

Data Mining Cluster Analysis: Basic Concepts and Algorithms

Lecture Notes for Chapter 7

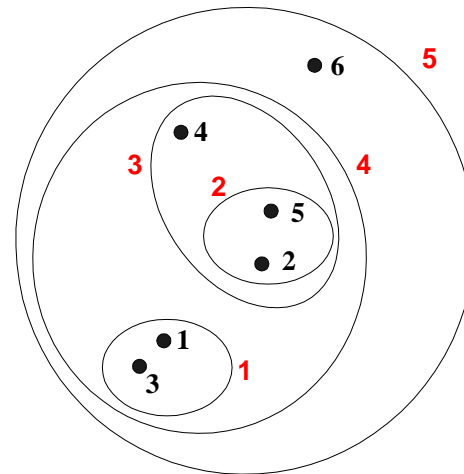
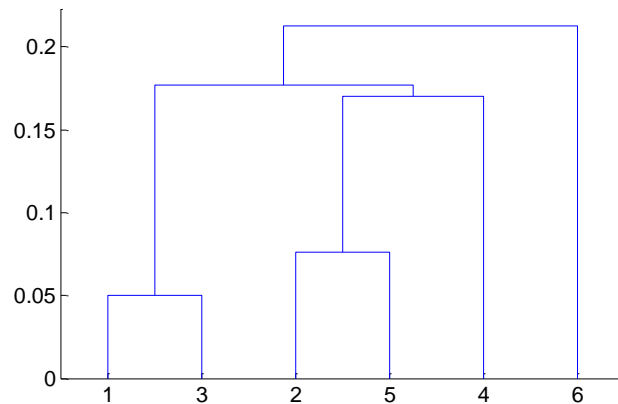
Introduction to Data Mining, 2nd Edition

by

Tan, Steinbach, Karpatne, Kumar

Hierarchical Clustering

- Produces a set of nested clusters organized as a hierarchical tree
- Can be visualized as a dendrogram
 - A tree like diagram that records the sequences of merges or splits



Strengths of Hierarchical Clustering

- Do not have to assume any particular number of clusters
 - Any desired number of clusters can be obtained by ‘cutting’ the dendrogram at the proper level
- They may correspond to meaningful taxonomies
 - Example in biological sciences (e.g., animal kingdom, phylogeny reconstruction, ...)

Hierarchical Clustering

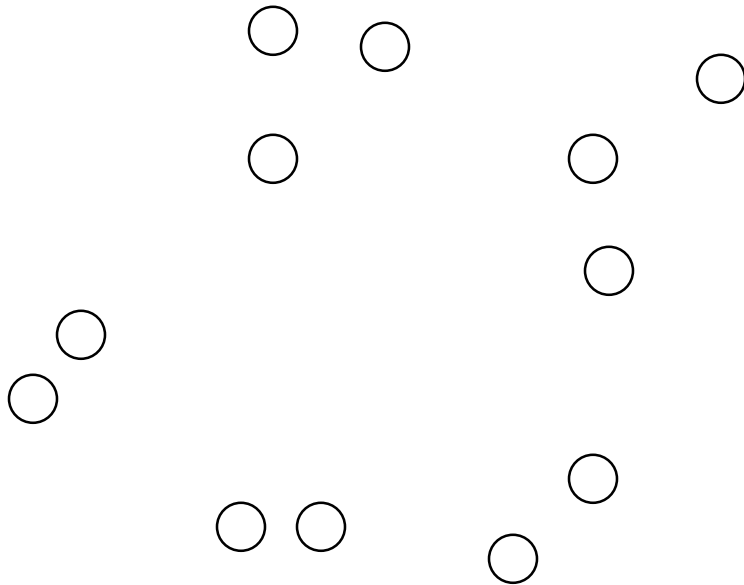
- Two main types of hierarchical clustering
 - Agglomerative:
 - ◆ Start with the points as individual clusters
 - ◆ At each step, merge the closest pair of clusters until only one cluster (or k clusters) left
 - Divisive:
 - ◆ Start with one, all-inclusive cluster
 - ◆ At each step, split a cluster until each cluster contains an individual point (or there are k clusters)
- Traditional hierarchical algorithms use a similarity or distance matrix
 - Merge or split one cluster at a time

Agglomerative Clustering Algorithm

- Most popular hierarchical clustering technique
- Basic algorithm is straightforward
 1. Compute the proximity matrix
 2. Let each data point be a cluster
 3. **Repeat**
 4. Merge the two closest clusters
 5. Update the proximity matrix
 6. **Until** only a single cluster remains
- Key operation is the computation of the proximity of two clusters
 - Different approaches to defining the distance between clusters distinguish the different algorithms

Starting Situation

- Start with clusters of individual points and a proximity matrix



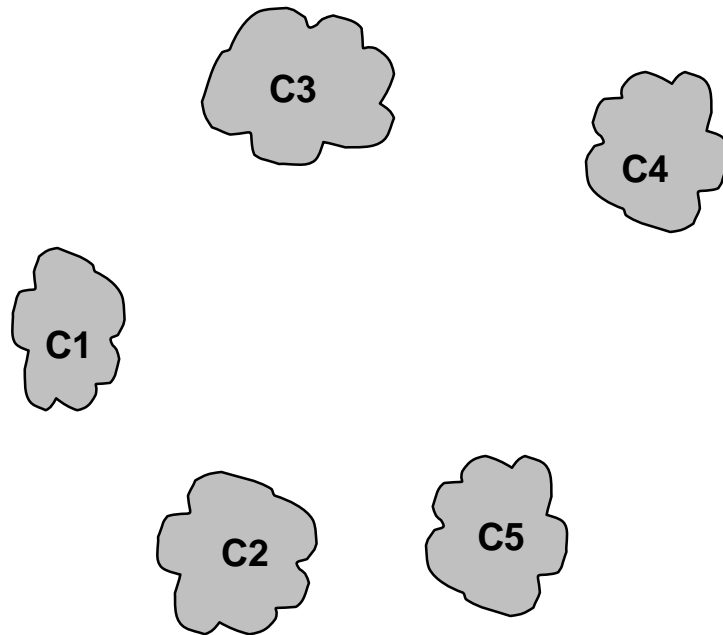
	p1	p2	p3	p4	p5	...
p1						
p2						
p3						
p4						
p5						
.						
.						
.						

Proximity Matrix



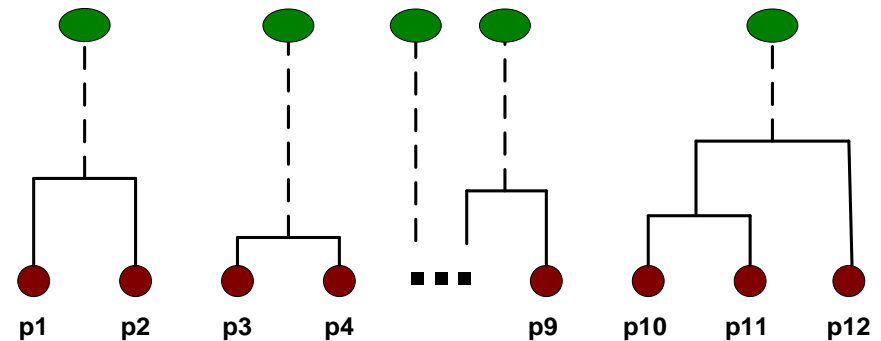
Intermediate Situation

- After some merging steps, we have some clusters



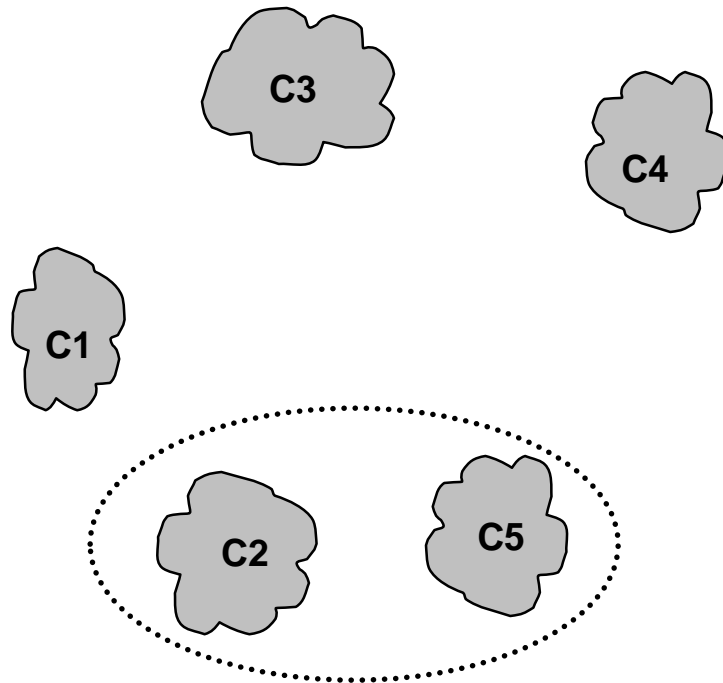
	C1	C2	C3	C4	C5
C1					
C2					
C3					
C4					
C5					

Proximity Matrix



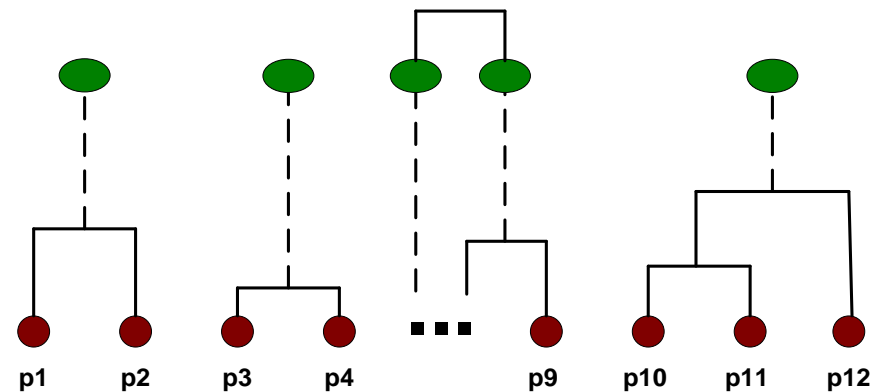
Intermediate Situation

- We want to merge the two closest clusters (C2 and C5) and update the proximity matrix.



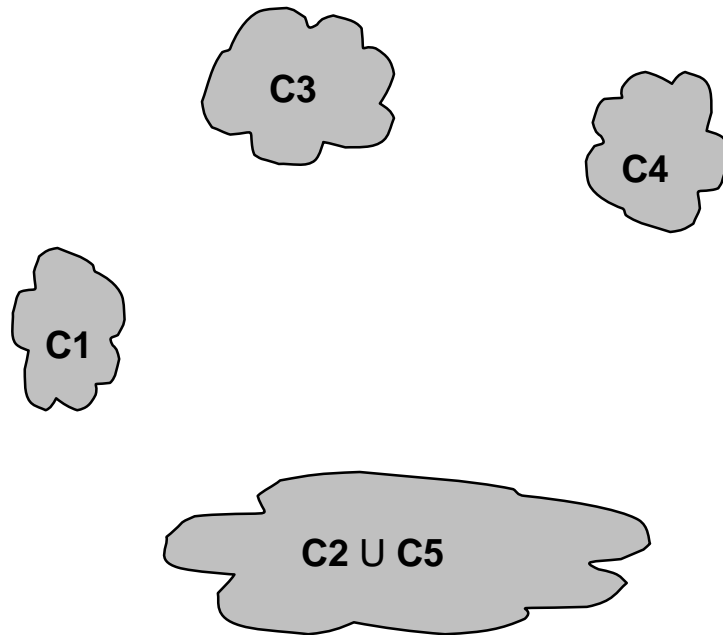
	C1	C2	C3	C4	C5
C1					
C2					
C3					
C4					
C5					

Proximity Matrix



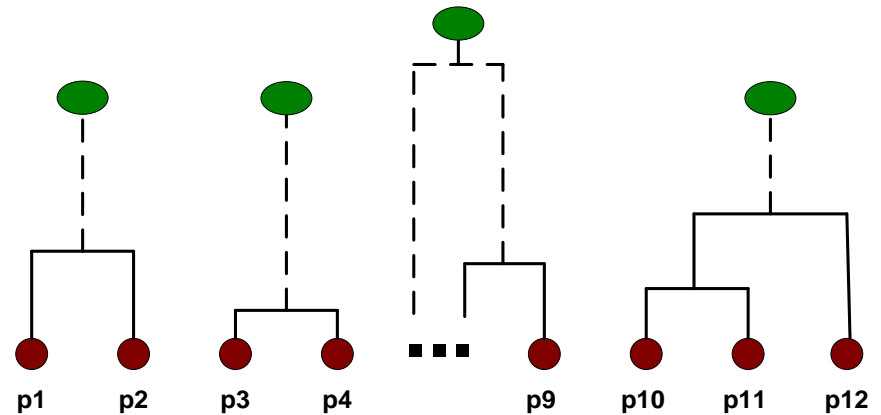
After Merging

- The question is “How do we update the proximity matrix?”

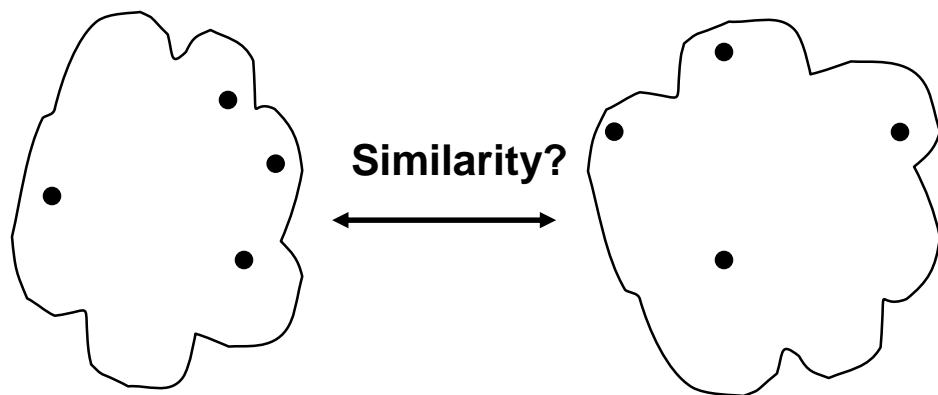


	C1	C2 U C5	C3	C4
C1		?		
C2 U C5	?	?	?	?
C3		?		
C4		?		

Proximity Matrix



How to Define Inter-Cluster Distance

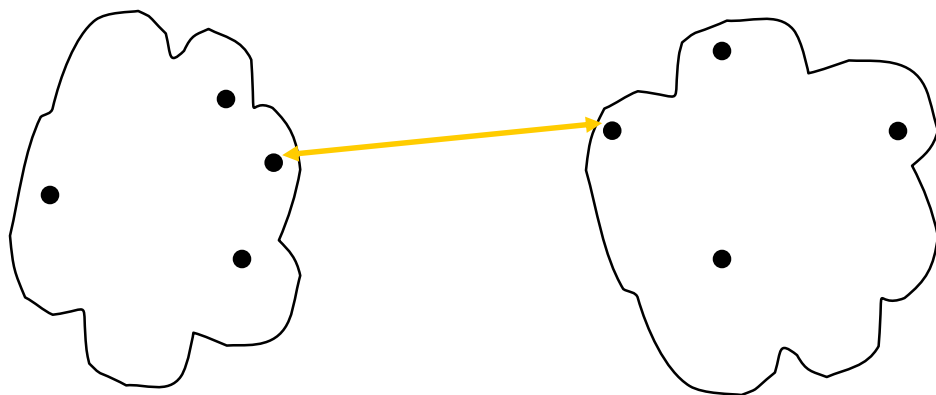


- MIN
- MAX
- Group Average
- Distance Between Centroids
- Other methods driven by an objective function
 - Ward's Method uses squared error

	p1	p2	p3	p4	p5	...
p1						
p2						
p3						
p4						
p5						
.						
.						
.						

Proximity Matrix

How to Define Inter-Cluster Similarity

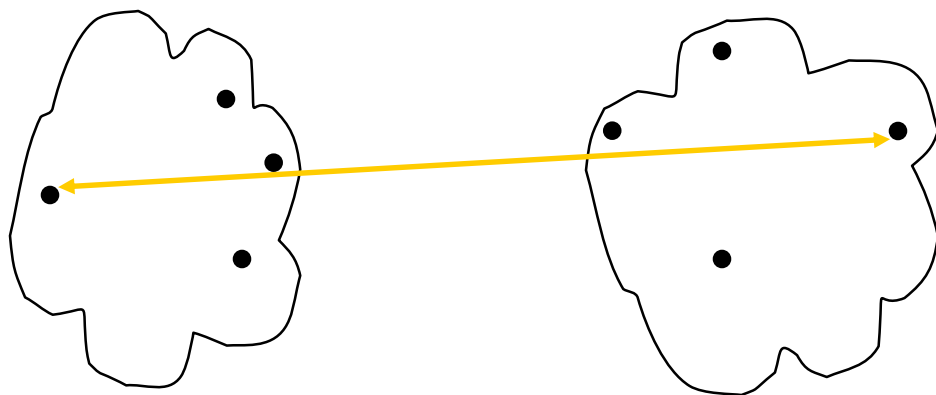


- **MIN**
- **MAX**
- **Group Average**
- **Distance Between Centroids**
- **Other methods driven by an objective function**
 - Ward's Method uses squared error

	p1	p2	p3	p4	p5	...
p1						
p2						
p3						
p4						
p5						
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.						

· **Proximity Matrix**

How to Define Inter-Cluster Similarity

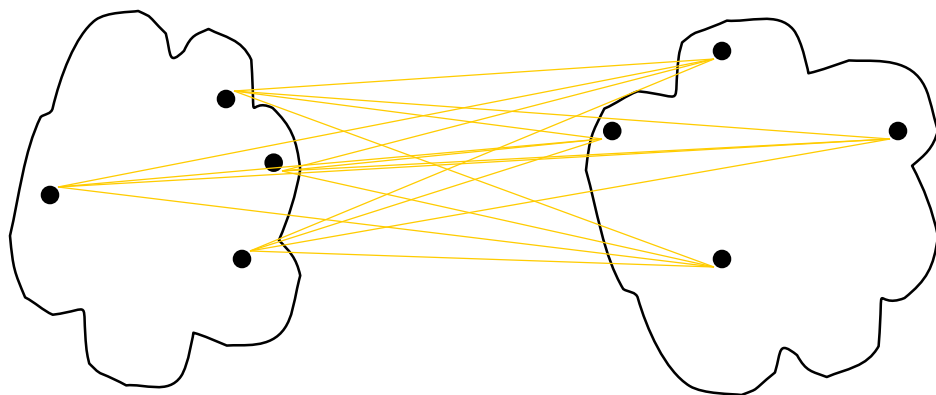


- MIN
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	p1	p2	p3	p4	p5	...
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p2						
p3						
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p5						
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.						

Proximity Matrix

How to Define Inter-Cluster Similarity

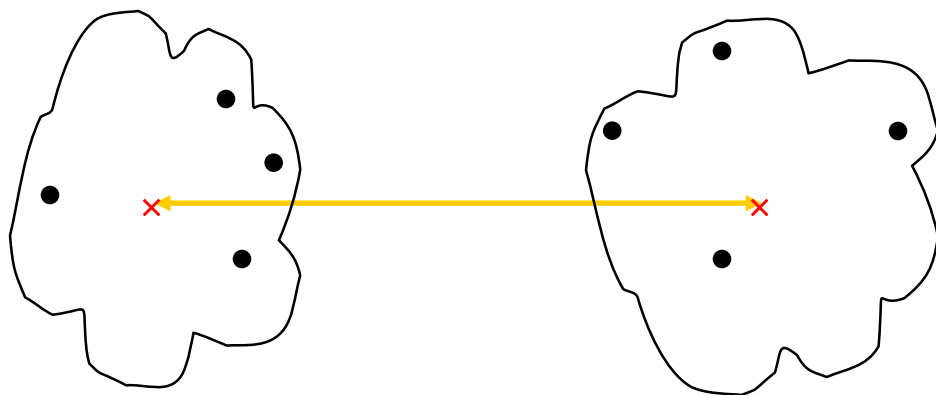


- MIN
- MAX
- **Group Average**
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	p1	p2	p3	p4	p5	...
p1						
p2						
p3						
p4						
p5						
.						
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.						

· **Proximity Matrix**

How to Define Inter-Cluster Similarity



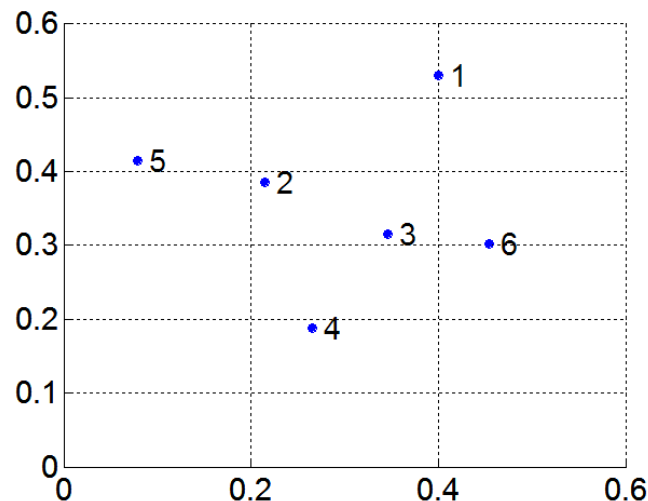
- MIN
- MAX
- Group Average
- **Distance Between Centroids**
- Other methods driven by an objective function
 - Ward's Method uses squared error

	p1	p2	p3	p4	p5	...
p1						
p2						
p3						
p4						
p5						
.						
.						
.						

Proximity Matrix

MIN or Single Link

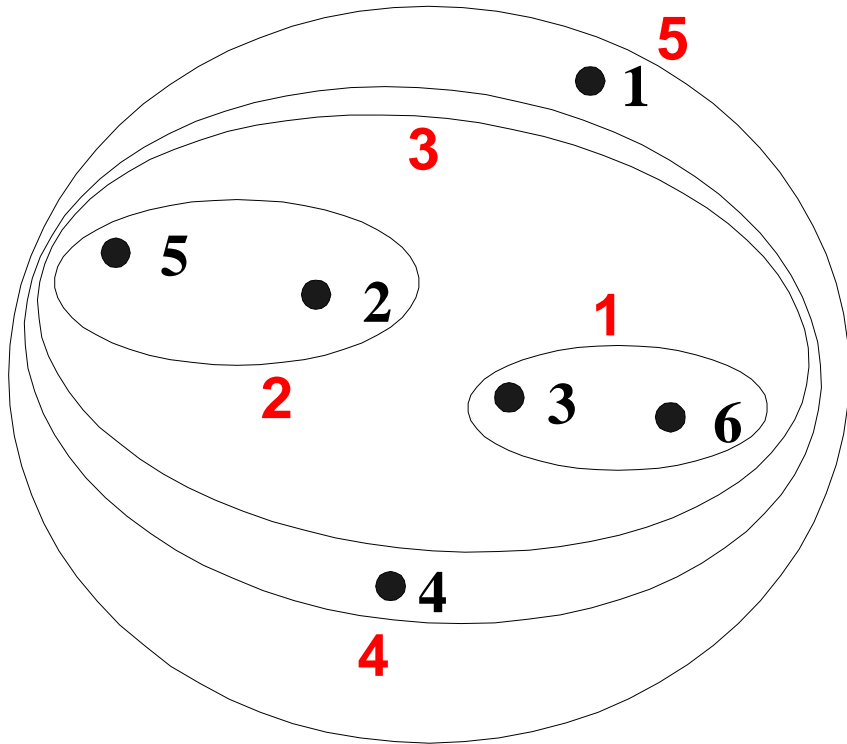
- Proximity of two clusters is based on the two closest points in the different clusters
 - Determined by one pair of points, i.e., by one link in the proximity graph
- Example:



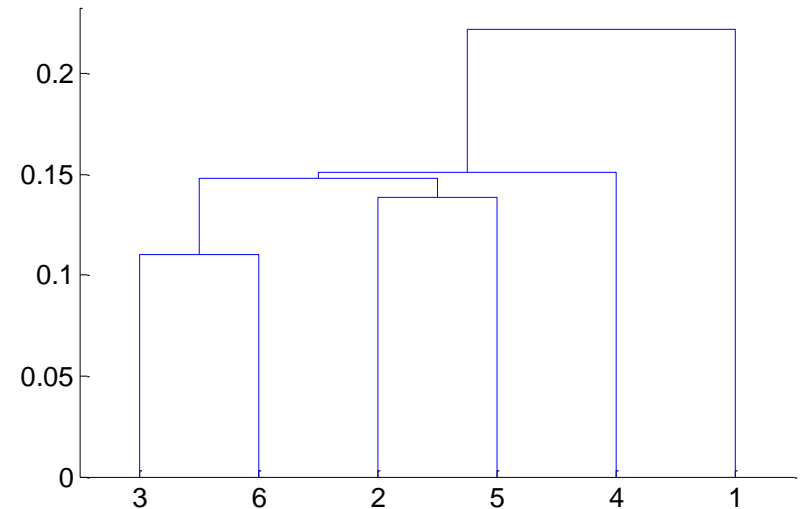
Distance Matrix:

	p1	p2	p3	p4	p5	p6
p1	0.00	0.24	0.22	0.37	0.34	0.23
p2	0.24	0.00	0.15	0.20	0.14	0.25
p3	0.22	0.15	0.00	0.15	0.28	0.11
p4	0.37	0.20	0.15	0.00	0.29	0.22
p5	0.34	0.14	0.28	0.29	0.00	0.39
p6	0.23	0.25	0.11	0.22	0.39	0.00

Hierarchical Clustering: MIN

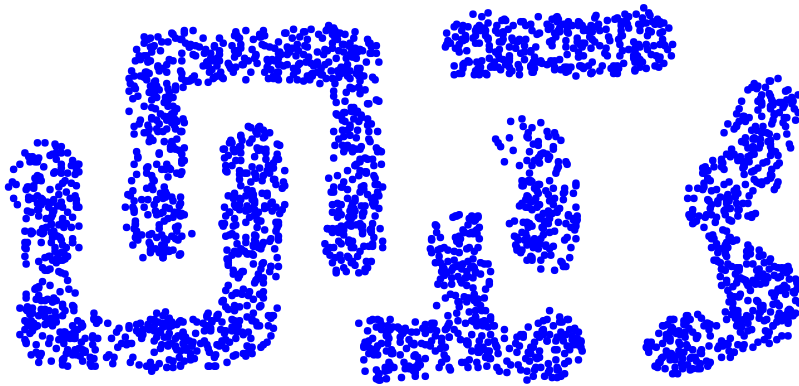


Nested Clusters

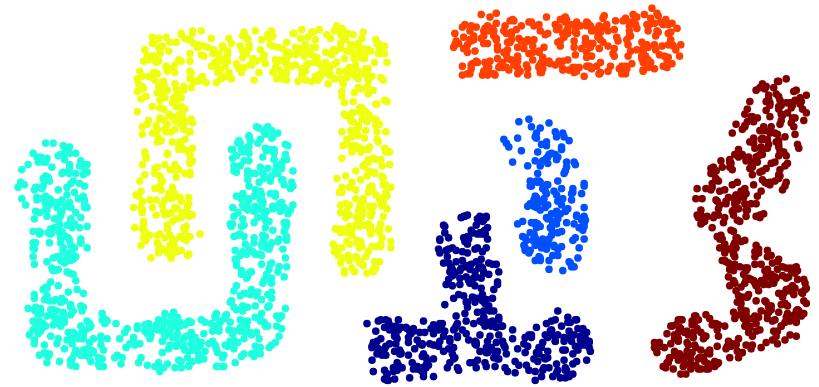


Dendrogram

Strength of MIN



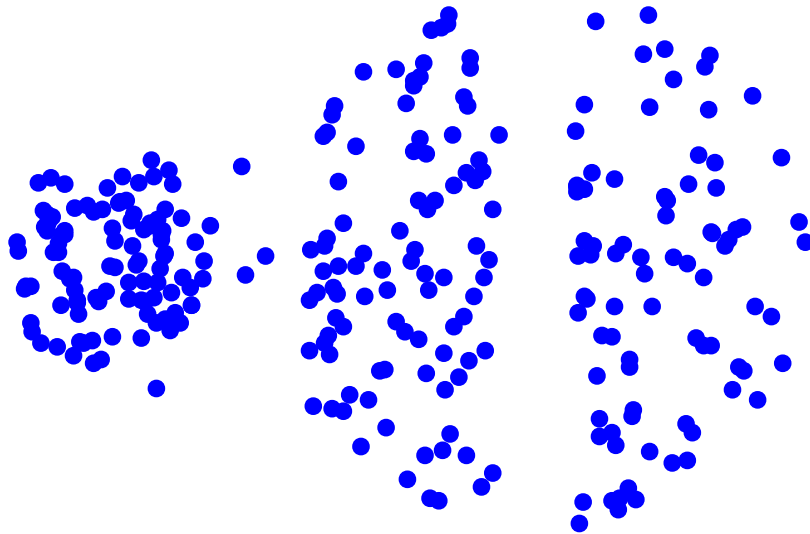
Original Points



Six Clusters

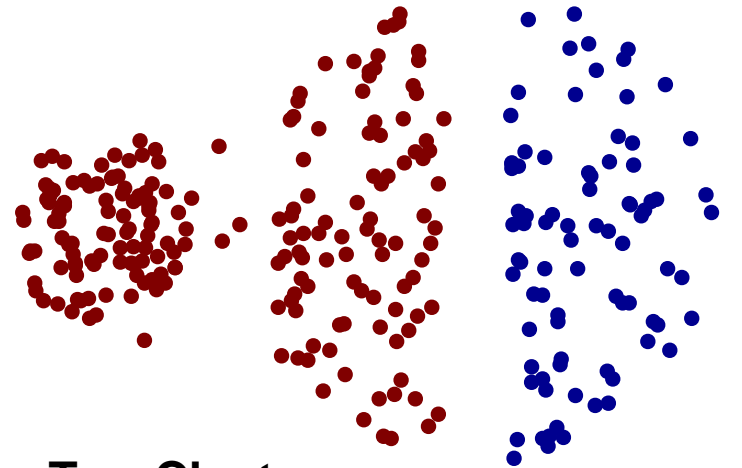
- Can handle non-elliptical shapes

Limitations of MIN

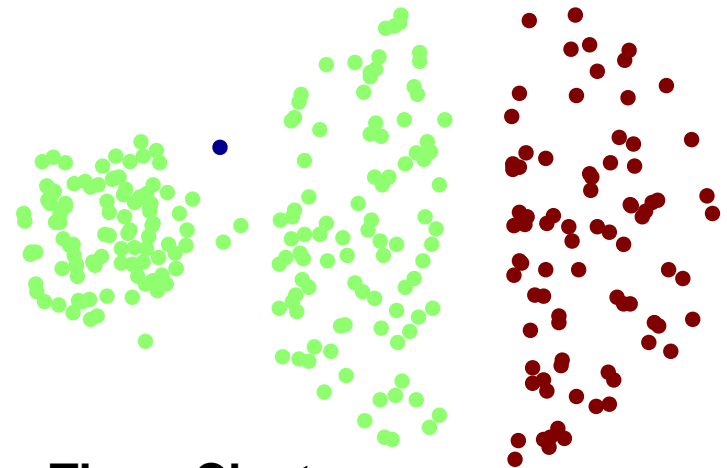


Original Points

- Sensitive to noise and outliers



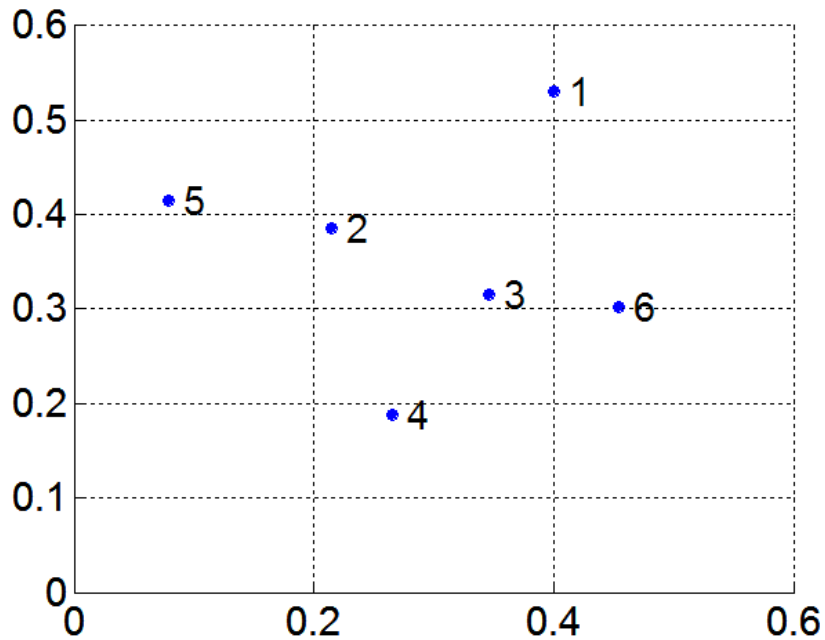
Two Clusters



Three Clusters

MAX or Complete Linkage

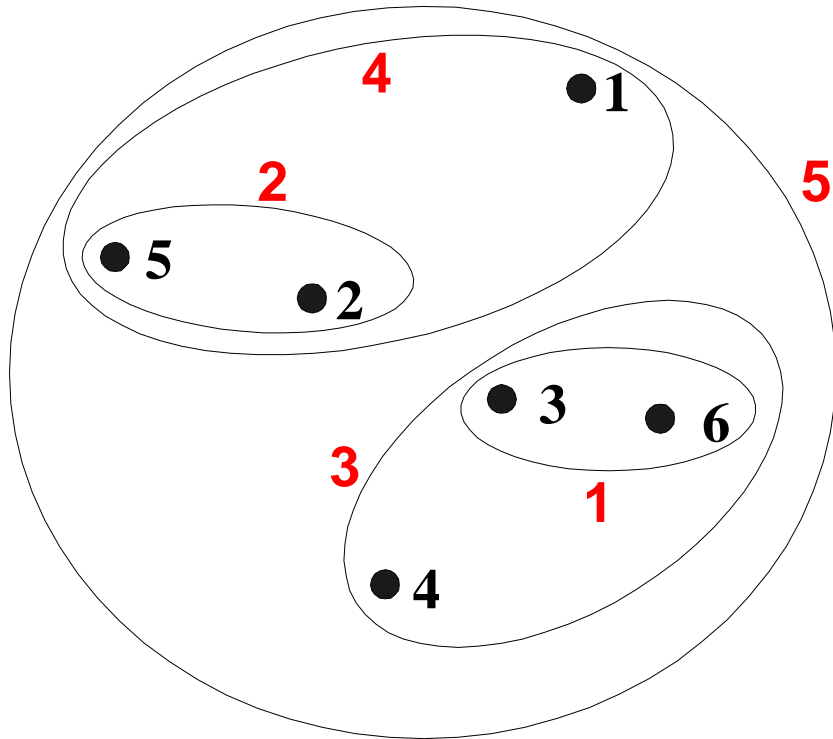
- Proximity of two clusters is based on the two most distant points in the different clusters
 - Determined by all pairs of points in the two clusters



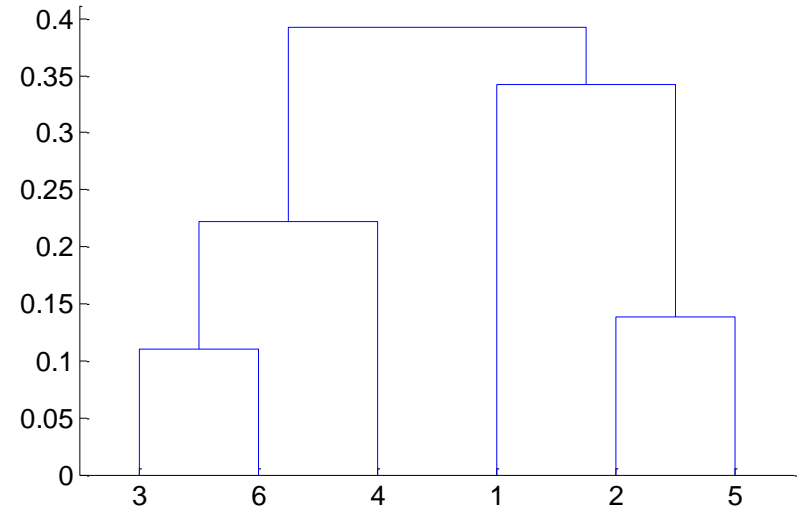
Distance Matrix:

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p1	0.00	0.24	0.22	0.37	0.34	0.23
p2	0.24	0.00	0.15	0.20	0.14	0.25
p3	0.22	0.15	0.00	0.15	0.28	0.11
p4	0.37	0.20	0.15	0.00	0.29	0.22
p5	0.34	0.14	0.28	0.29	0.00	0.39
p6	0.23	0.25	0.11	0.22	0.39	0.00

Hierarchical Clustering: MAX

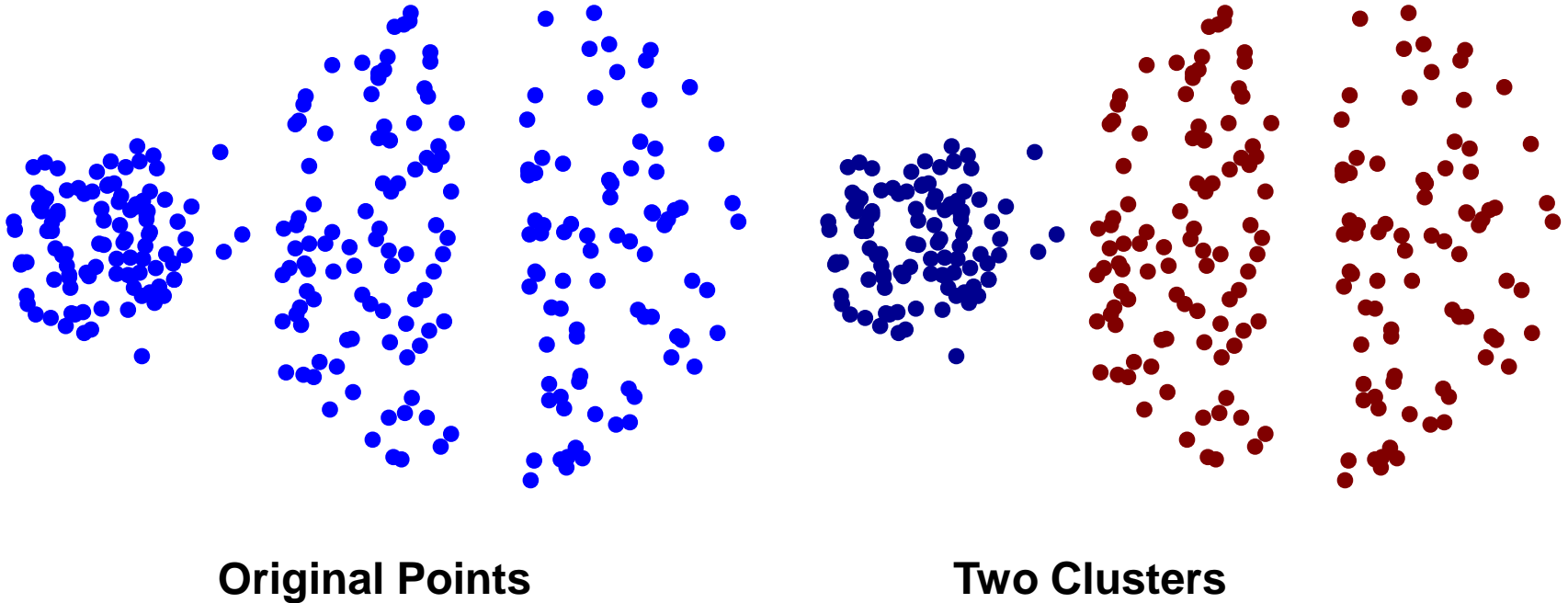


Nested Clusters



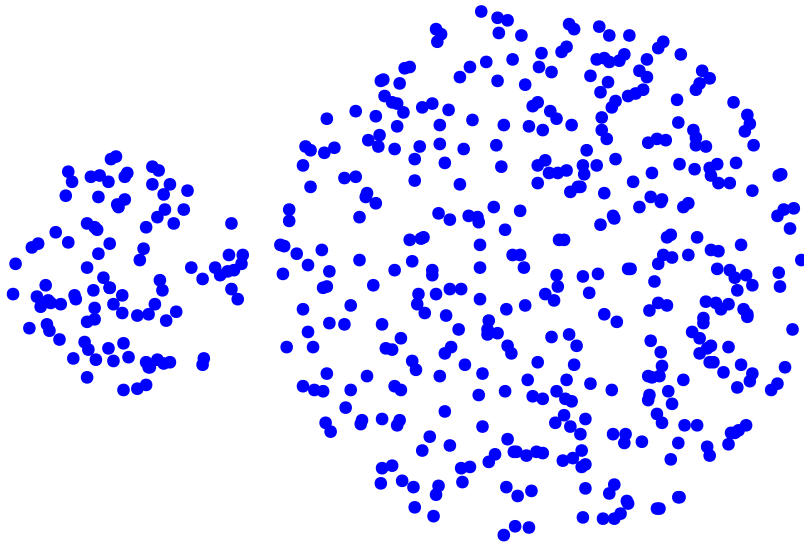
Dendrogram

Strength of MAX

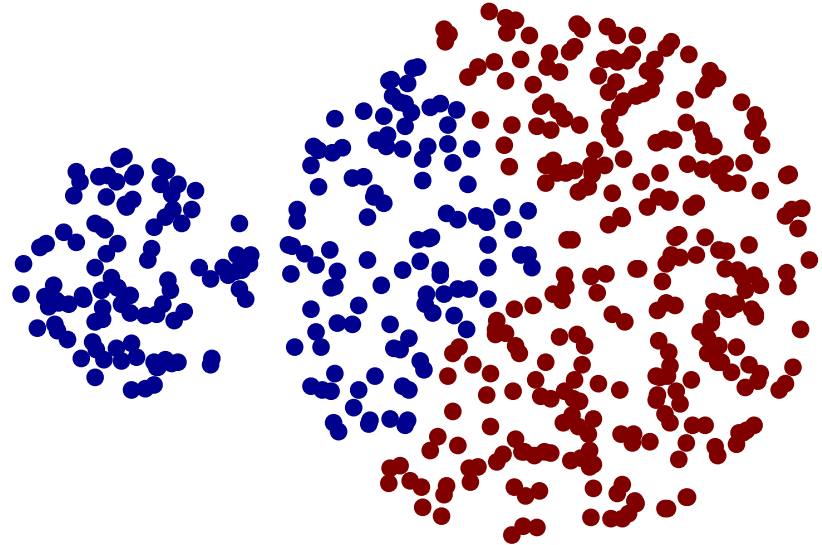


- Less susceptible to noise and outliers

Limitations of MAX



Original Points



Two Clusters

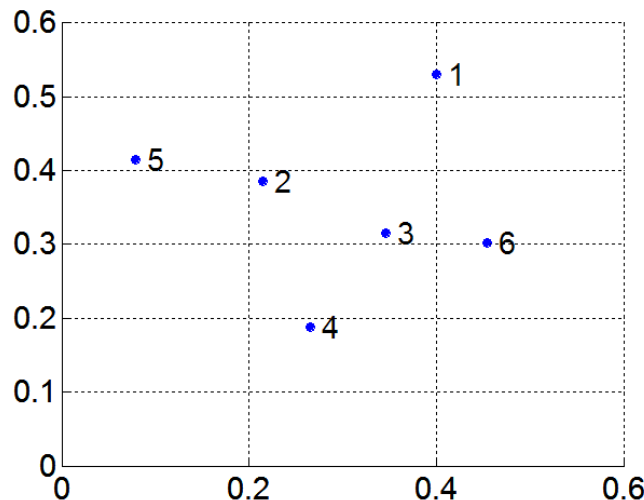
- Tends to break large clusters
- Biased towards globular clusters

Group Average

- Proximity of two clusters is the average of pairwise proximity between points in the two clusters.

$$\text{proximity}(\text{Cluster}_i, \text{Cluster}_j) = \frac{\sum_{\substack{p_i \in \text{Cluster}_i \\ p_j \in \text{Cluster}_j}} \text{proximity}(p_i, p_j)}{|\text{Cluster}_i| \times |\text{Cluster}_j|}$$

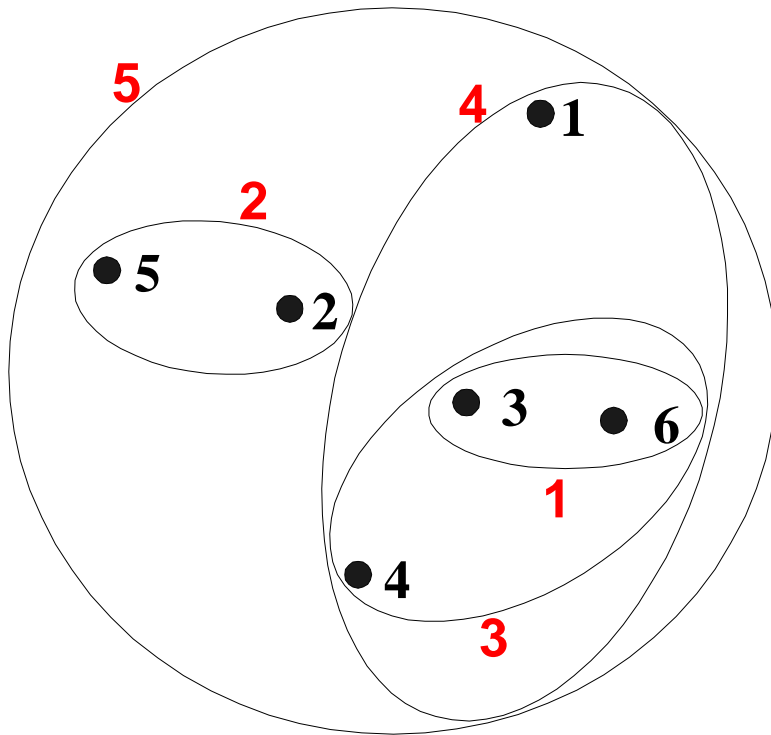
- Need to use average connectivity for scalability since total proximity favors large clusters



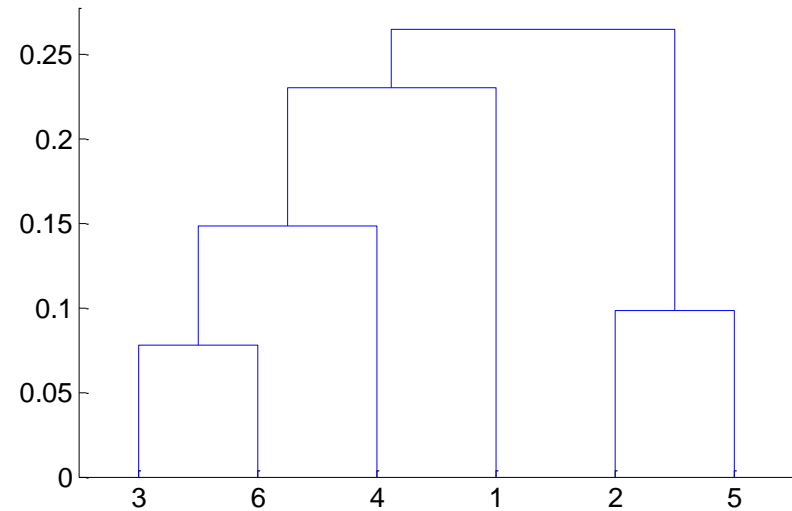
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Hierarchical Clustering: Group Average



Nested Clusters



Dendrogram

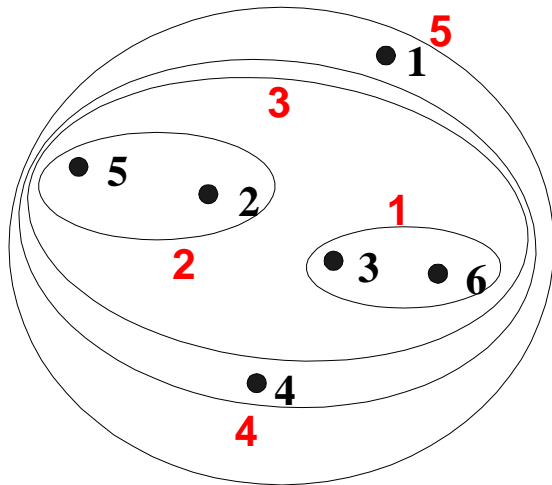
Hierarchical Clustering: Group Average

- Compromise between Single and Complete Link
- Strengths
 - Less susceptible to noise and outliers
- Limitations
 - Biased towards globular clusters

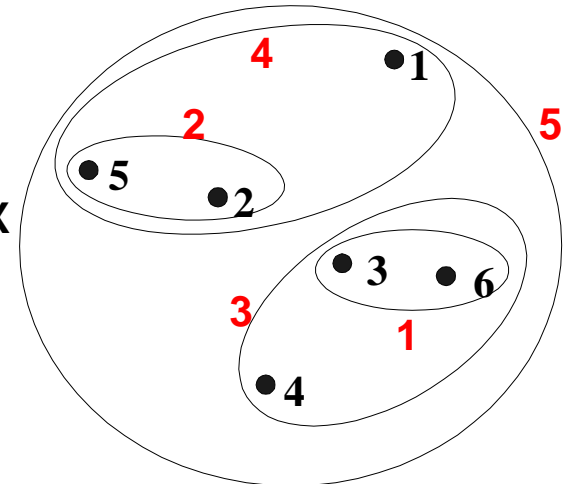
Cluster Similarity: Ward's Method

- Similarity of two clusters is based on the increase in squared error when two clusters are merged
 - Similar to group average if distance between points is distance squared
- Less susceptible to noise and outliers
- Biased towards globular clusters
- Hierarchical analogue of K-means
 - Can be used to initialize K-means

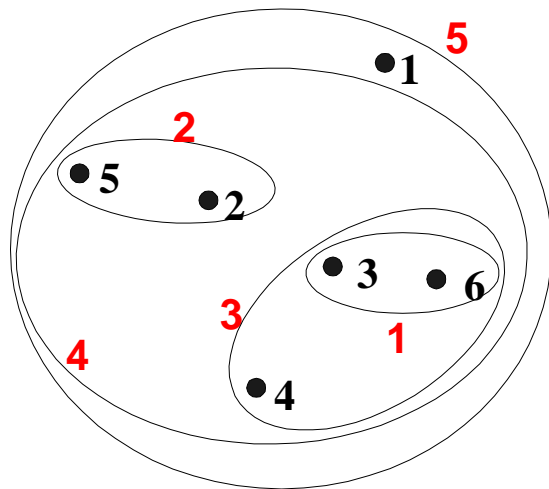
Hierarchical Clustering: Comparison



MIN

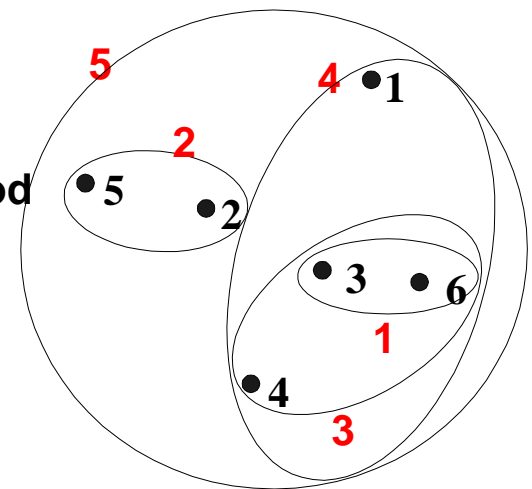


MAX



Group Average

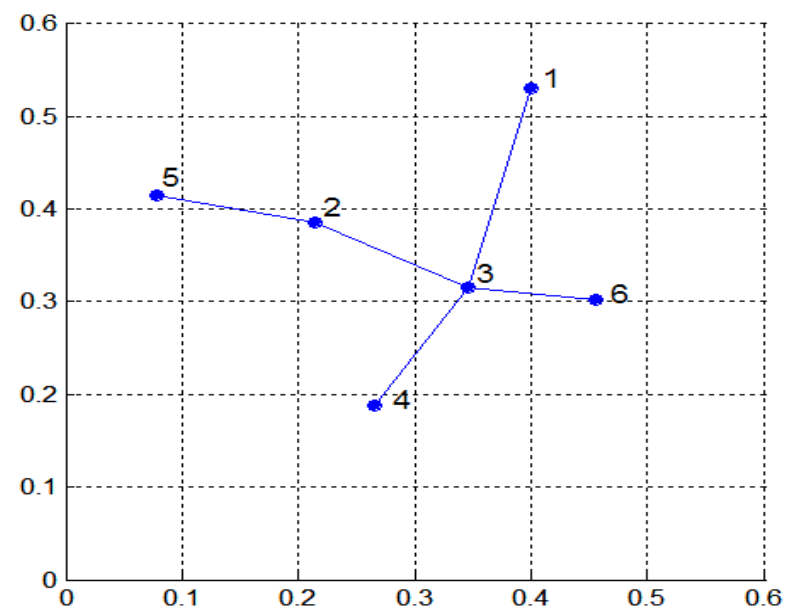
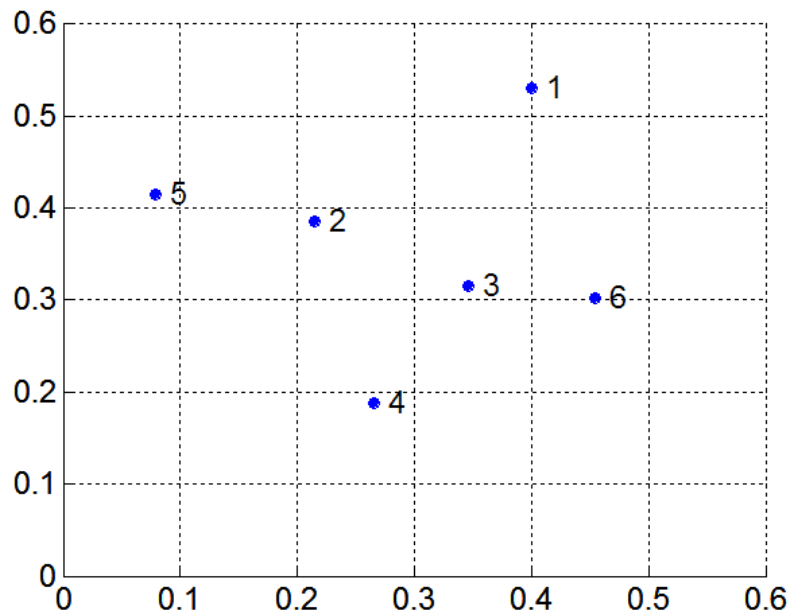
Ward's Method



MST: Divisive Hierarchical Clustering

● Build MST (Minimum Spanning Tree)

- Start with a tree that consists of any point
- In successive steps, look for the closest pair of points (p, q) such that one point (p) is in the current tree but the other (q) is not
- Add q to the tree and put an edge between p and q



MST: Divisive Hierarchical Clustering

- Use MST for constructing hierarchy of clusters

Algorithm 7.5 MST Divisive Hierarchical Clustering Algorithm

- 1: Compute a minimum spanning tree for the proximity graph.
 - 2: **repeat**
 - 3: Create a new cluster by breaking the link corresponding to the largest distance (smallest similarity).
 - 4: **until** Only singleton clusters remain
-

Hierarchical Clustering: Time and Space requirements

- $O(N^2)$ space since it uses the proximity matrix.
 - N is the number of points.

- $O(N^3)$ time in many cases
 - There are N steps and at each step the size, N^2 , proximity matrix must be updated and searched
 - Complexity can be reduced to $O(N^2 \log(N))$ time with some cleverness

Hierarchical Clustering: Problems and Limitations

- Once a decision is made to combine two clusters, it cannot be undone
- No global objective function is directly minimized
- Different schemes have problems with one or more of the following:
 - Sensitivity to noise and outliers
 - Difficulty handling clusters of different sizes and non-globular shapes
 - Breaking large clusters