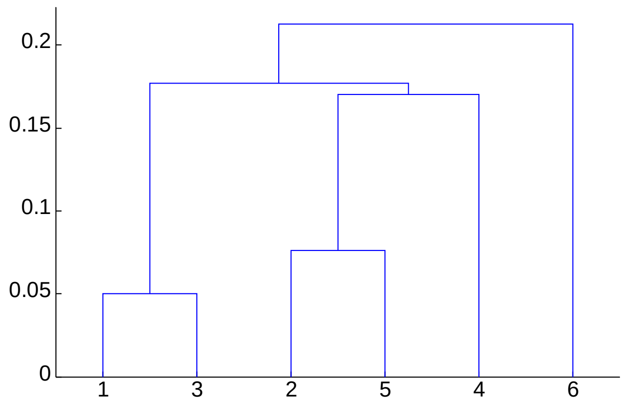
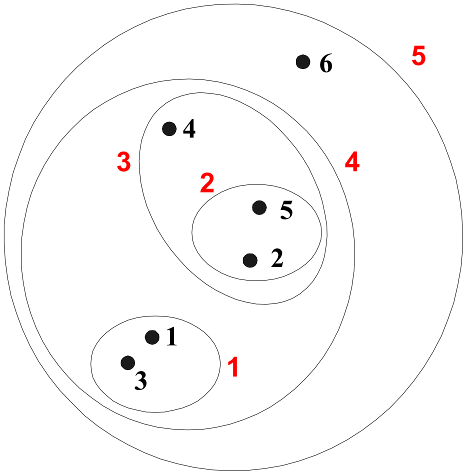
Hierarchical Clustering

- 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 dendogram at the proper level

- They may correspond to meaningful taxonomies
  - Example in biological sciences (e.g., animal kingdom, phylogeny reconstruction, …)

Hierarchical Clustering

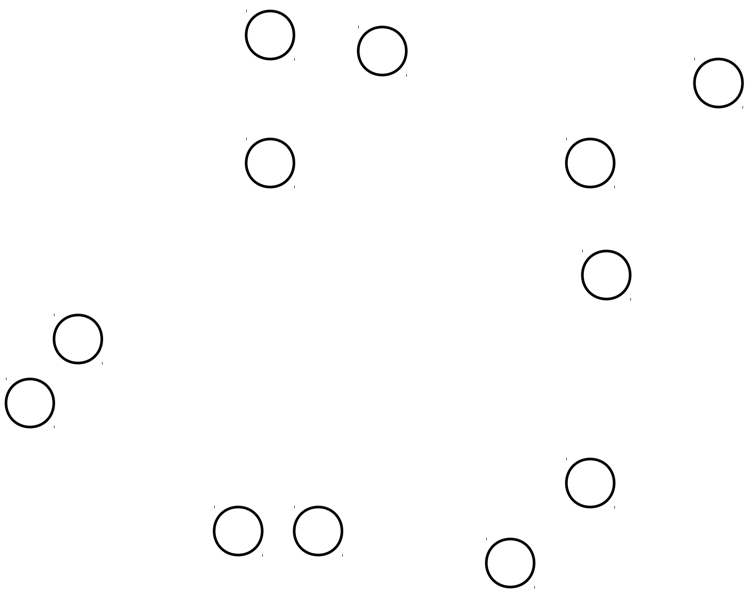
- Two main types of hierarchical clustering
  - Agglomerative:
    - Start with the points as individual clusters
    - At each step, merge the closest pair of clusters until only one cluster (or k clusters) left
  - Divisive:
    - Start with one, all-inclusive cluster
    - At each step, split a cluster until each cluster contains a 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

- More popular hierarchical clustering technique
- Basic algorithm is straightforward
  - *Compute the proximity matrix*
  - *Let each data point be a cluster*
  - ***Repeat***
  - *Merge the two closest clusters*
  - *Update the proximity matrix*
  - ***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

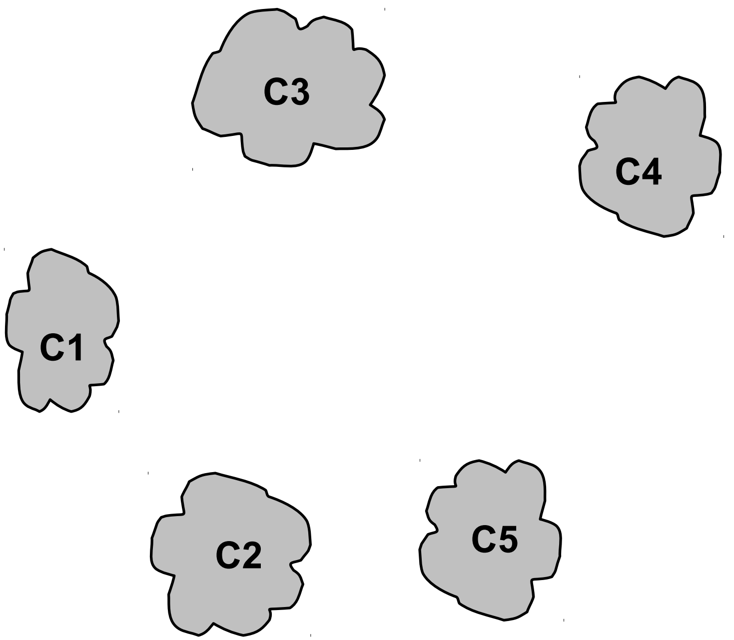


	p1	p2	p3	p4	p5	. . .
p1						
p2						
p3						
p4						
p5						
.						
.						
.						

Proximity Matrix

Intermediate Situation

- After some merging steps, we have some clusters

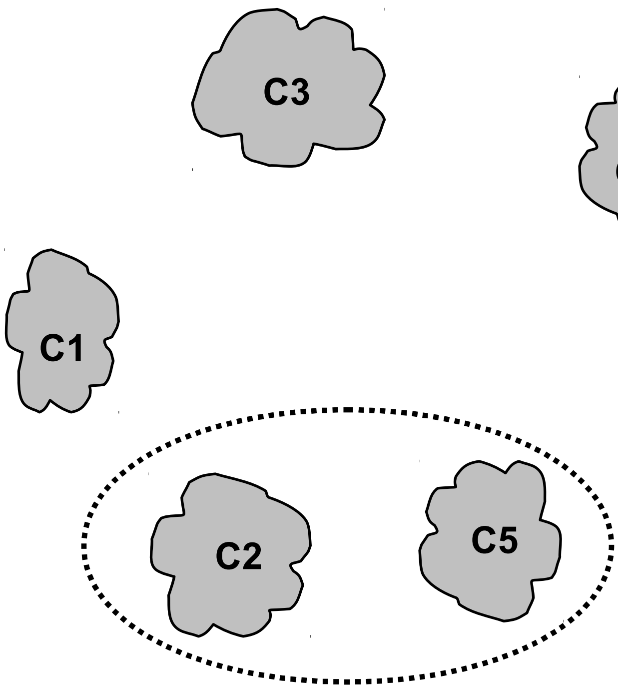


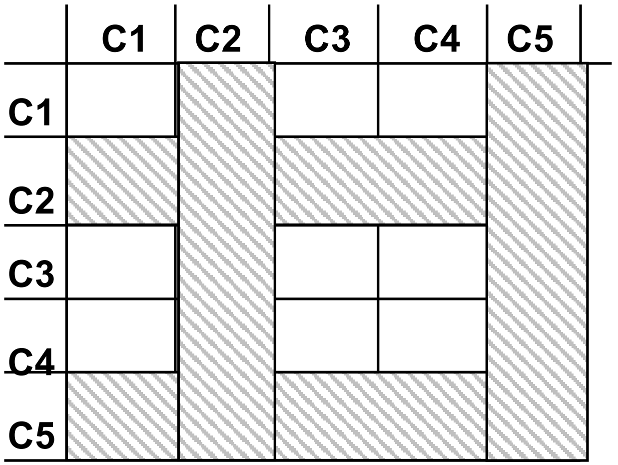
	C1	C2	C3	C4	C5
C1					
C2					
C3					
C4					
C5					

Proximity Matrix

Intermediate Situation

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

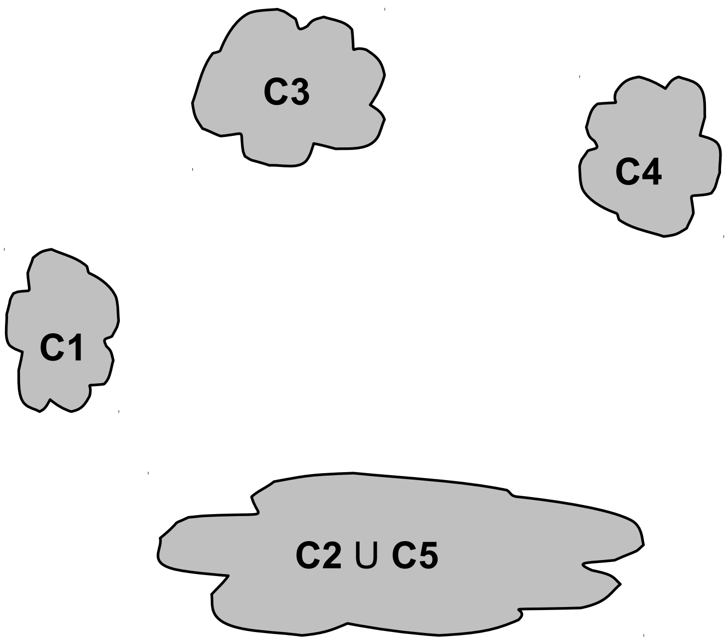




Proximity Matrix

After Merging

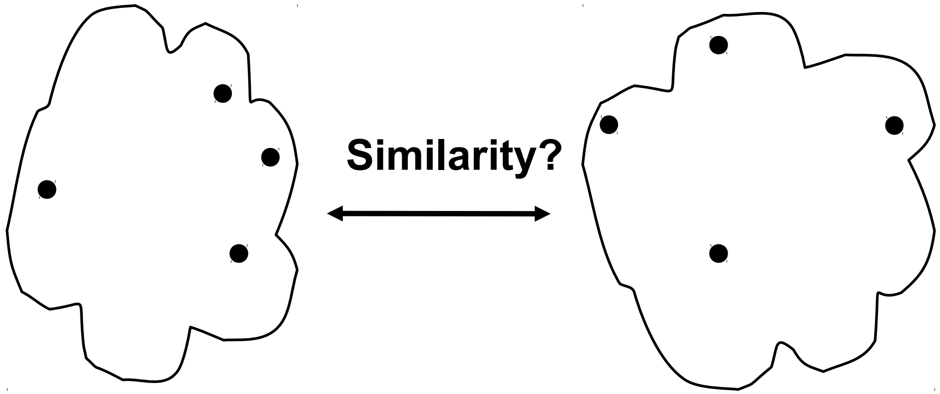
- The question is “How do we update the proximity matrix?”



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

Proximity Matrix

How to Define Inter-Cluster Similarity

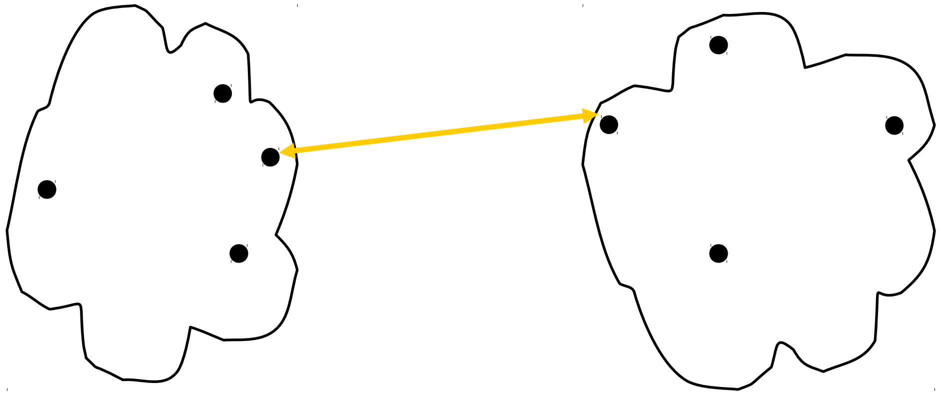


	p1	p2	p3	p4	p5	. . .
p1						
p2						
p3						
p4						
p5						
.						
.						
.						

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 Similarity



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

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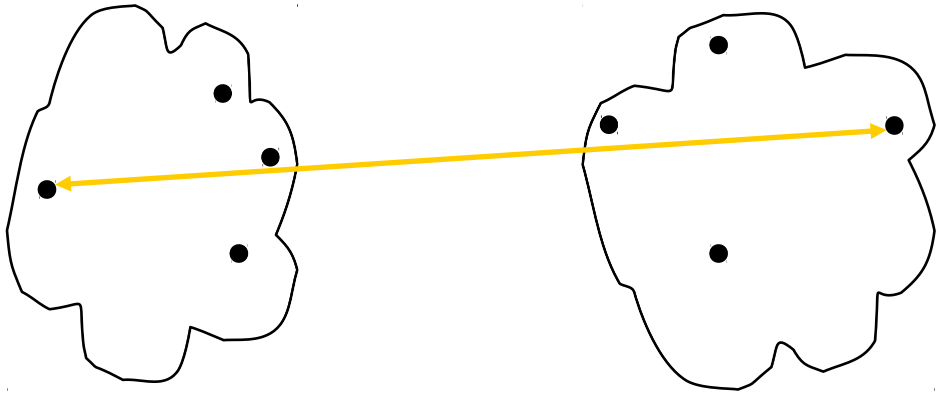
How to Define Inter-Cluster Similarity



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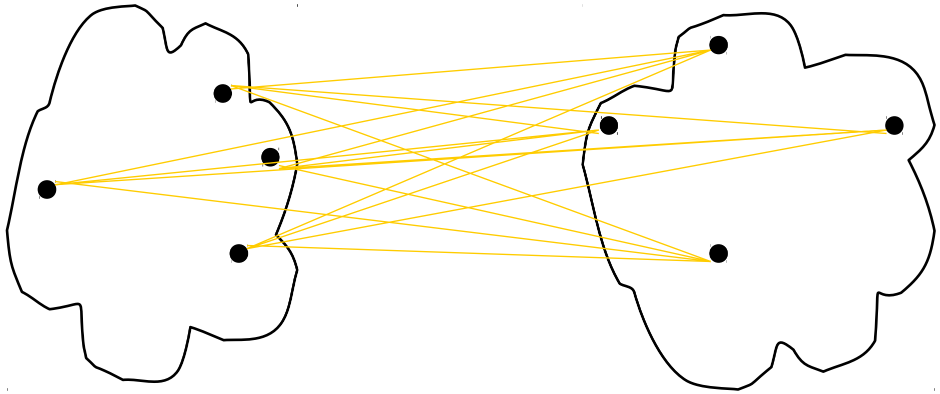
How to Define Inter-Cluster Similarity



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

Proximity Matrix

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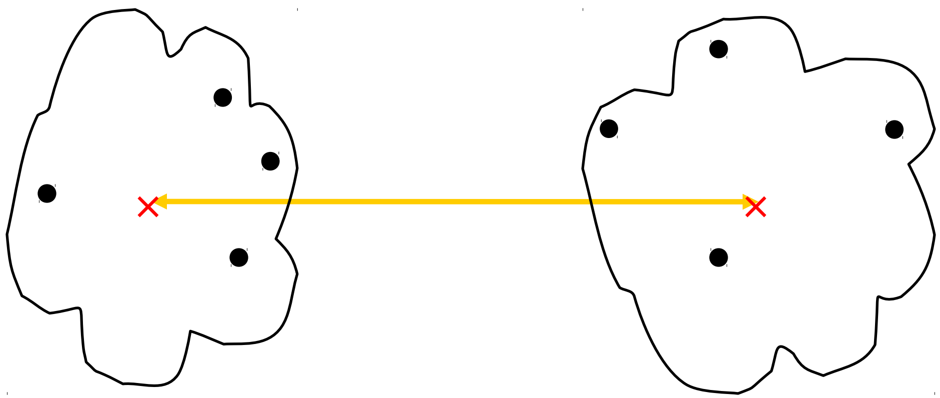
How to Define Inter-Cluster Similarity



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

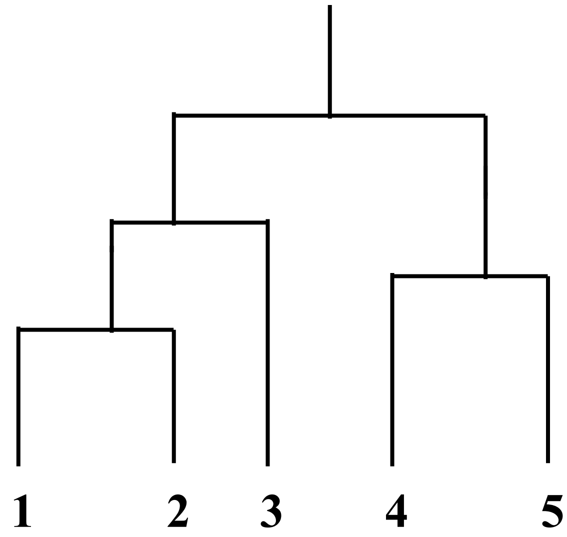
Proximity Matrix

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

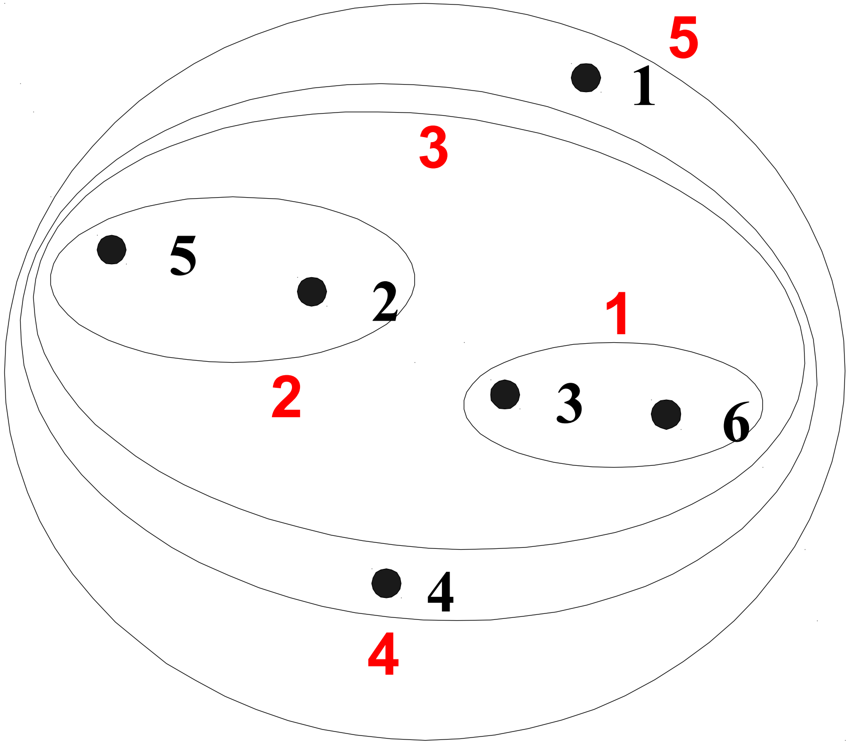
Cluster Similarity: MIN or Single Link

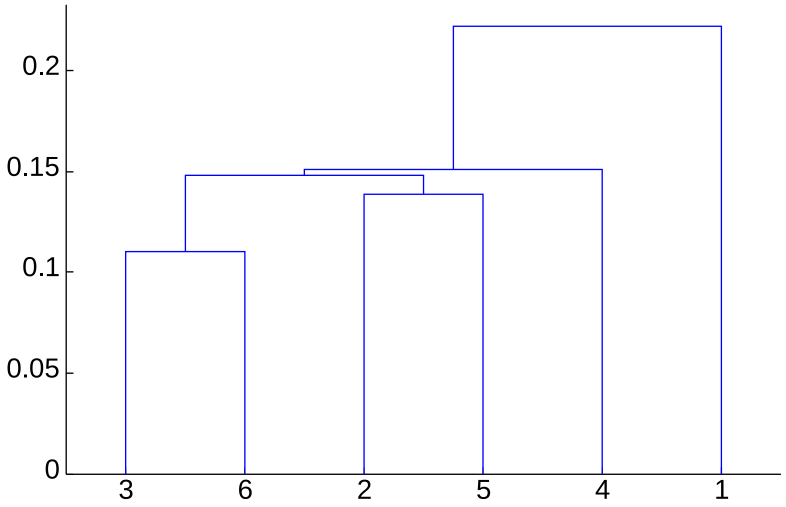
- Similarity of two clusters is based on the two most similar (closest) points in the different clusters
  - Determined by one pair of points, i.e., by one link in the proximity graph.

	I1	I2	I3	I4	I5
I1	1,00	0,90	0,10	0,65	0,20
I2	0,90	1,00	0,70	0,60	0,50
I3	0,10	0,70	1,00	0,40	0,30
I4	0,65	0,60	0,40	1,00	0,80
I5	0,20	0,50	0,30	0,80	1,00



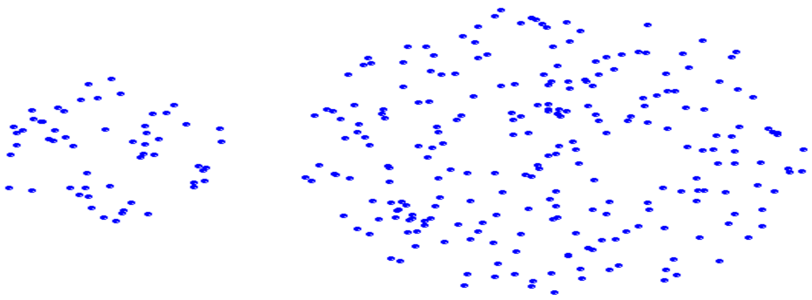
Hierarchical Clustering: MIN



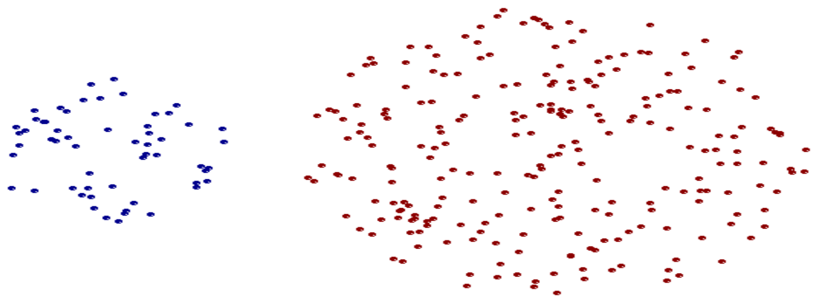


Nested Clusters **Dendrogram**

Strength of MIN



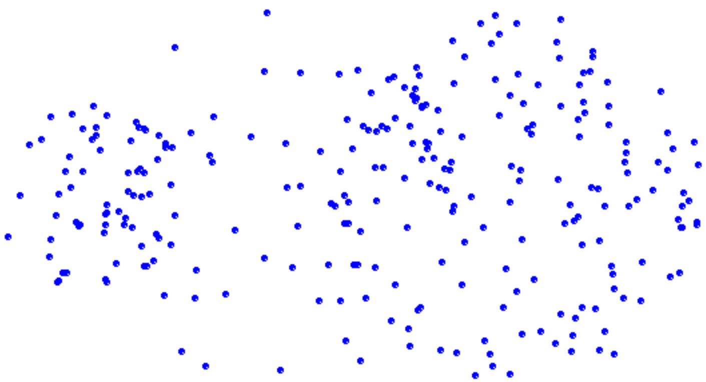
Original Points



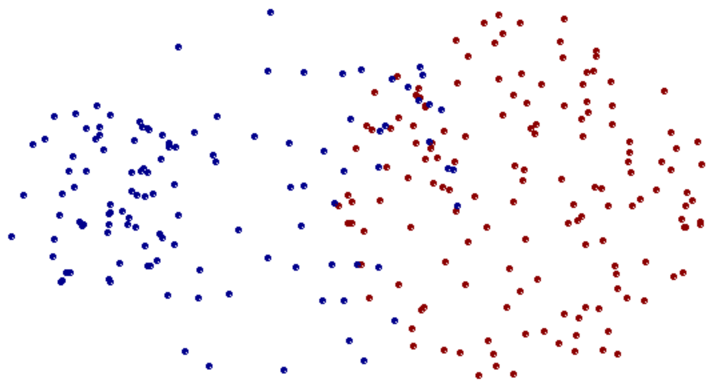
Two Clusters

- Can handle non-elliptical shapes

Limitations of MIN

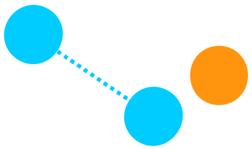


Original Points



Two Clusters

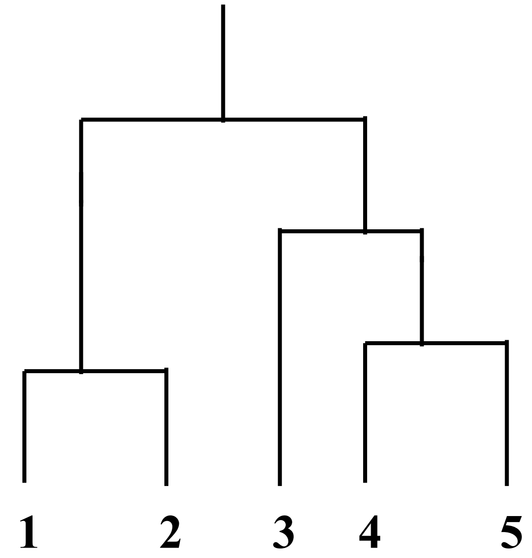
- **Sensitive to noise and outliers**
  - **Particular case: chain effect**



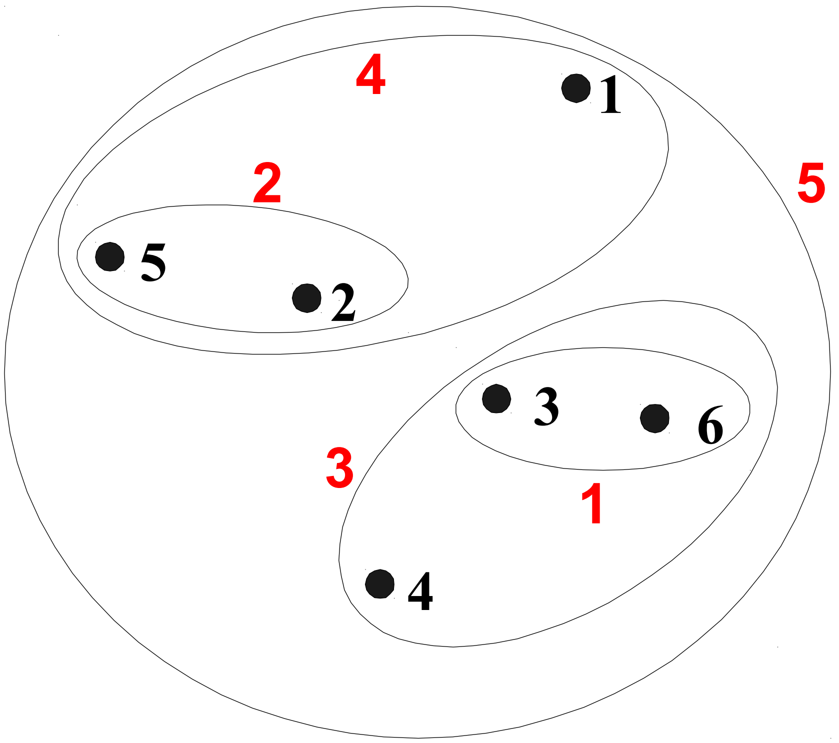
Cluster Similarity: MAX or Complete Linkage

- Similarity of two clusters is based on the two least similar (most distant) points in the different clusters
  - Determined by all pairs of points in the two clusters

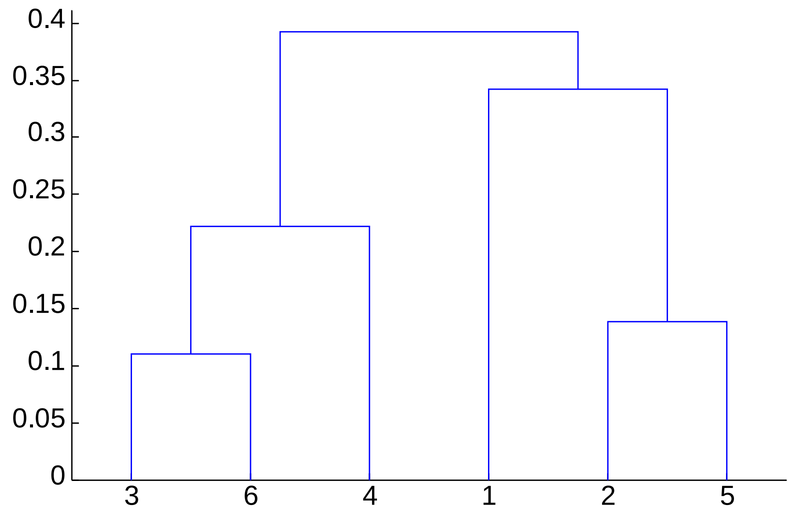
	I1	I2	I3	I4	I5
I1	1,00	0,90	0,10	0,65	0,20
I2	0,90	1,00	0,70	0,60	0,50
I3	0,10	0,70	1,00	0,40	0,30
I4	0,65	0,60	0,40	1,00	0,80
I5	0,20	0,50	0,30	0,80	1,00



Hierarchical Clustering: MAX

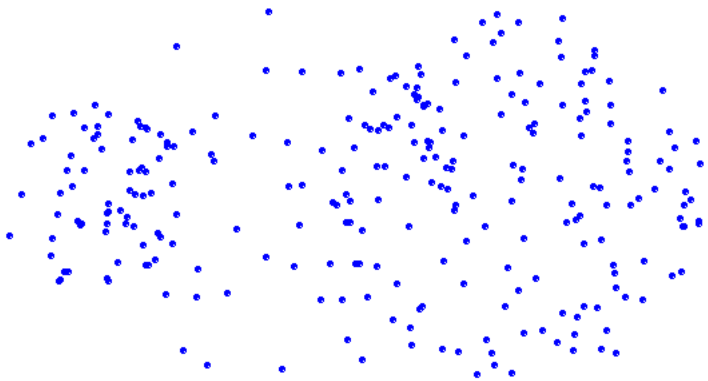


Nested Clusters

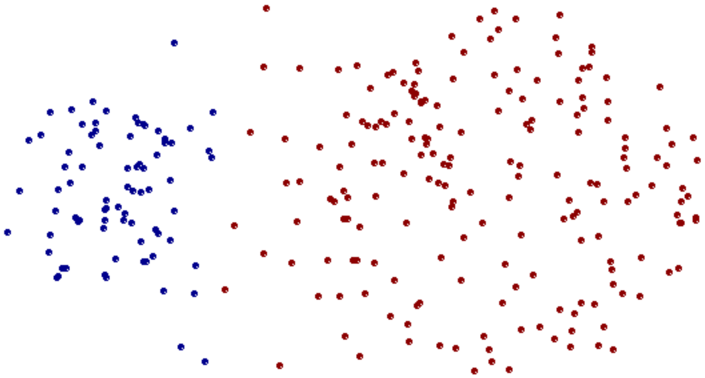


Dendrogram

Strength of MAX



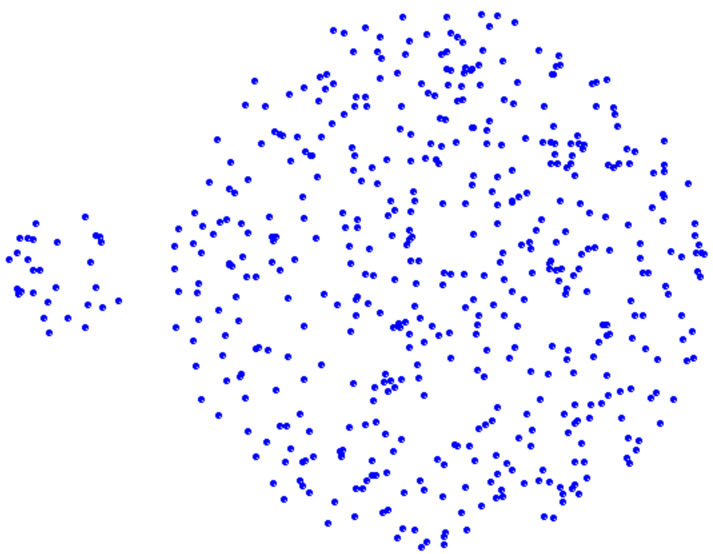
Original Points



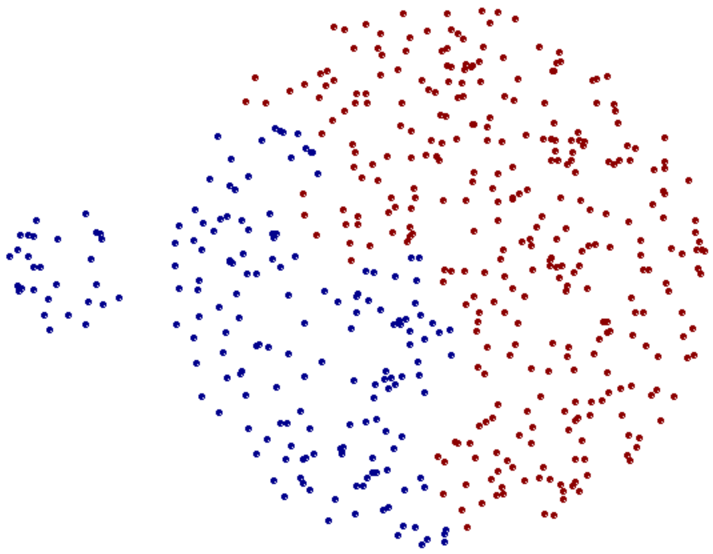
Two Clusters

- Less susceptible to noise and outliers

Limitations of MAX



Original Points



Two Clusters

•Tends to break large clusters

•Biased towards globular clusters

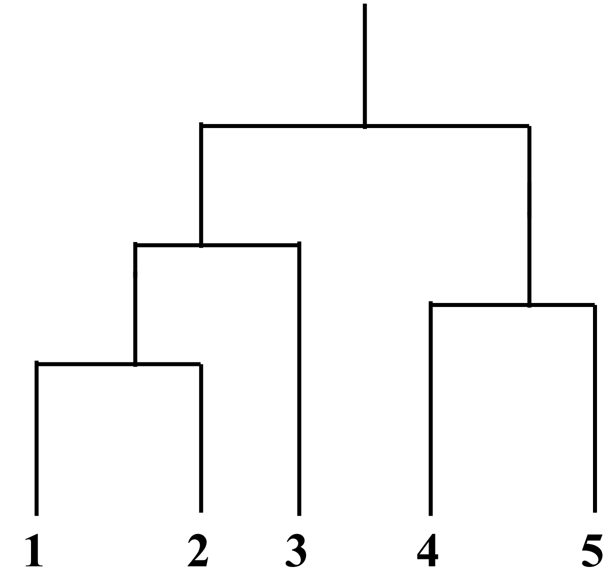
Cluster Similarity: Group Average

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

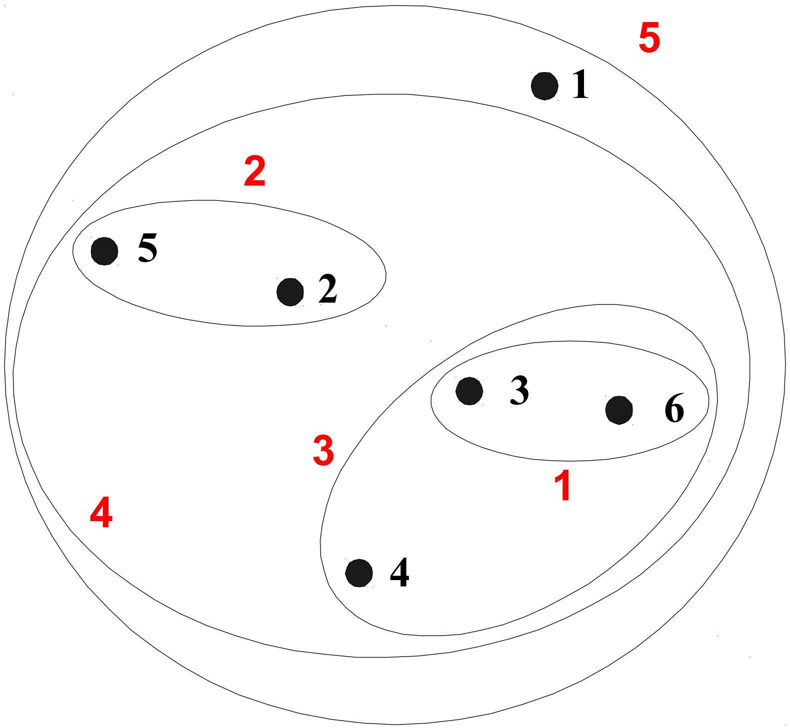
$$proximity(C_i, C_j) = \frac{\sum_{\substack{\mathbf{x} \in C_i \\ \mathbf{y} \in C_j}} proximity(\mathbf{x}, \mathbf{y})}{m_i * m_j}$$

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

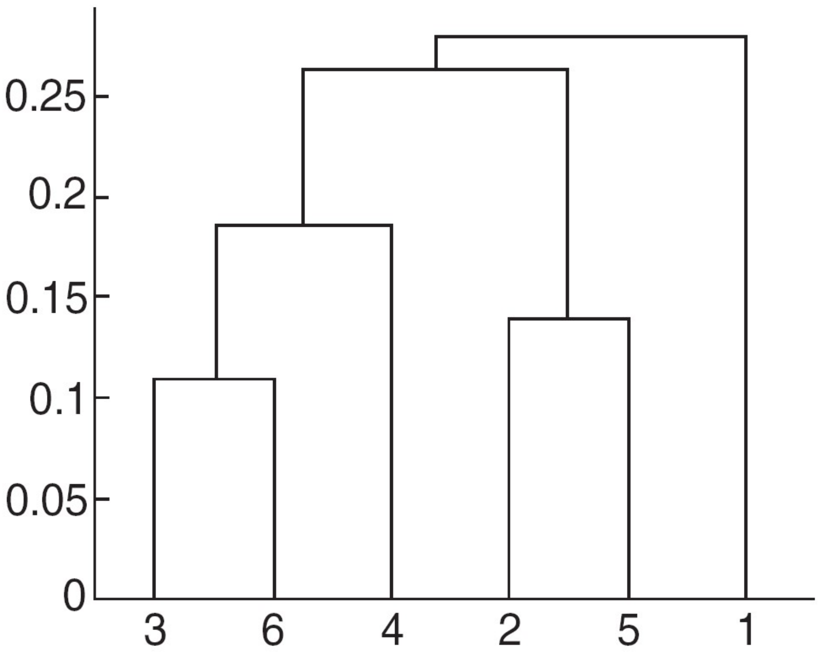
	I1	I2	I3	I4	I5
I1	1,00	0,90	0,10	0,65	0,20
I2	0,90	1,00	0,70	0,60	0,50
I3	0,10	0,70	1,00	0,40	0,30
I4	0,65	0,60	0,40	1,00	0,80
I5	0,20	0,50	0,30	0,80	1,00



Hierarchical Clustering: Group Average



Nested Clusters



Dendrogram

Hierarchical Clustering: Group Average

- Compromise between Single and Complete Link

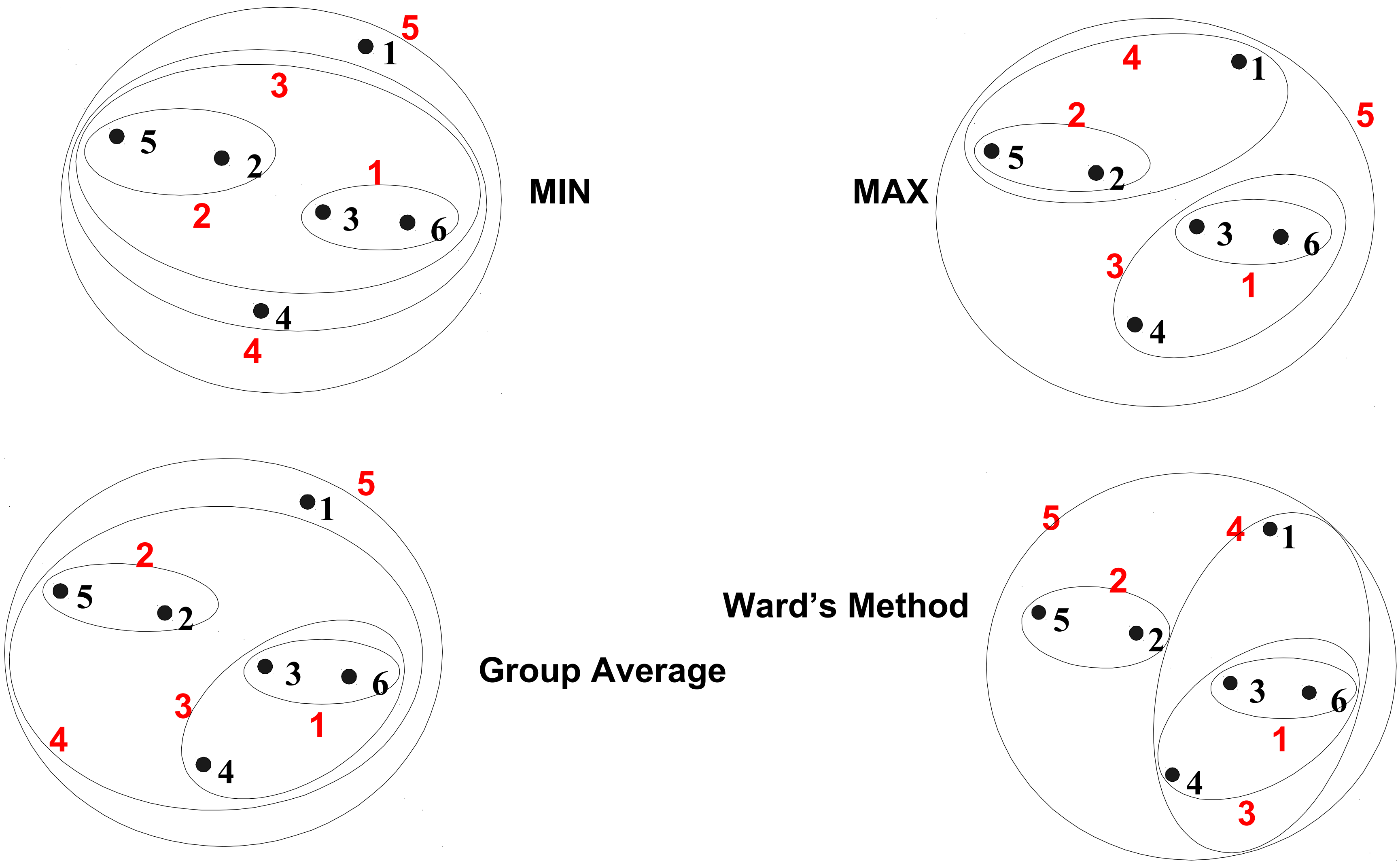
- Strengths
  – Less susceptible to noise and outliers

- 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



Hierarchical Clustering: Time and Space requirements

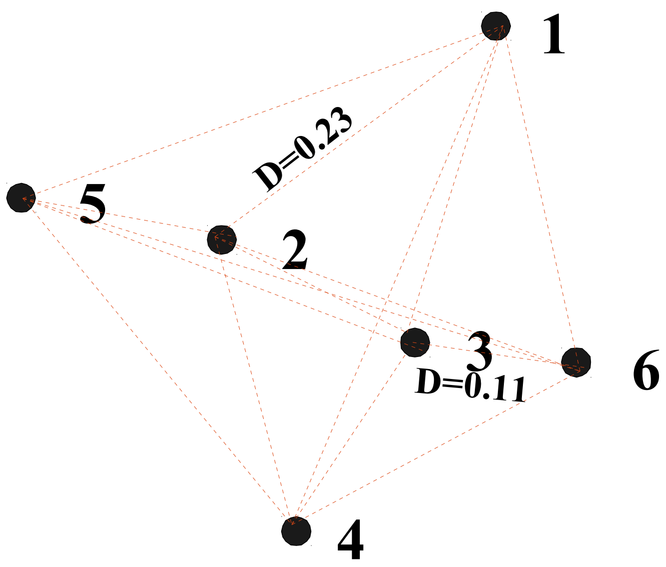
- $O(N^2)$ space since it uses the proximity matrix.
  - N is the number of points.

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

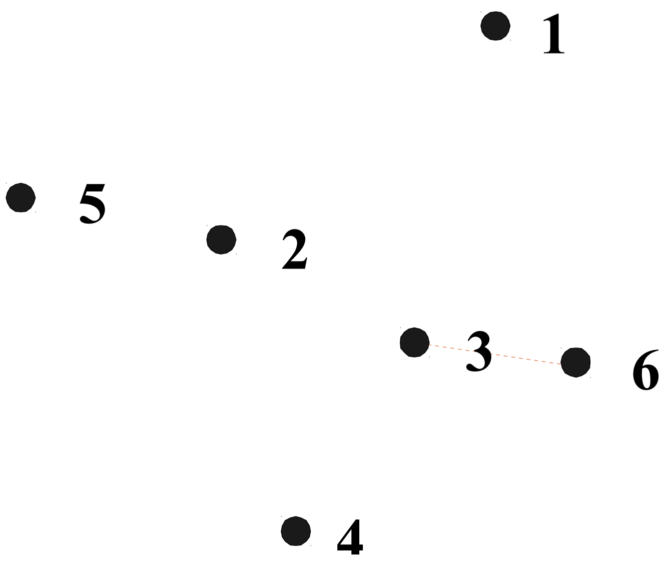
Hierarchical Clustering: Problems and Limitations

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

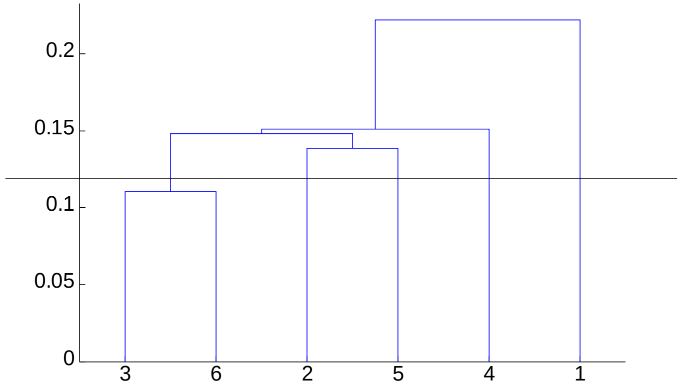
Single-link HAC vs Graphs



Cut edges with D>0.12

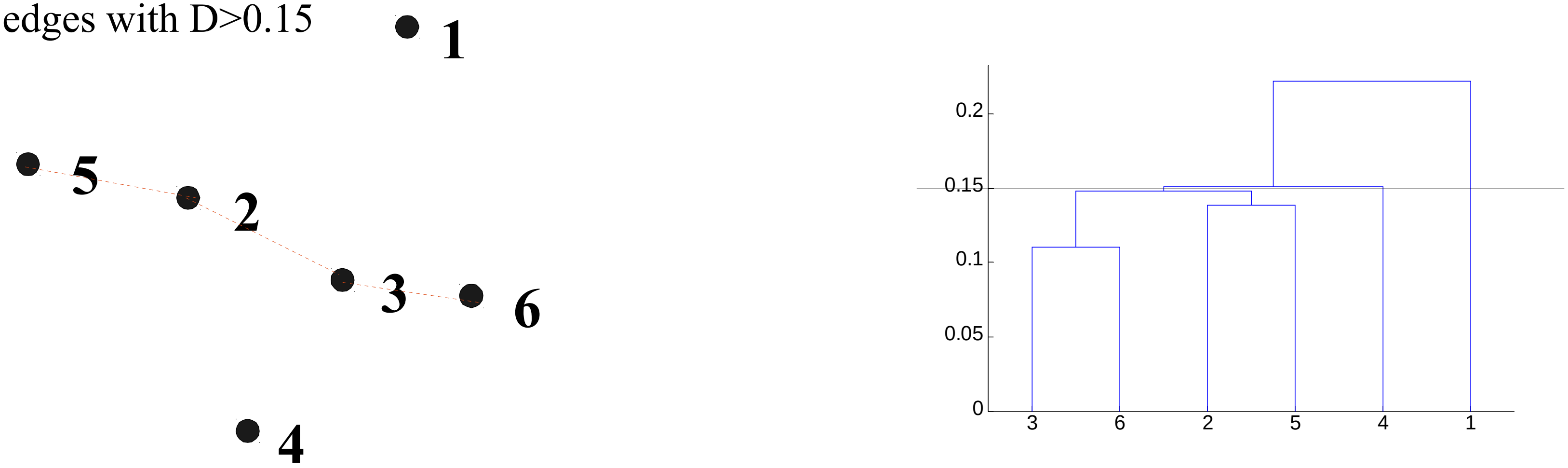


Clusters = connected components

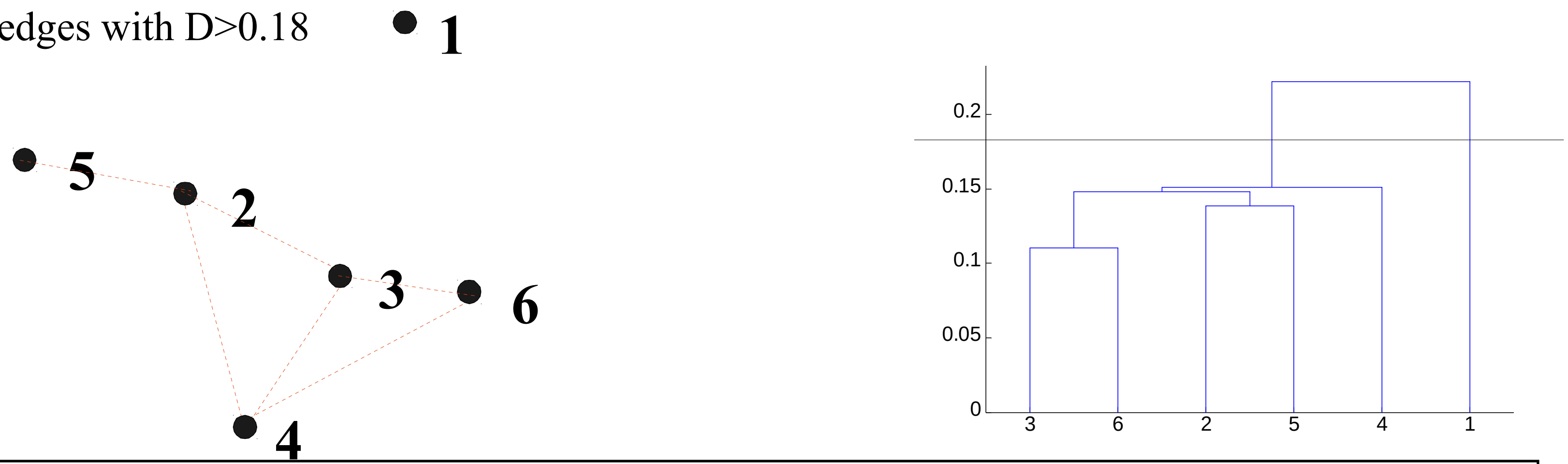


Single-link HAC vs Graphs

Cut edges with D>0.15



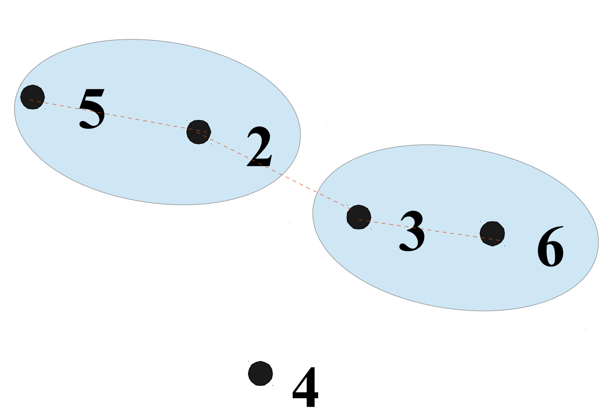
Cut edges with D>0.18

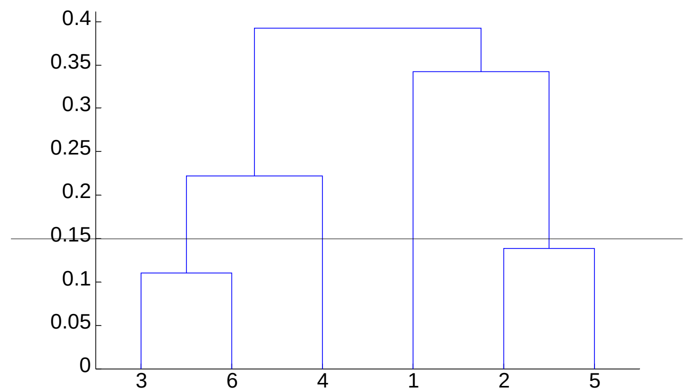


Complete-link HAC vs Graphs

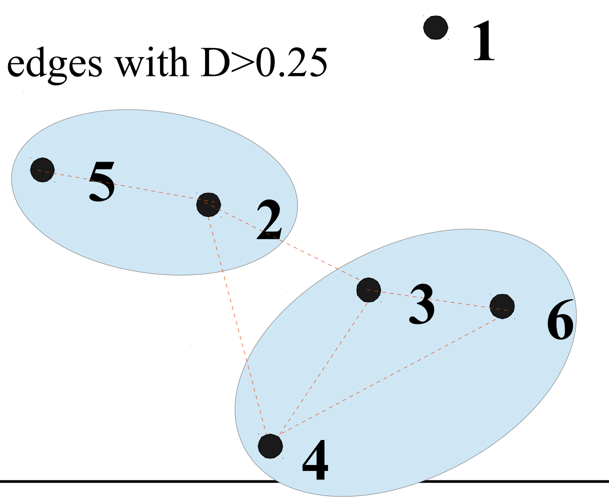
Clusters ~ cliques – constraint: earlier cliques have precedence

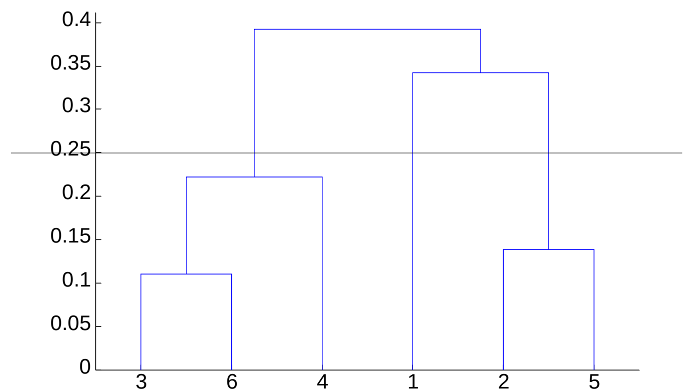
Cut edges with D>0.15





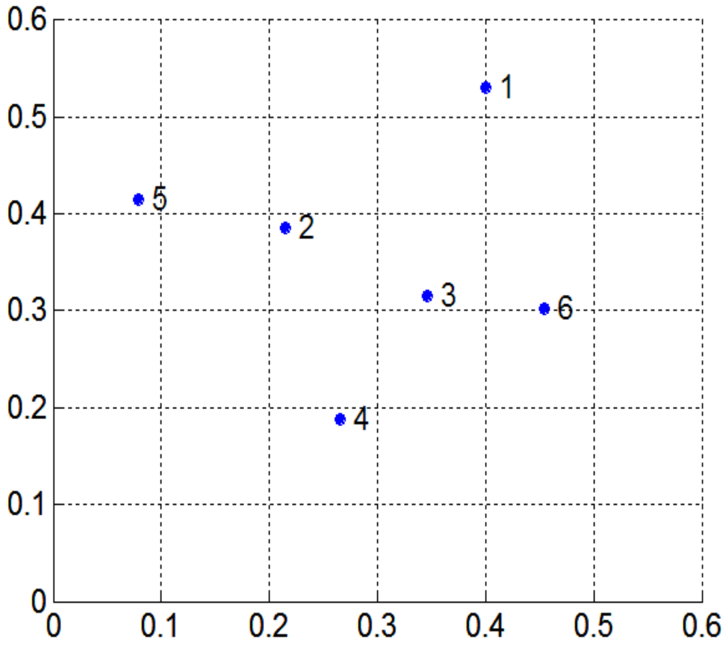
Cut edges with D>0.25

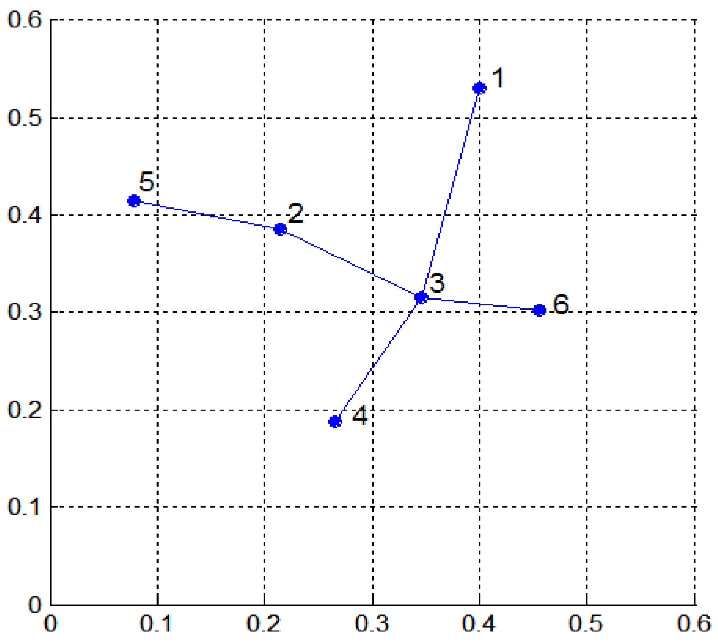




MST: Divisive Hierarchical Clustering

- 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

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