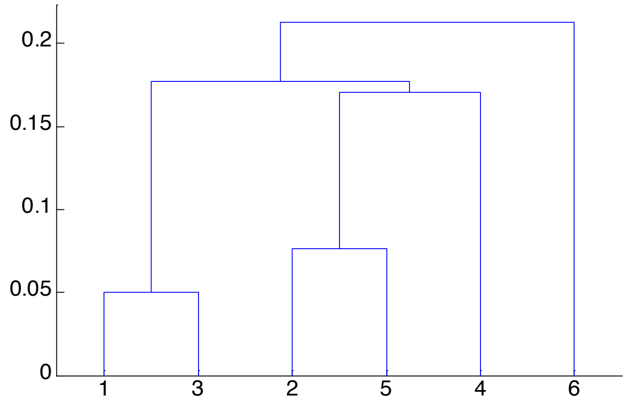
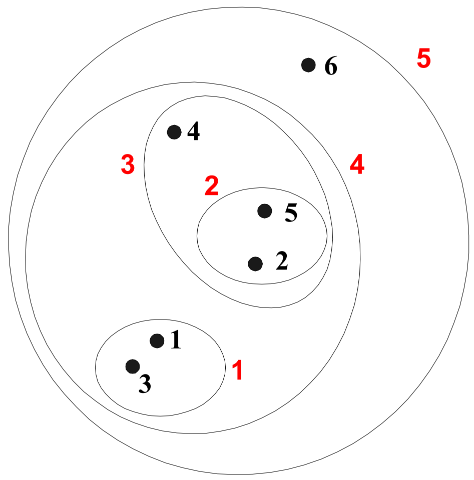
Hierarchical Clustering

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

- Does 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

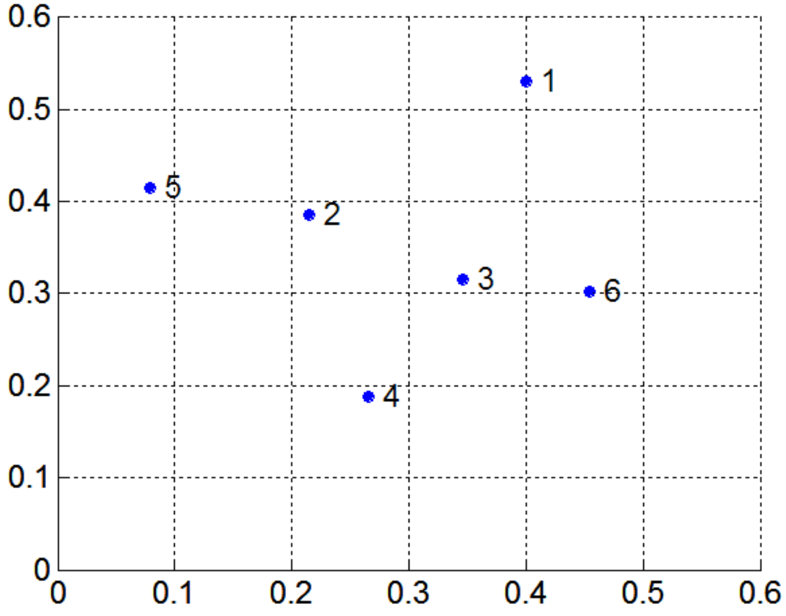
- The dendrogram may correspond to meaningful taxonomies

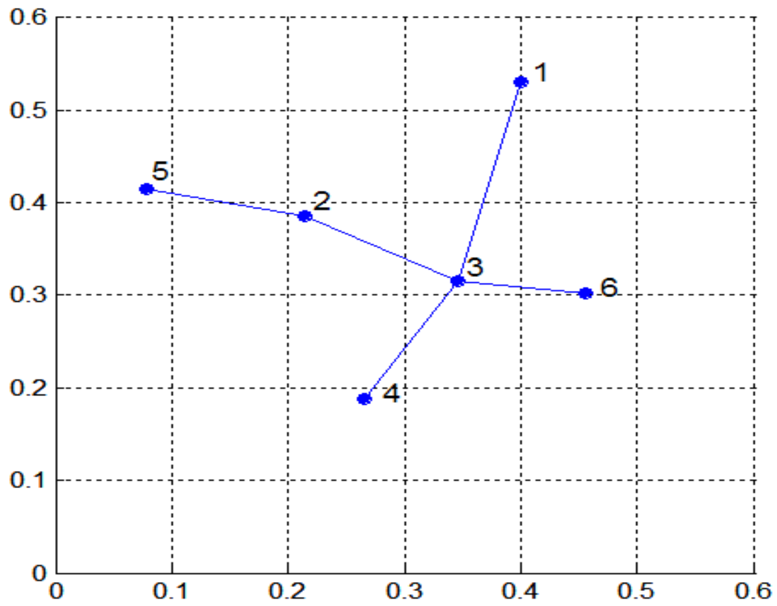
Hierarchical Clustering

- 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 a point (or there are k clusters)
- Traditional hierarchical algorithms use a similarity or distance matrix
  - Merge or split one cluster at a time

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





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

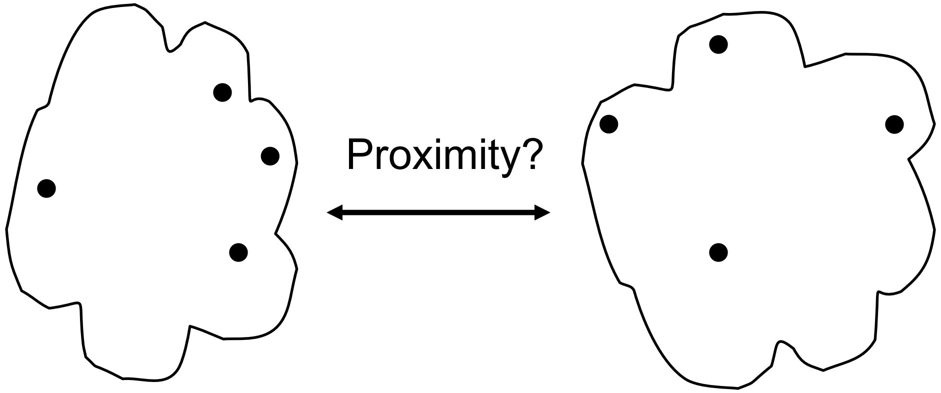
Agglomerative Clustering Algorithm

- More 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

How to Define Inter-Cluster Proximity

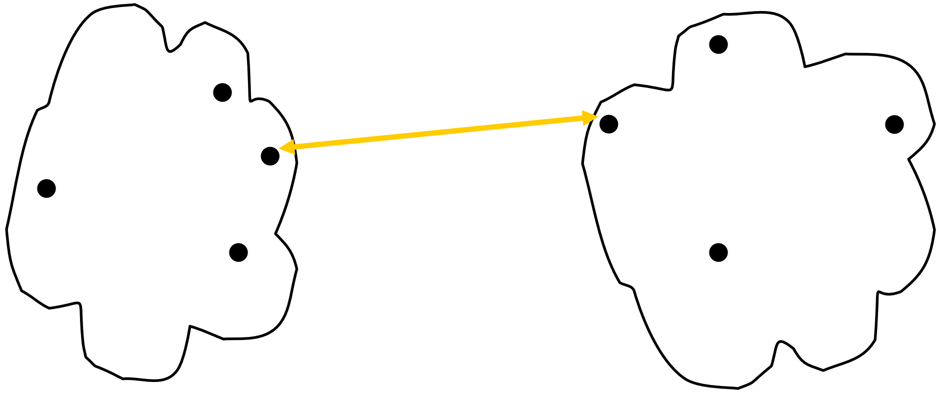


	p1	p2	p3	p4	p5	. . .
p1						
p2						
p3						
p4						
p5						
.						
.						
.						

Proximity Matrix

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

How to Define Inter-Cluster Proximity



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

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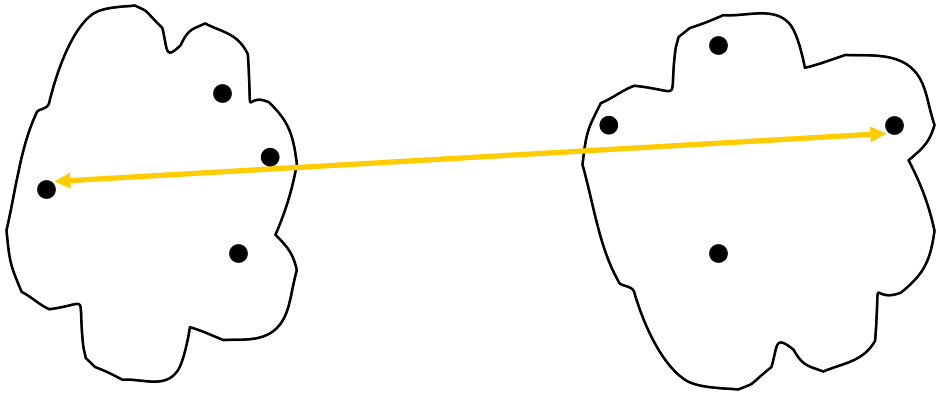
How to Define Inter-Cluster Proximity



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

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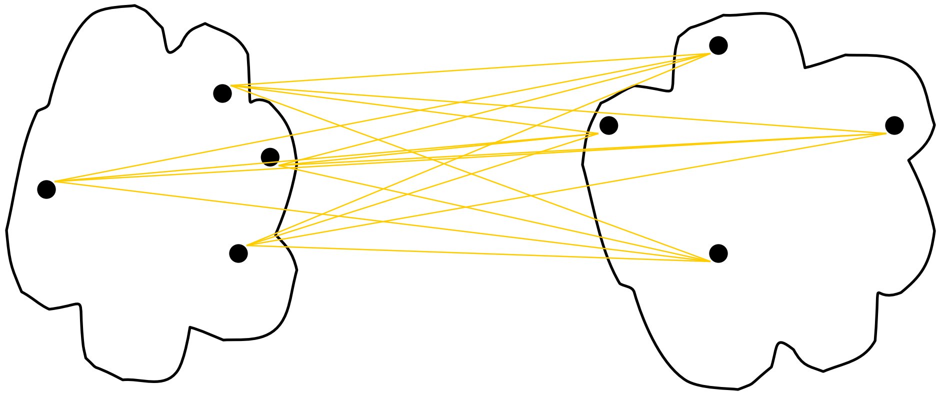
How to Define Inter-Cluster Proximity



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

Proximity Matrix

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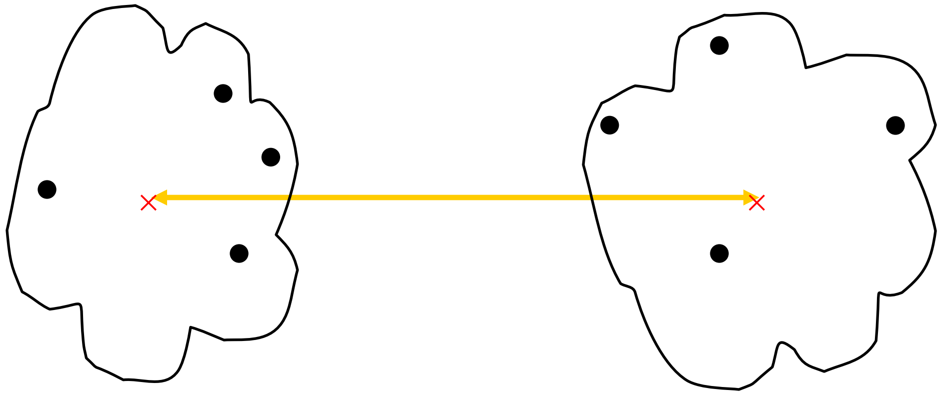
How to Define Inter-Cluster Proximity



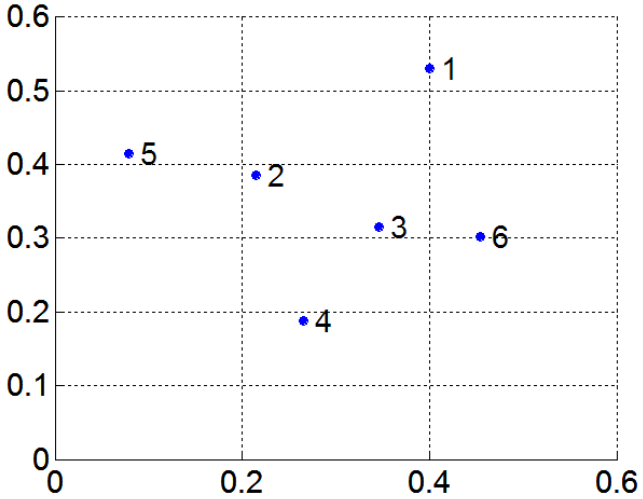
	p1	p2	p3	p4	p5	. . .
p1						
p2						
p3						
p4						
p5						
.						
.						
.						

Proximity Matrix

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

MIN

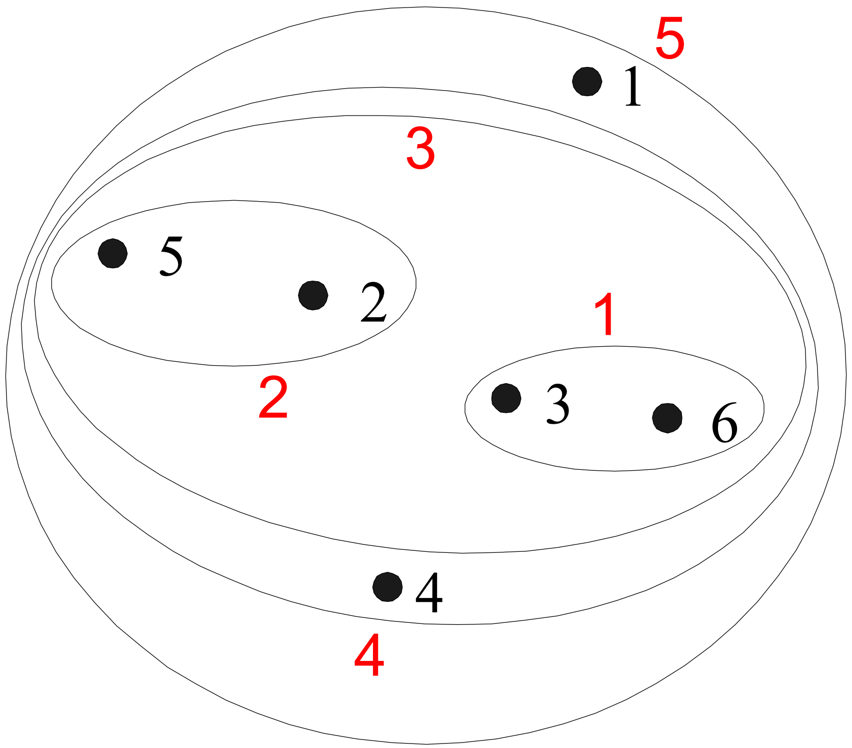
- Proximity of two clusters is based on the two closest points in the different clusters
  - Determined by one pair of points
- Example:



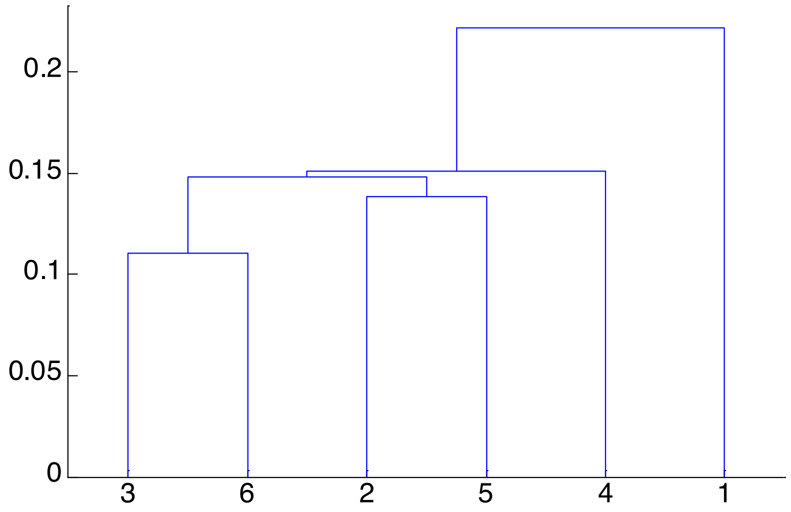
Distance Matrix:

	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

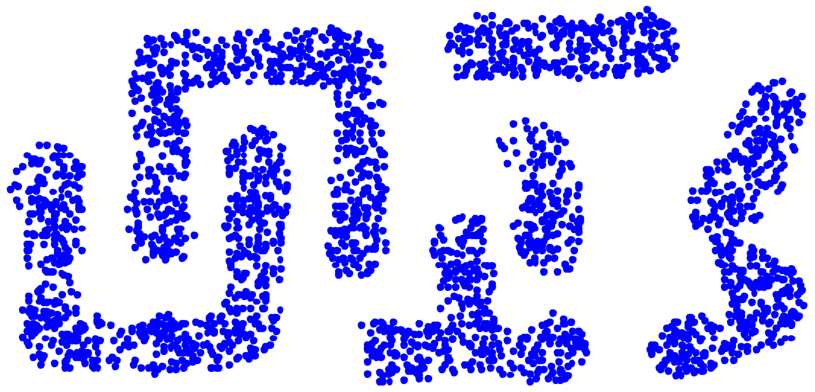


Nested Clusters

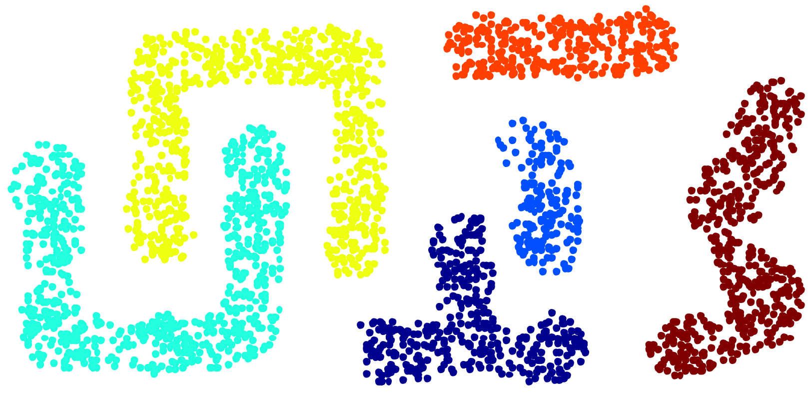


Dendrogram

Strength of MIN



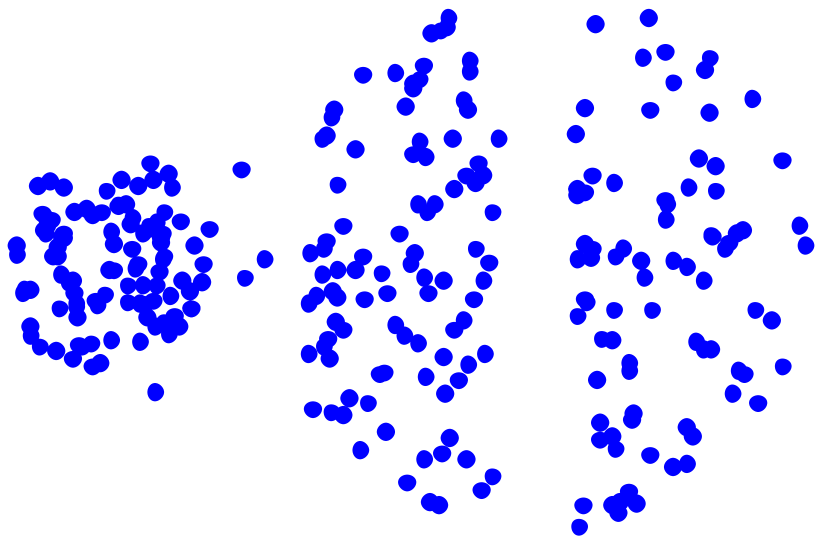
Original Points



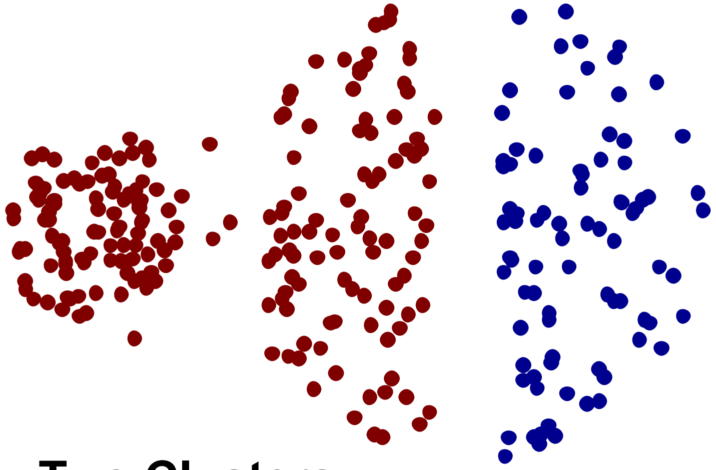
Six Clusters

- Can handle non-elliptical shapes

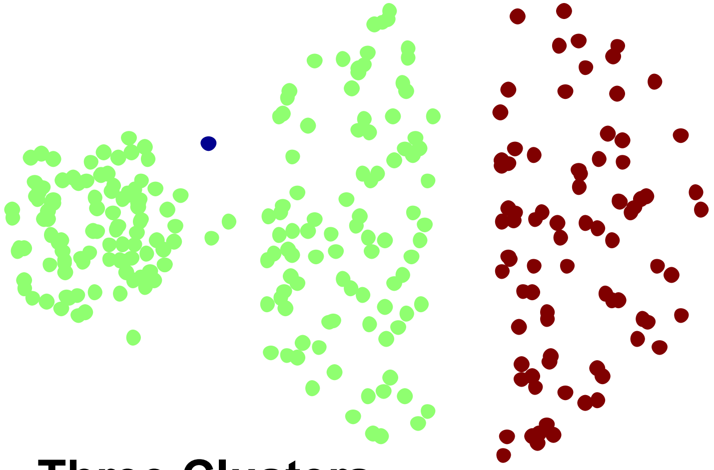
Limitations of MIN



Original Points



Two Clusters

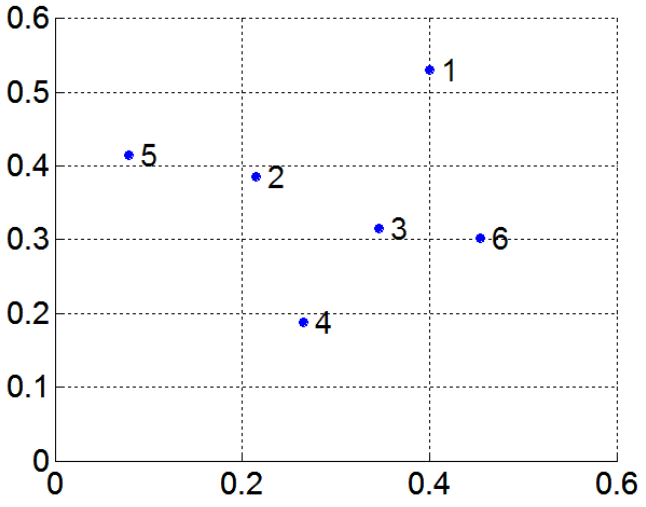


Three Clusters

- **Sensitive to noise**

MAX

- Similarity 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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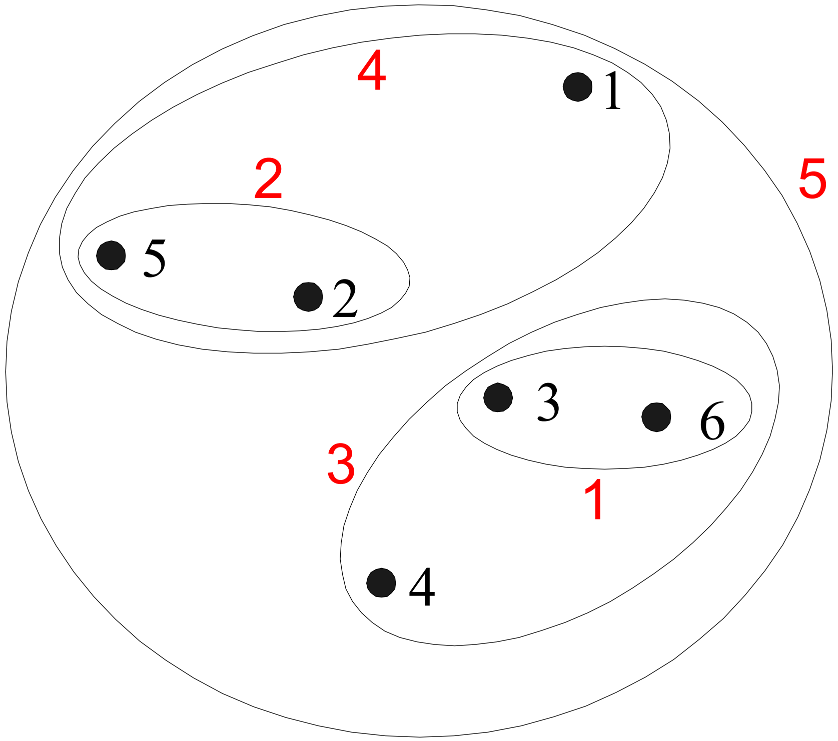
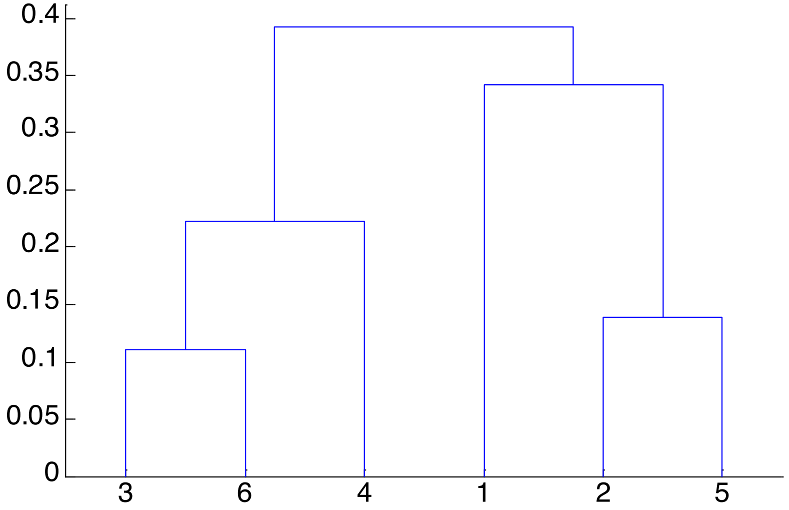
p6	0.23	0.25	0.11	0.22	0.39	0.00

Hierarchical Clustering: MAX

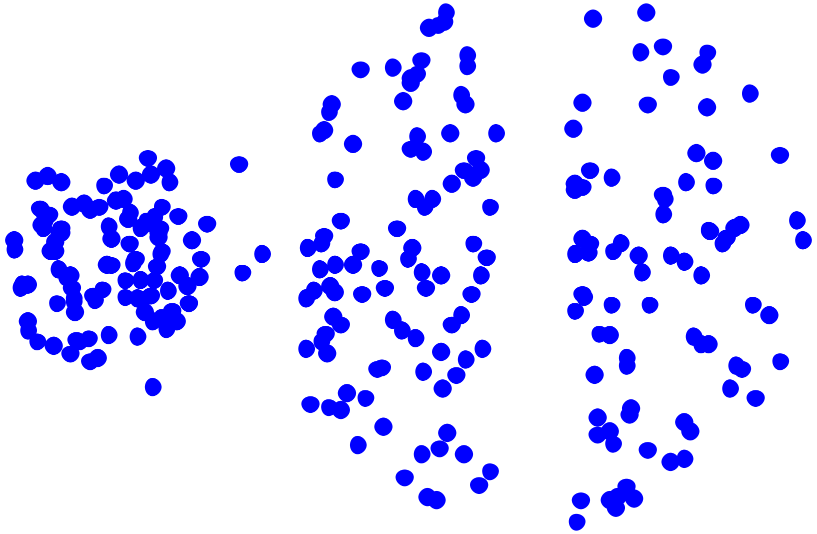


Nested Clusters

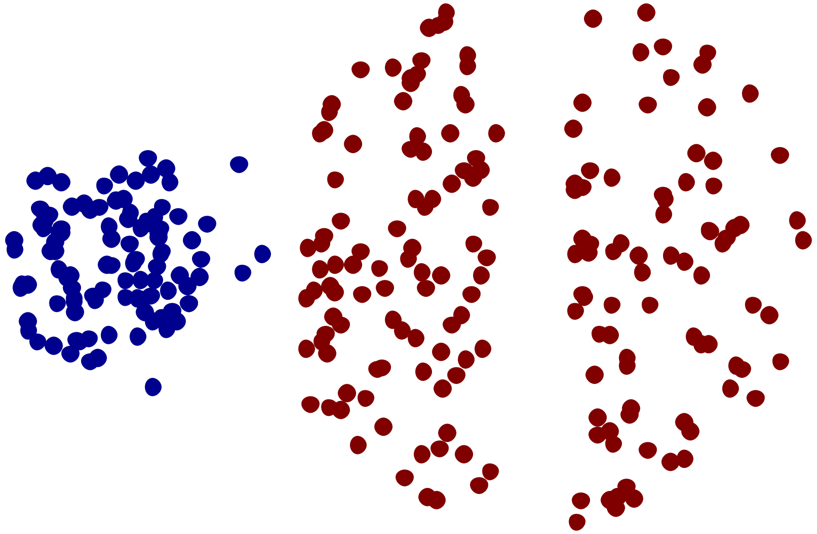


Dendrogram

Strength of MAX



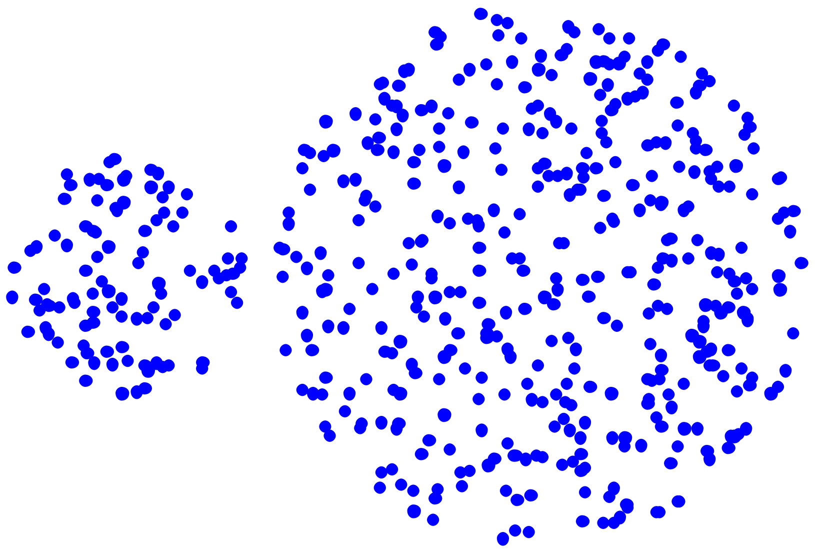
Original Points



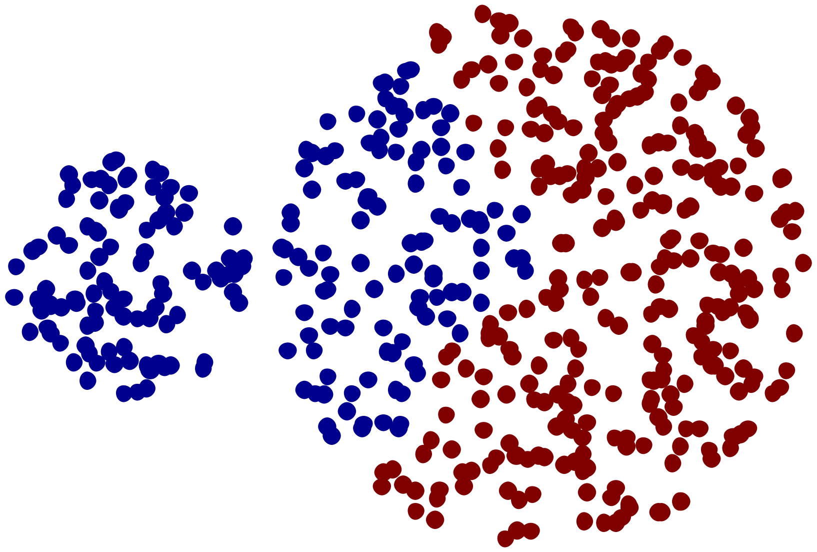
Two Clusters

- Less susceptible to noise

Limitations of MAX



Original Points



Two Clusters

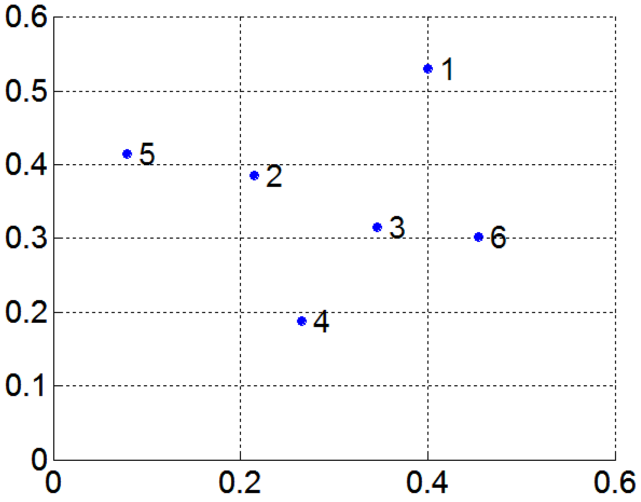
- Tends to break large clusters

Group Average

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

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

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



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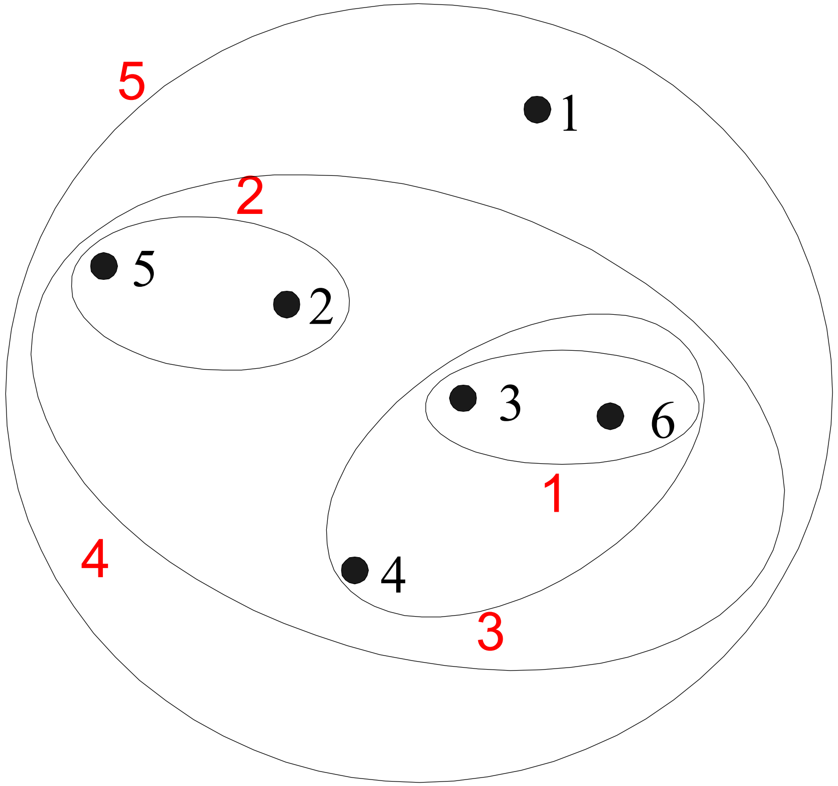
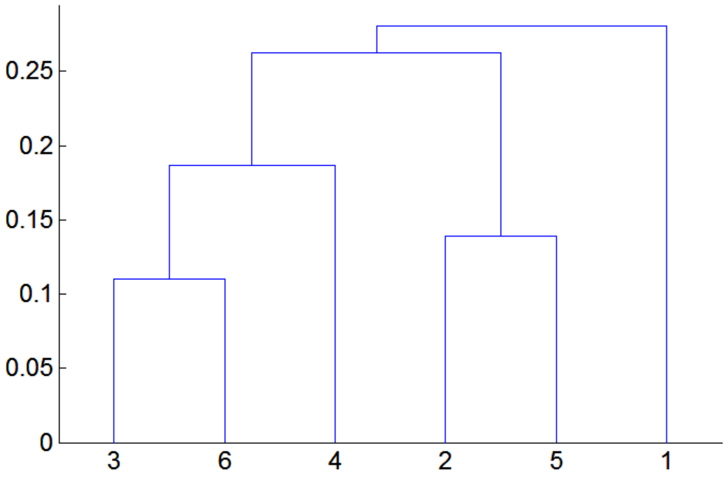
p3	0.22	0.15	0.00	0.15	0.28	0.11
p4	0.37	0.20	0.15	0.00	0.29	0.22
p5	0.34	0.14	0.28	0.29	0.00	0.39
p6	0.23	0.25	0.11	0.22	0.39	0.00

Hierarchical Clustering: Group Average



Nested Clusters



Dendrogram

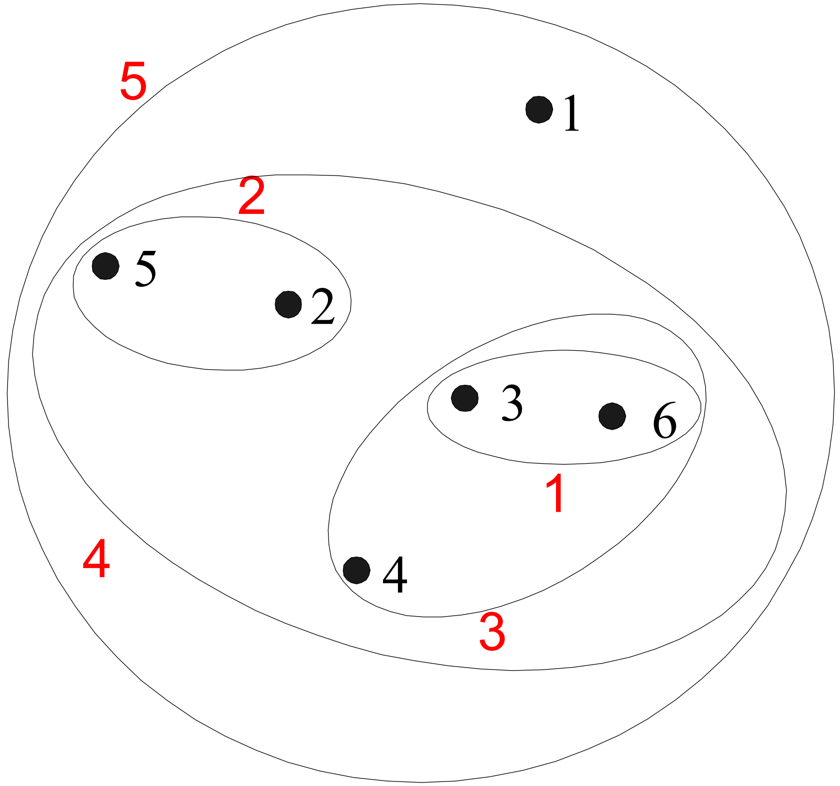
Hierarchical Clustering: Group Average

- Compromise between MIN and MAX
- Strengths
  - Less susceptible to noise
- Limitations
  - Biased towards globular clusters

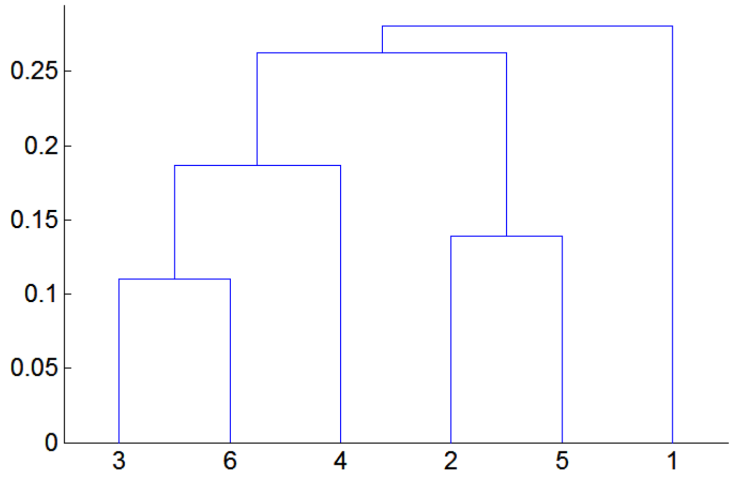
Centroid Methods

- Similarity of two clusters is based on proximity between centroids of clusters
- Less susceptible to noise
- Biased towards globular clusters

Hierarchical Clustering: Centroid



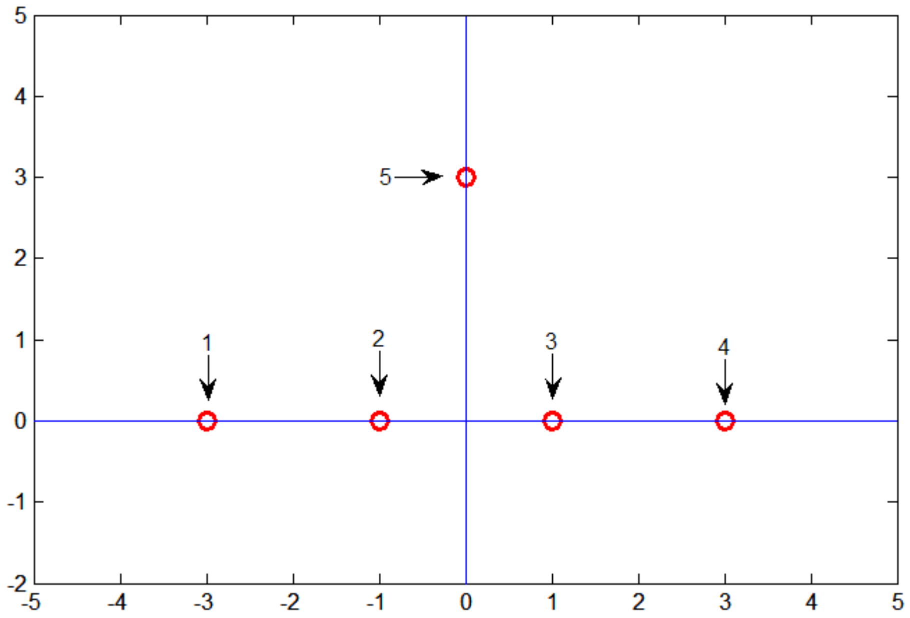
Nested Clusters

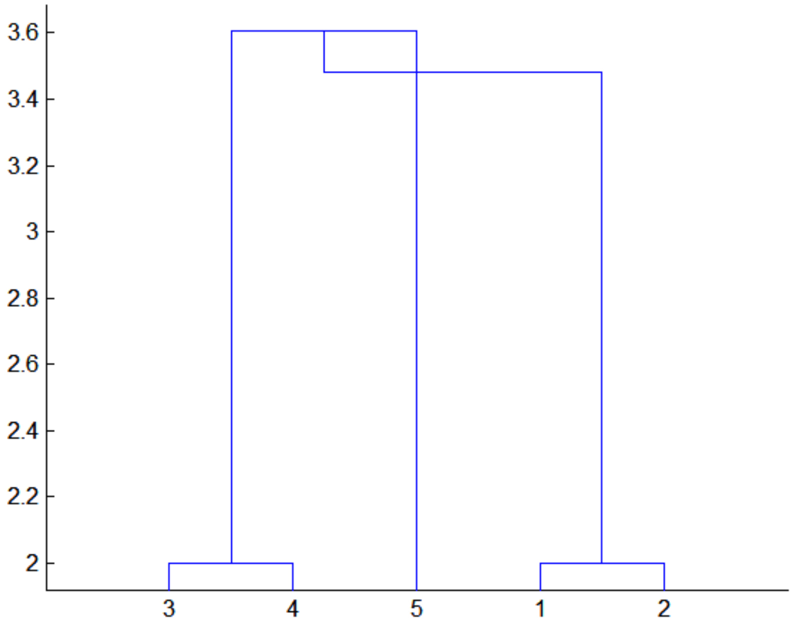


Dendrogram

Inversion

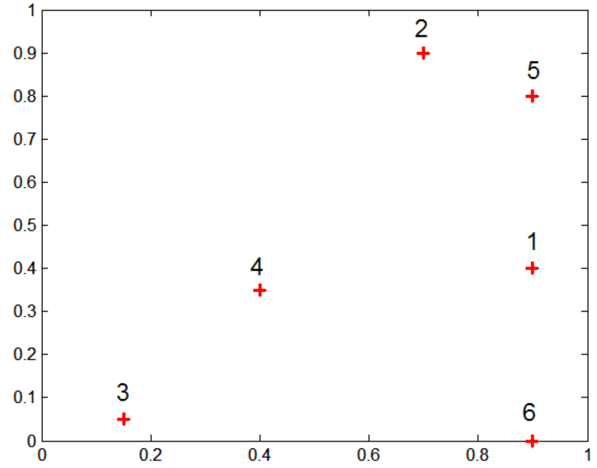
- Two clusters that are merged may be more similar than the pair of clusters that were merged in a previous step

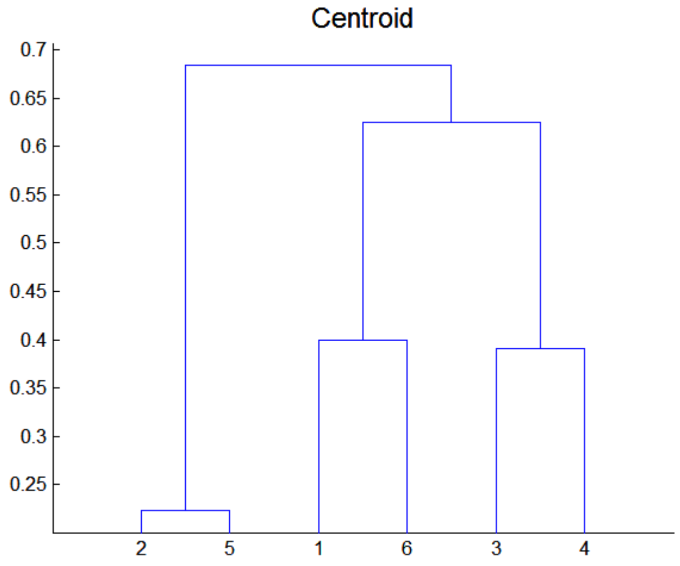


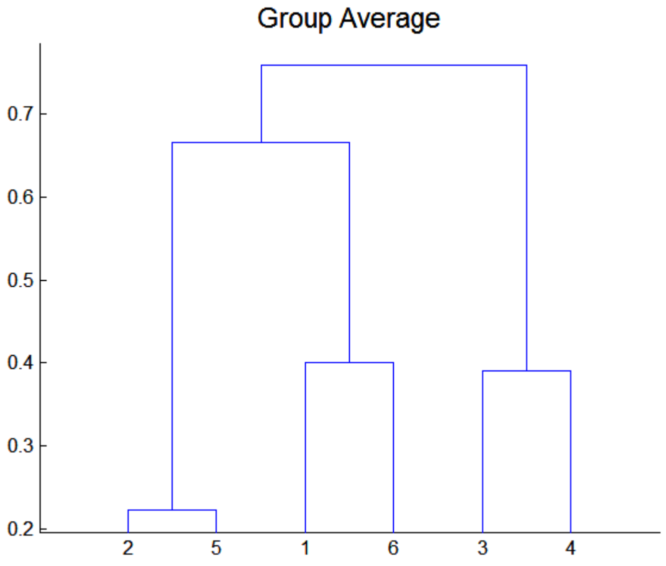


Centroid vs Group Average

X	Y
0.9	0.4
0.7	0.9
0.15	0.05
0.4	0.35
0.9	0.8
0.9	0



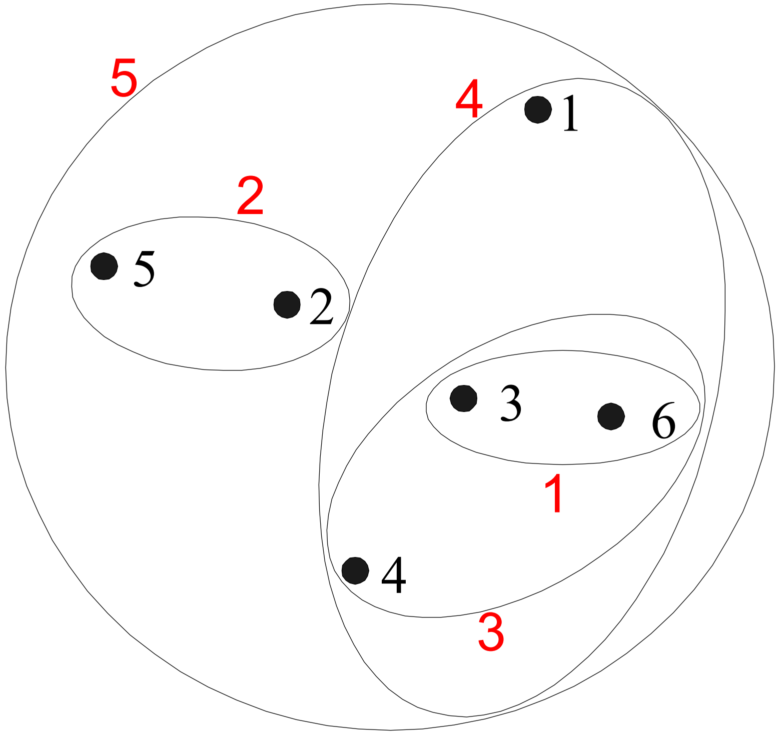




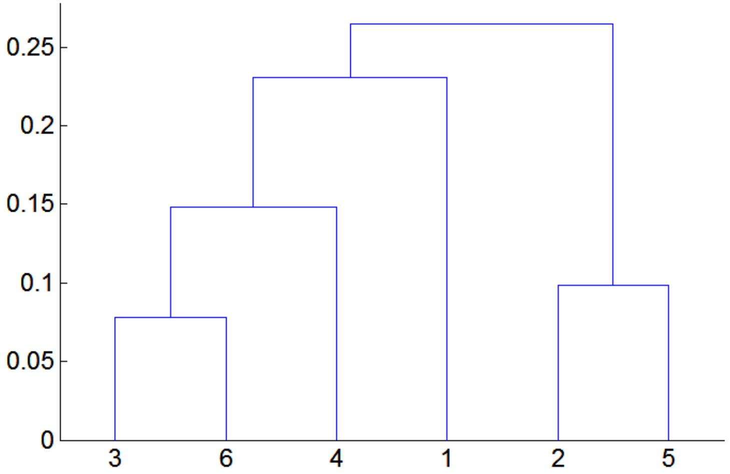
Cluster Similarity: Ward's Method

- Proximity 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
- Biased towards globular clusters

Hierarchical Clustering: Ward's Method

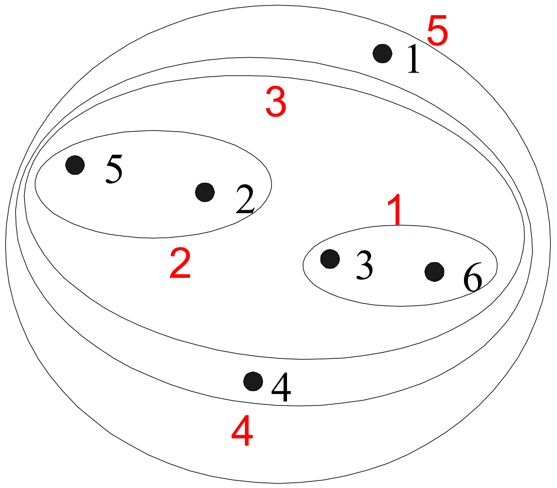


Nested Clusters



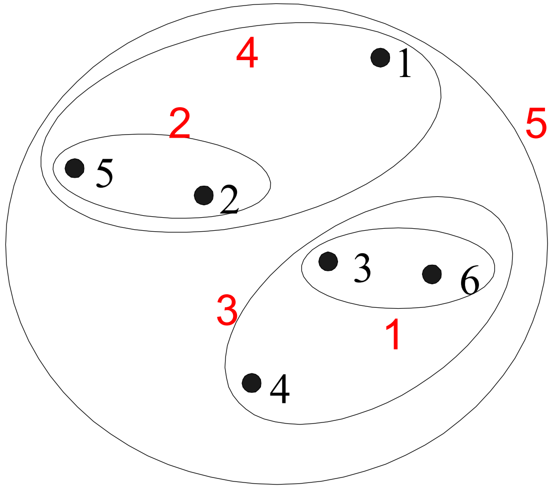
Dendrogram

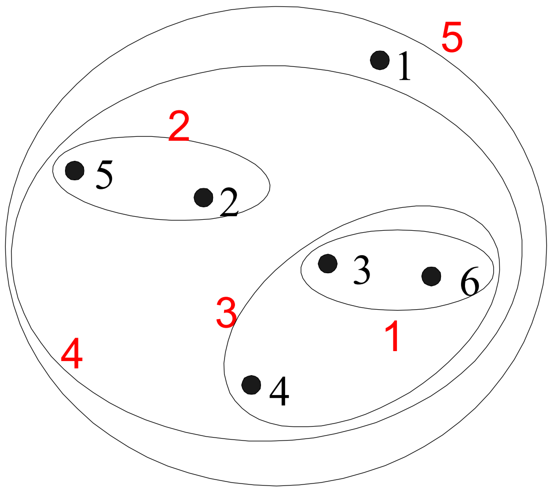
Hierarchical Clustering: Comparison



MIN

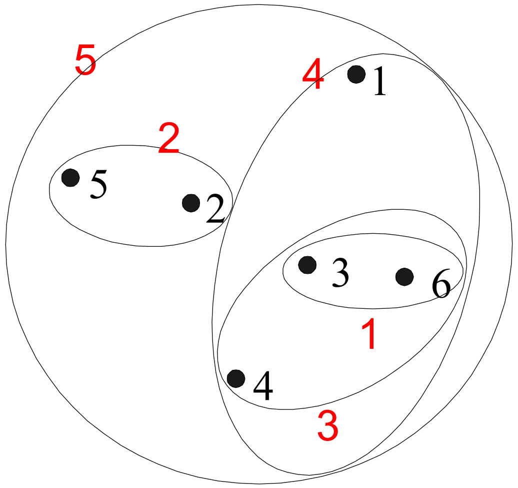
MAX





Group Average

Ward's Method



Lance-Williams Formula

- Proximity between clusters Q and R, where R is formed by merging clusters A and B

$$p(R,Q) = \alpha_A p(A,Q) + \alpha_B p(B,Q) + \beta p(A,B) + \gamma |p(A,Q) - p(B,Q)|$$

Clustering Method	$\alpha_{\mathbf{A}}$	$\alpha_{\mathbf{B}}$	β	γ
MIN	1/2	1/2	0	-1/2
MAX	1/2	1/2	0	1/2
Group Average	$\frac{m_A}{m_A+m_B}$	$\frac{m_B}{m_A+m_B}$	0	0
Centroid	$\frac{m_A}{m_A+m_B}$	$\frac{m_B}{m_A+m_B}$	$\frac{-m_A m_B}{(m_A+m_B)^2}$	0
Ward's	$\frac{m_A+m_Q}{m_A+m_B+m_Q}$	$\frac{m_B+m_Q}{m_A+m_B+m_Q}$	$\frac{-m_Q}{m_A+m_B+m_Q}$	0

  - m_i is size of cluster i, p(i,j) is proximity of clusters i & j

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
  - Difficulty handling different sized clusters and convex shapes
  - Breaking large clusters