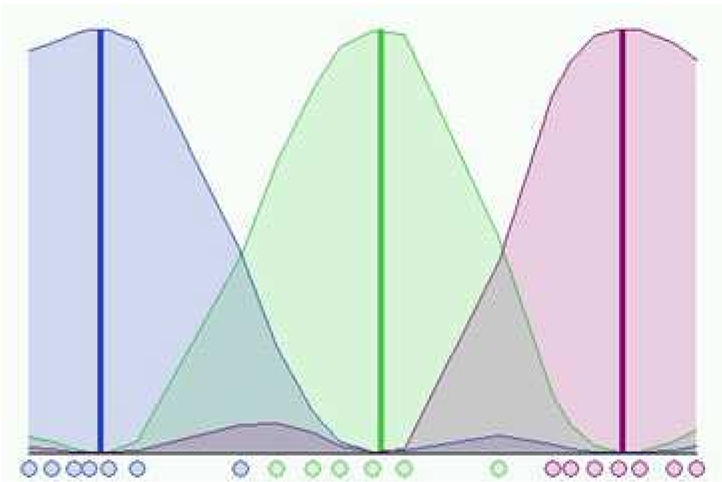
$$u_{ij} = \frac{1}{\sum_{k=1}^{C} \left(\frac{\|x_i - c_j\|}{\|x_i - c_k\|} \right)^{\frac{2}{m-1}}}$$

4. If $\|U^{(k+1)} - U^{(k)}\| < \varepsilon$ then STOP; otherwise return to step 2.

An Example



An Example



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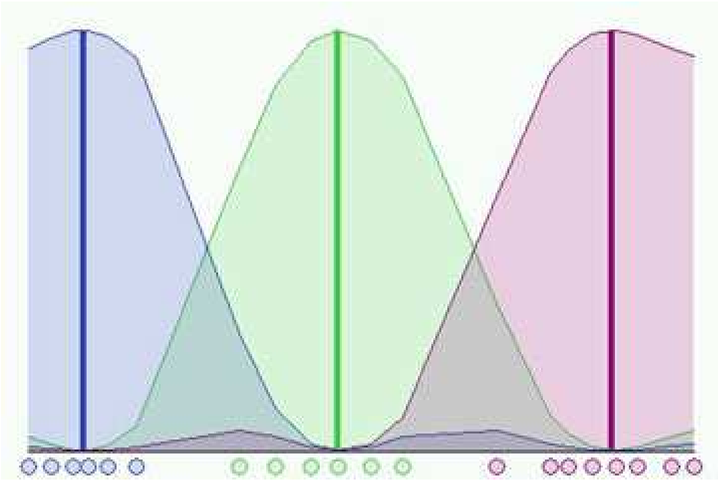


Hierarchical Clustering

- Top-down vs Bottom-up
- Top-down (or *divisive*):
  - Start with one universal cluster
  - Split it into two clusters
  - Proceed recursively on each subset
- Bottom-up (or *agglomerative*):
  - Start with single-instance clusters ("every item is a cluster")
  - At each step, join the two closest clusters
  - (design decision: distance between clusters)

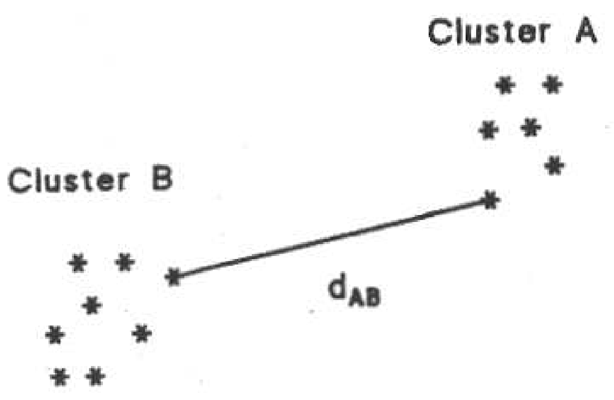
Agglomerative Hierarchical Clustering

Given a set of N items to be clustered, and an N*N distance (or dissimilarity) matrix, the basic process of agglomerative hierarchical clustering is the following:

1. Start by assigning each item to a cluster. Let the dissimilarities between the clusters be the same as the dissimilarities between the items they contain.
2. Find the closest (most similar) pair of clusters and merge them into a single cluster. Now, you have one cluster less.
3. Compute dissimilarities between the new cluster and each of the old ones.
4. Repeat Steps 2 and 3 until all items are clustered into a single cluster of size N.

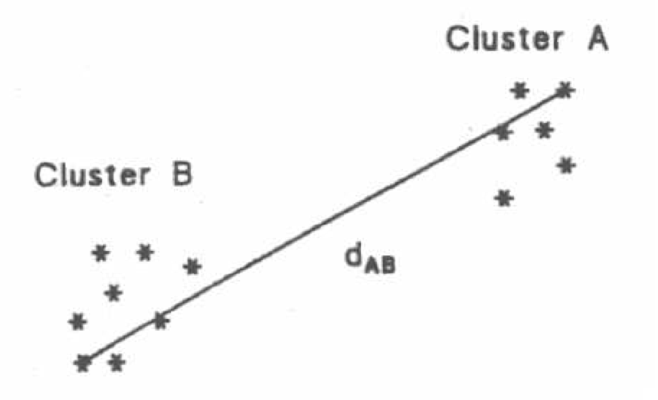
Single Linkage (SL) clustering

- We consider the distance between two clusters to be equal to the **shortest** distance from any member of one cluster to any member of the other one (**greatest** similarity).



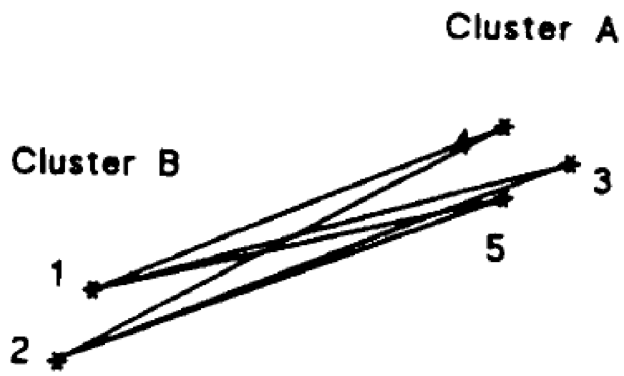
Complete Linkage (CL) clustering

- We consider the distance between two clusters to be equal to the **greatest** distance from any member of one cluster to any member of the other one (**smallest** similarity).



Group Average (GA) clustering

- We consider the distance between two clusters to be equal to the **average** distance from any member of one cluster to any member of the other one.



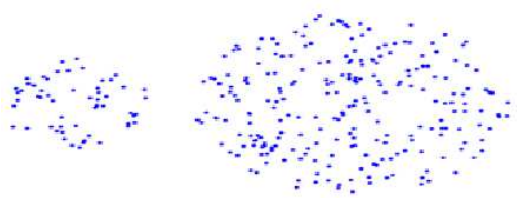
About distances

If the data exhibit strong clustering tendency, all 3 methods produce similar results.

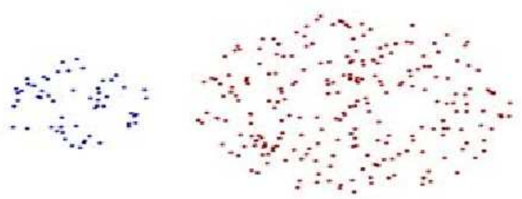
- **SL**: requires only a single dissimilarity to be small. Drawback: produced clusters can violate the “compactness” property (cluster with large diameters)
- **CL**: opposite extreme (compact clusters with small diameters, but can violate the “closeness” property)
- **GA**: compromise, it attempts to produce relatively compact clusters and relatively far apart. BUT it depends on the dissimilarity scale.

Hierarchical algorithms limits

Strength of MIN



Original Points

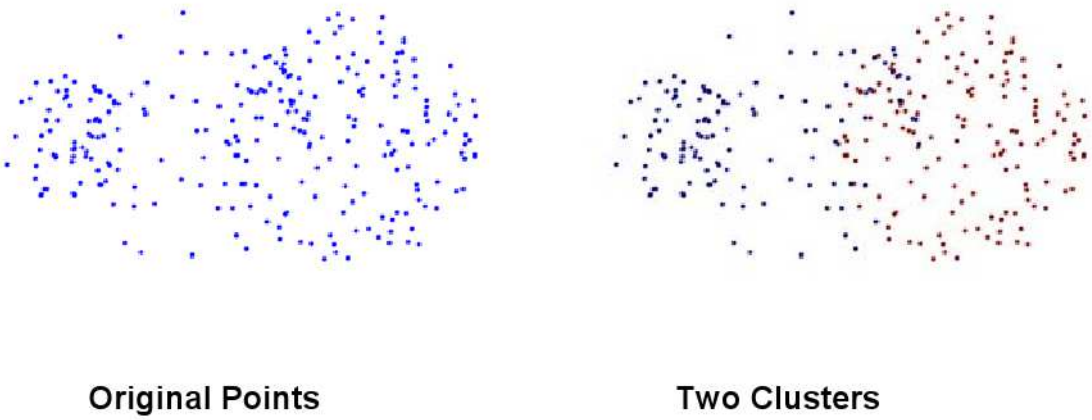


Two Clusters

- Easily handles clusters of different sizes
- Can handle non elliptical shapes

Hierarchical algorithms limits

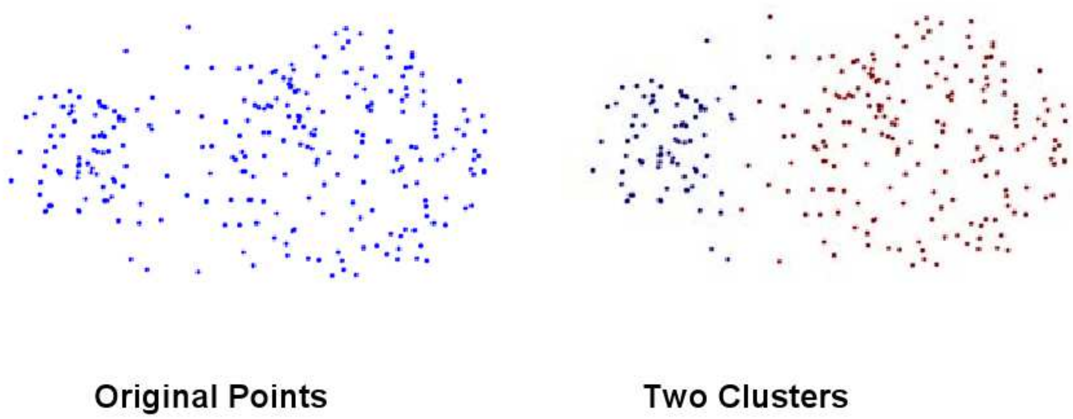
Limitations of MIN



- Sensitive to noise and outliers

Hierarchical algorithms limits

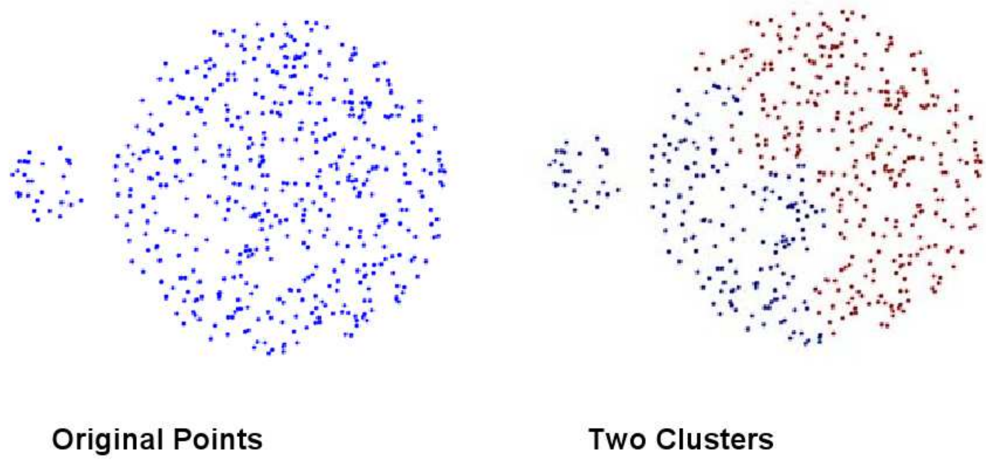
Strength of MAX



- Less sensitive to noise and outliers

Hierarchical algorithms limits

Limitations of MAX



- Tends to break large clusters
- Biased toward globular clusters

Hierarchical clustering: Summary

- Advantages
  - It's nice that you get a hierarchy instead of an amorphous collection of groups
  - If you want k groups, just cut the $(k-1)$ longest links
- Disadvantages
  - It doesn't scale well: time complexity of at least $O(n^2)$, where n is the number of objects

Bibliography

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