School of Computing
UNIVERSITY OF GEORGIA

CSCI 4380/6380 DATA MINING

Fei Dou

Assistant Professor
School of Computing
University of Georgia

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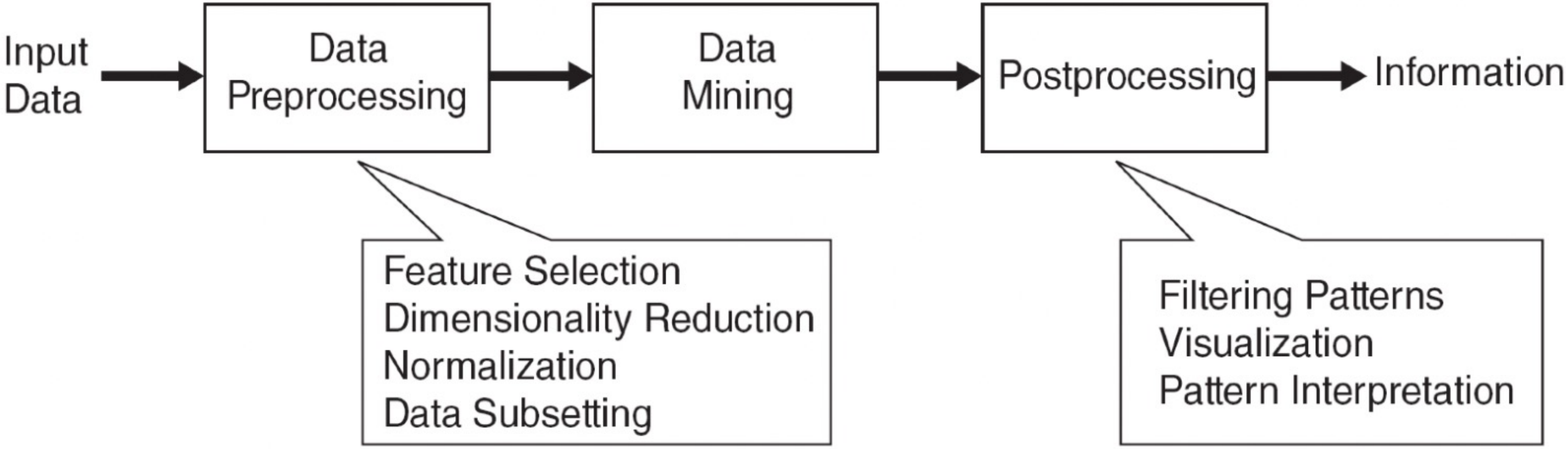
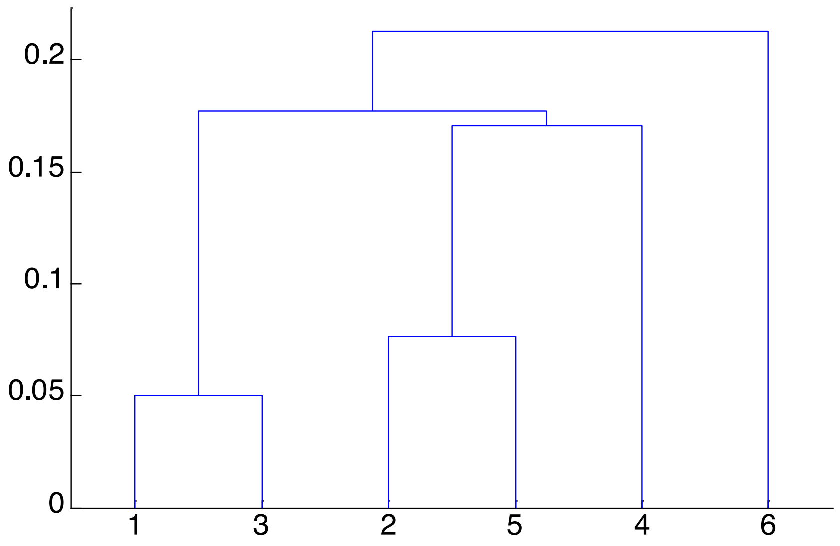
Recap: Data Mining Process

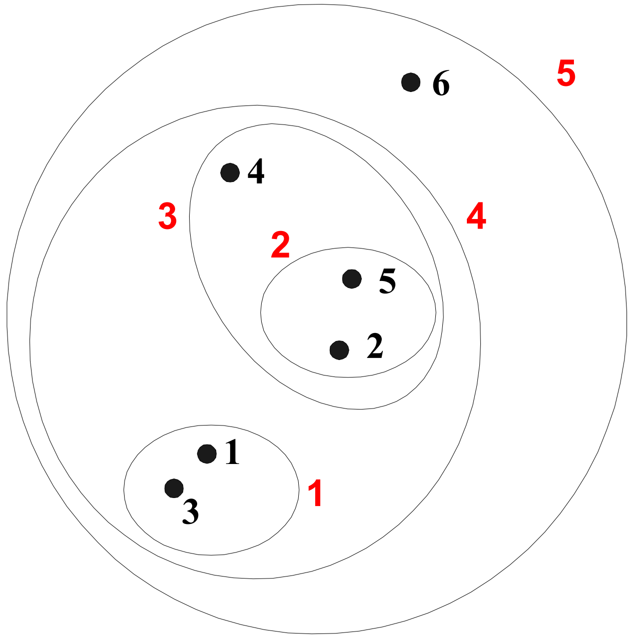


Hierarchical Clustering

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



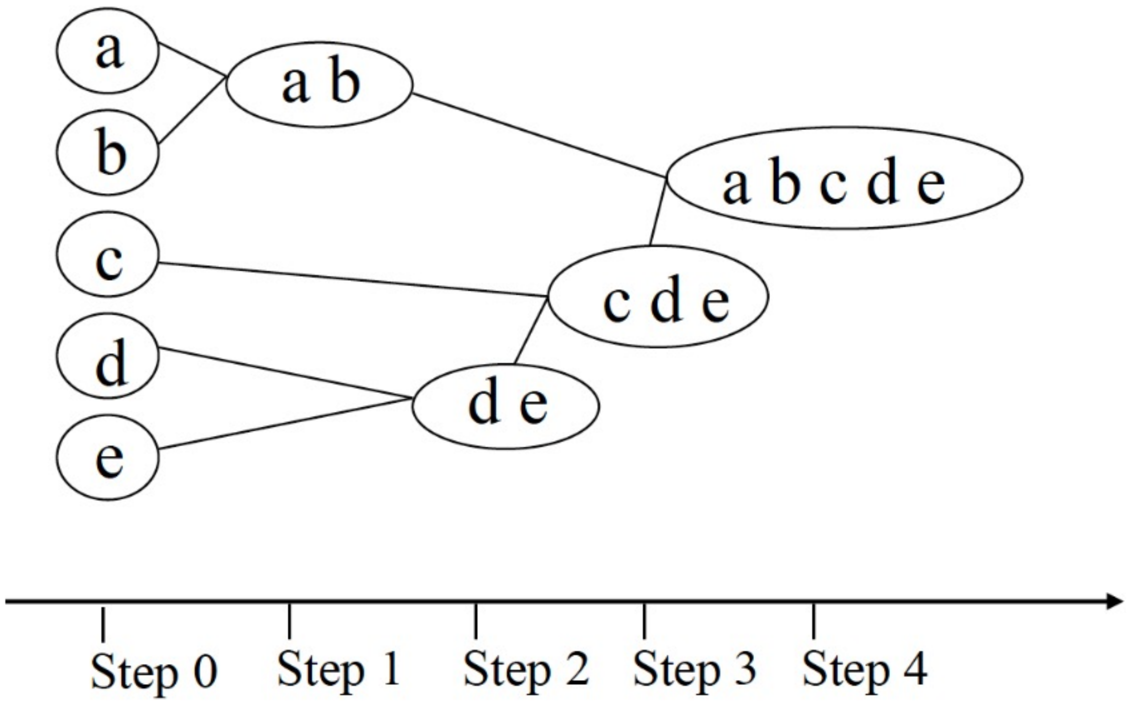


Hierarchical Clustering

- 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

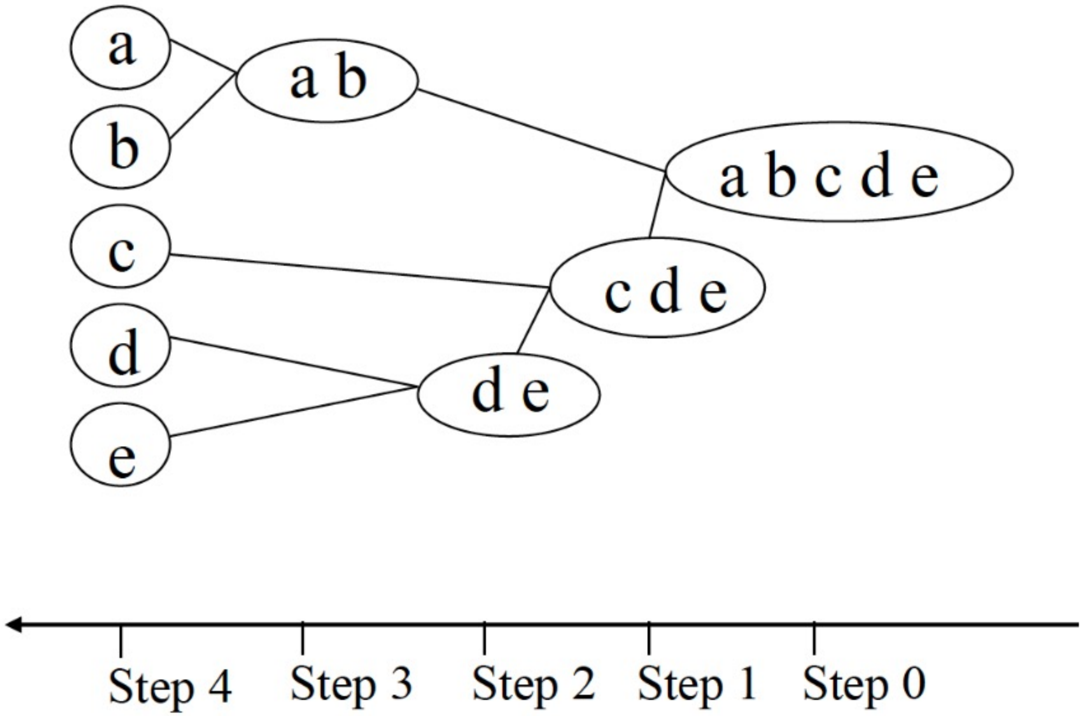
Agglomerative approach (bottom-up)

- **Initialization**: Each sample is a cluster
- **Iteration**:
  - Merge two clusters which are most similar to each other
  - Until all samples are merged into a single cluster

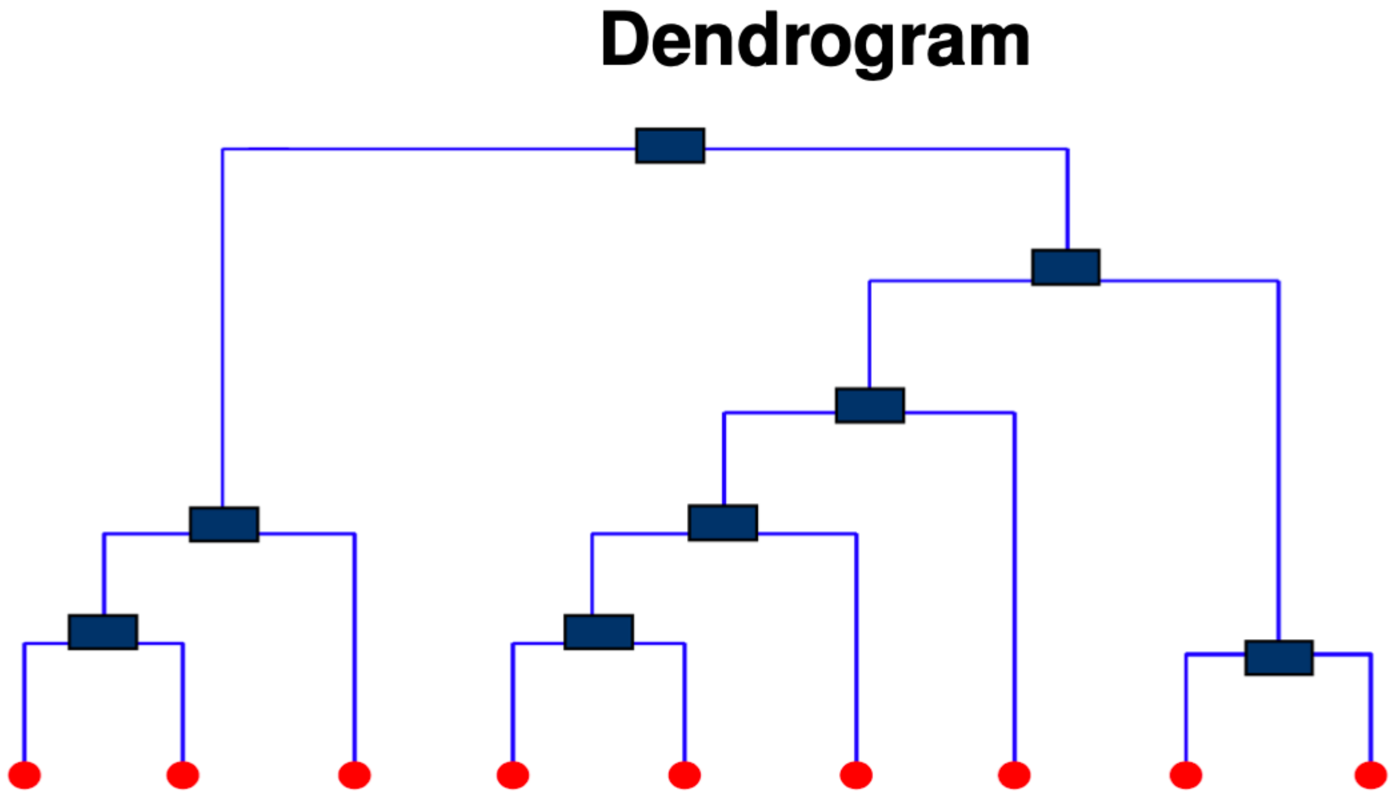


Divisive Approaches (top-down)

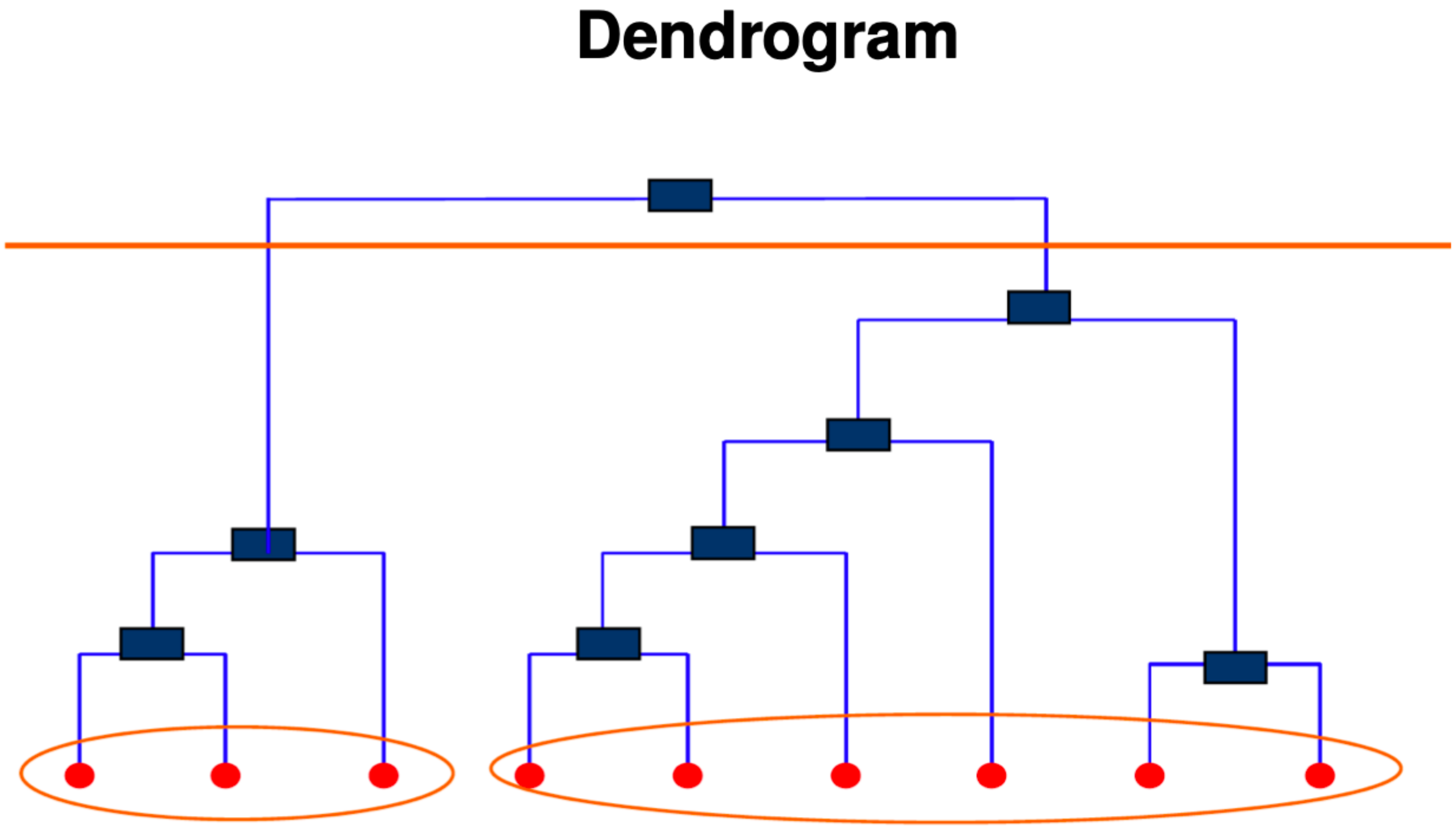
- **Initialization**: All samples stay in one cluster
- **Iteration**:
  - Select a cluster and split it into two sub clusters
  - Until each leaf cluster contains only one object



Hierarchical Clustering



Hierarchical Clustering



Agglomerative Clustering Algorithm

Key Idea: Successively merge closest clusters

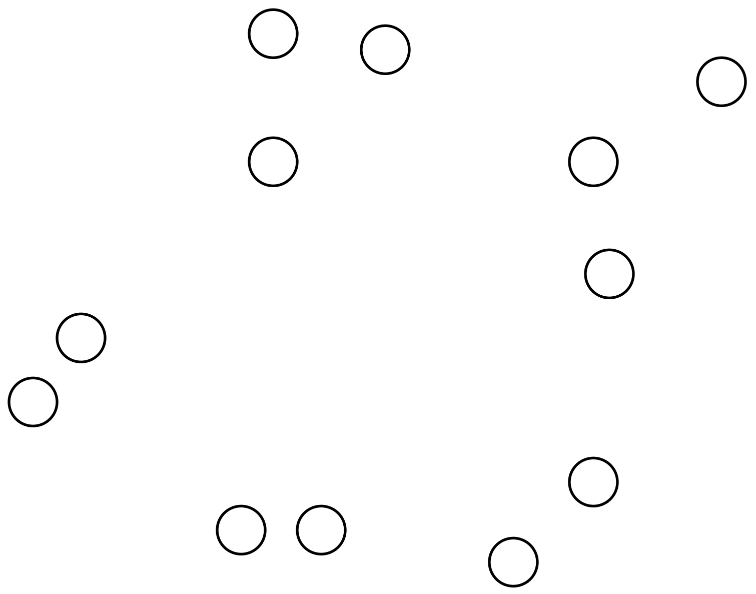
Basic algorithm

- 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

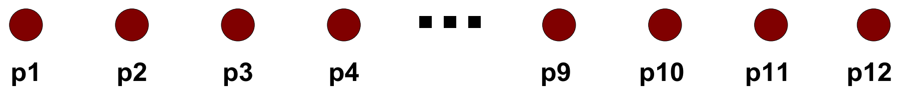
Steps 1 and 2

- Start with clusters of individual points and a proximity matrix



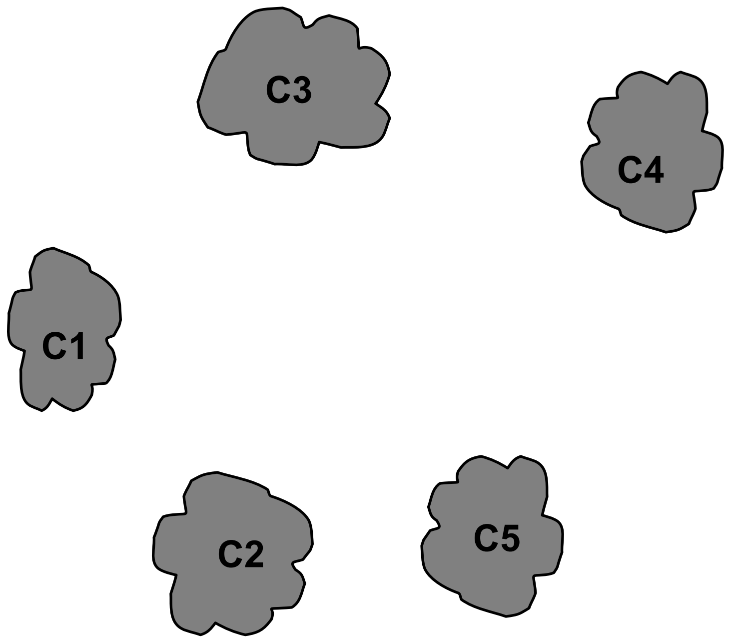
	p1	p2	p3	p4	p5	. . .
p1						
p2						
p3						
p4						
p5						
.						
.						
.						

Proximity Matrix



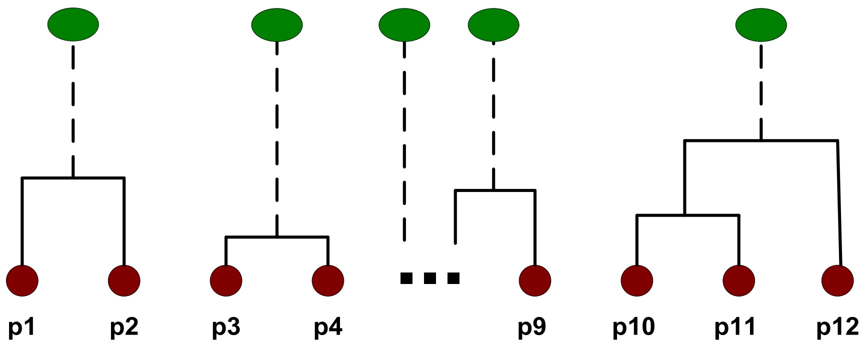
Step3: Intermediate Situation

- After some merging steps, we have some clusters



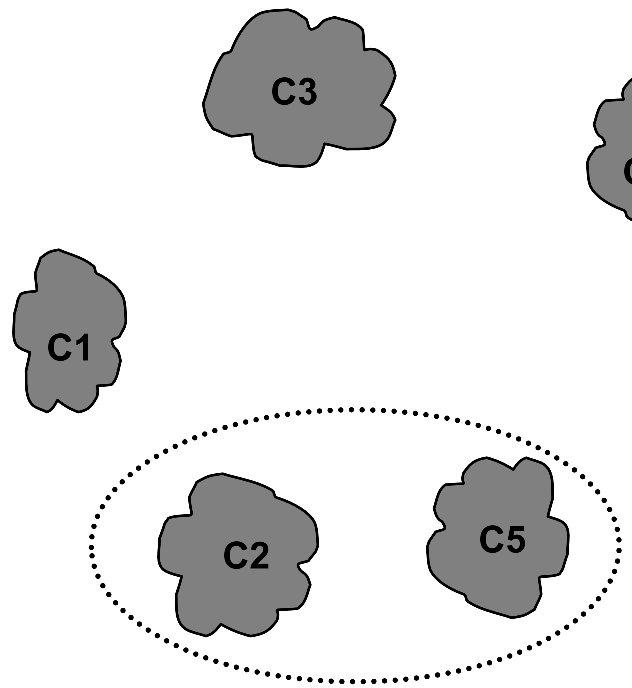
	C1	C2	C3	C4	C5
C1					
C2					
C3					
C4					
C5					

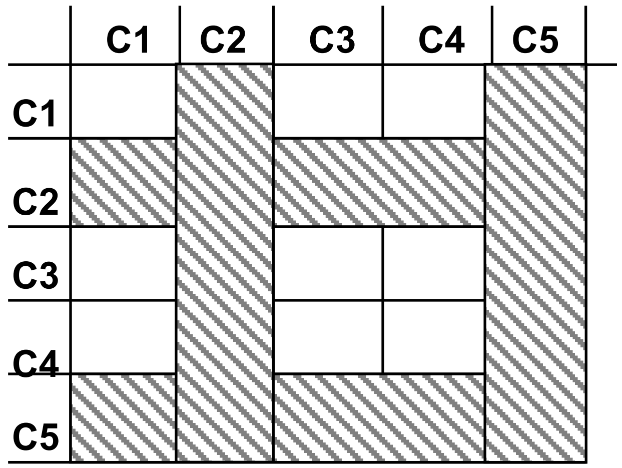
Proximity Matrix



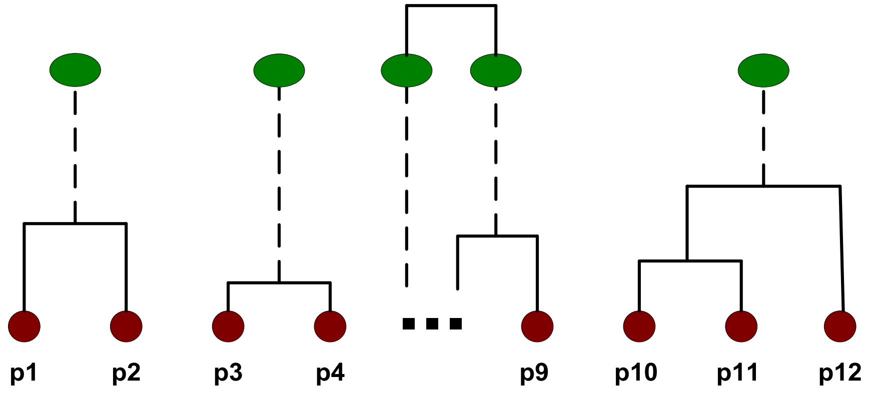
Step 4

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



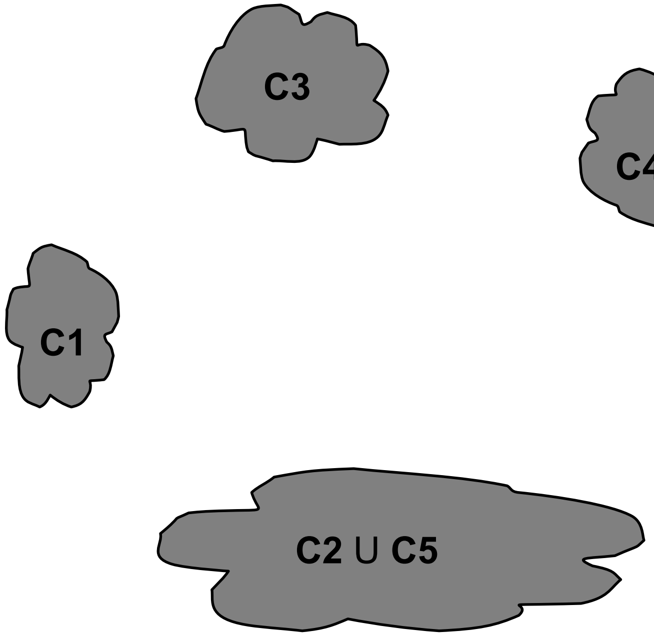


Proximity Matrix



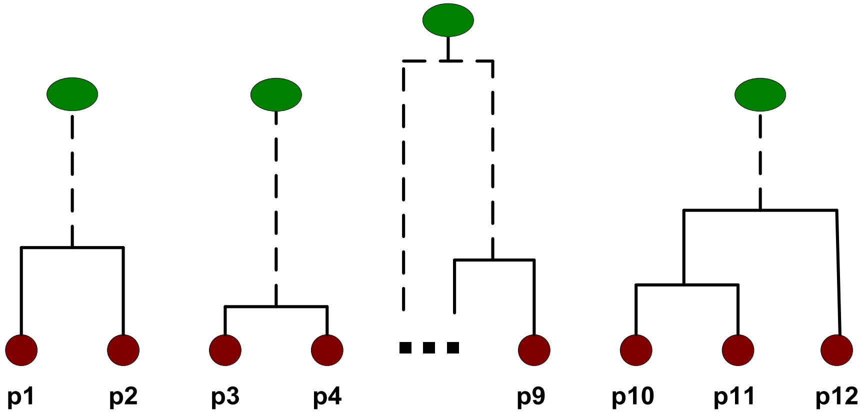
Step 5

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

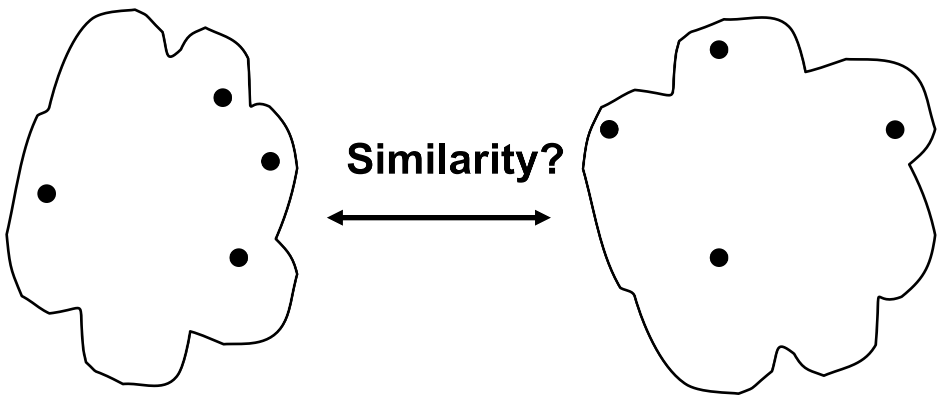


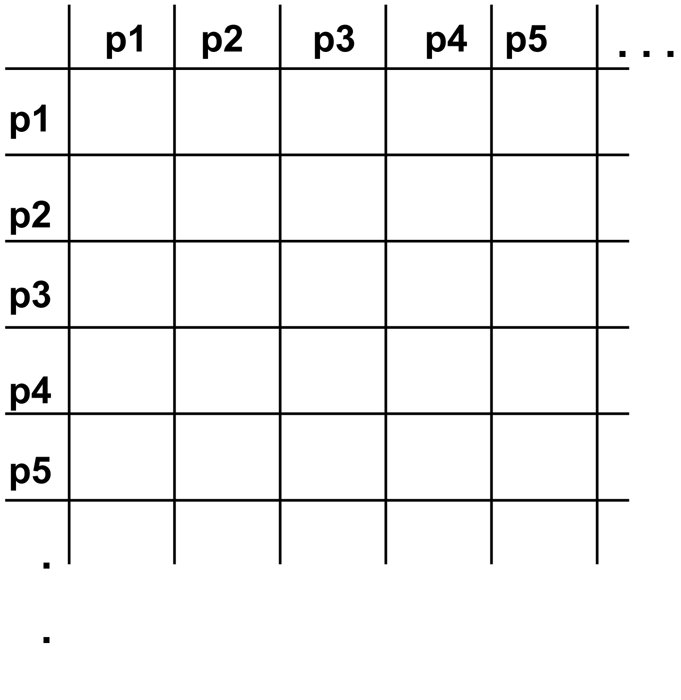
	C1	C2 U C5	C3	C4
C1		?		
C2 U C5	?	?	?	?
C3		?		
C4		?		

Proximity Matrix



How to Define Inter-Cluster Distance

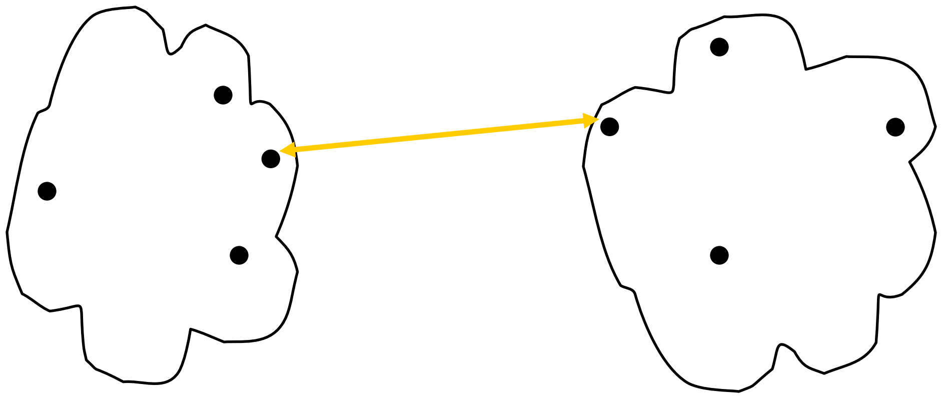




Proximity Matrix

- 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	. . .
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p3						
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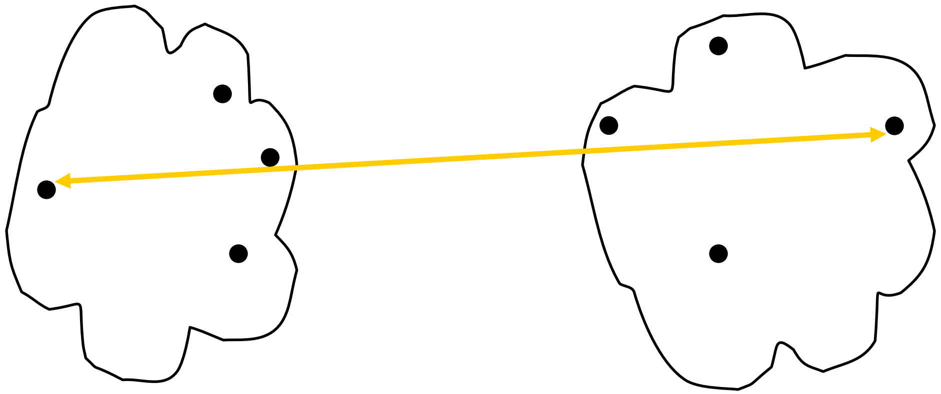

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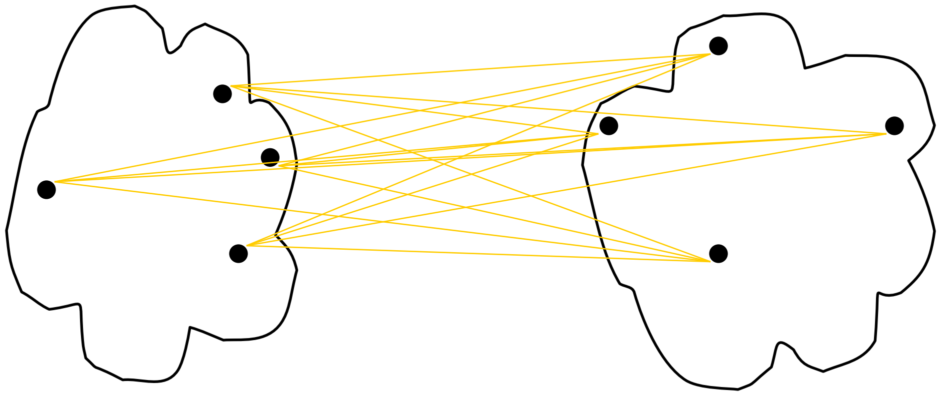

	p1	p2	p3	p4	p5	. . .
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p3						
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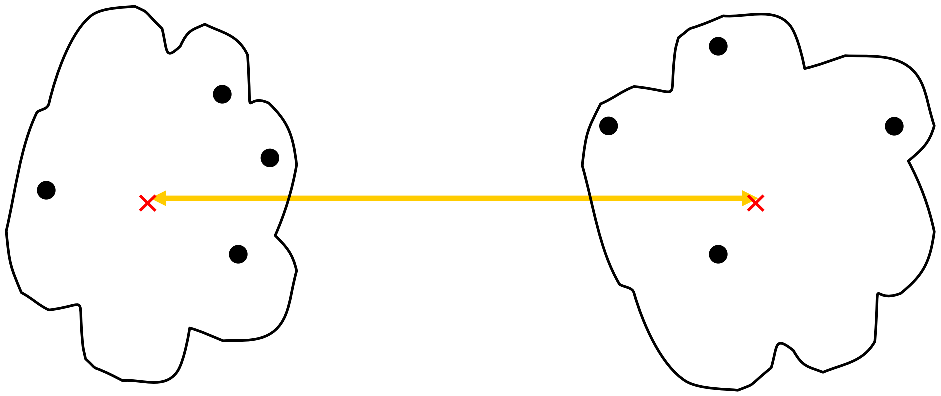
How to Define Inter-Cluster Similarity



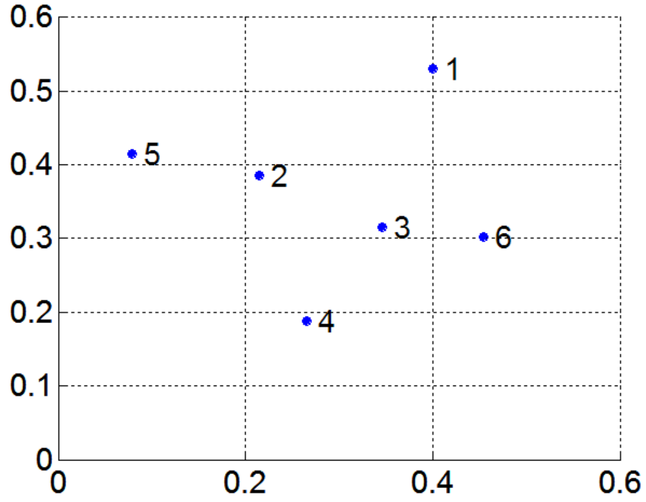
	p1	p2	p3	p4	p5	. . .
p1						
p2						
p3						
p4						
p5						
.						
.						
.						

Proximity Matrix

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

MIN or Single Link

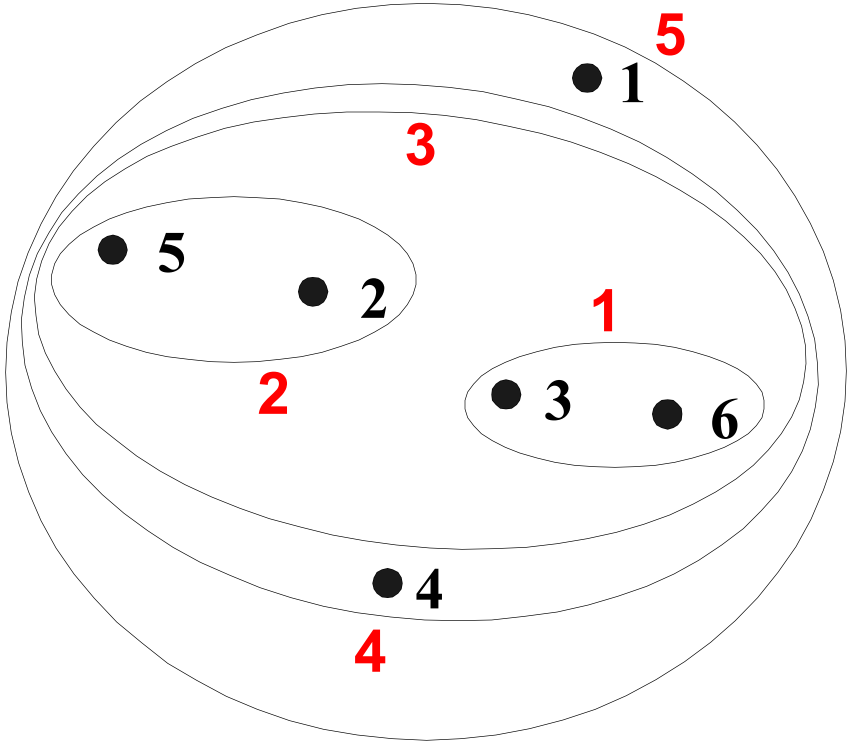
- Proximity of two clusters is based on the two closest points in the different clusters
  - Determined by one pair of points, i.e., by one link in the proximity graph
- Example:



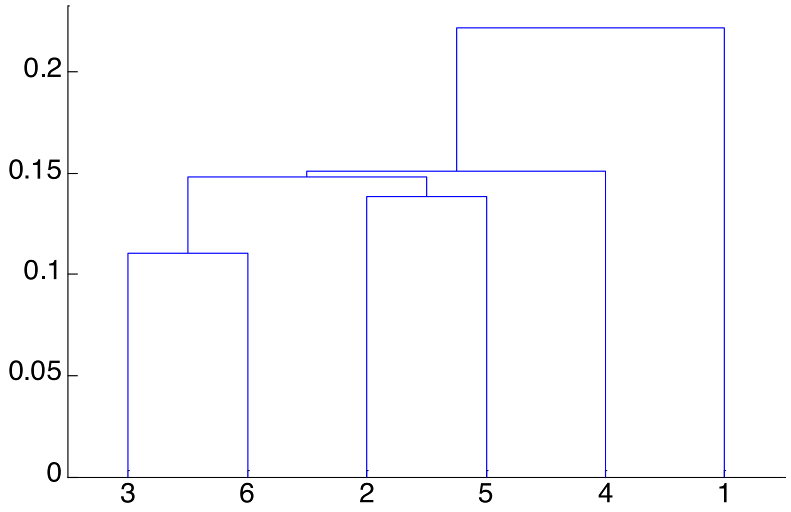
Distance Matrix:

	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

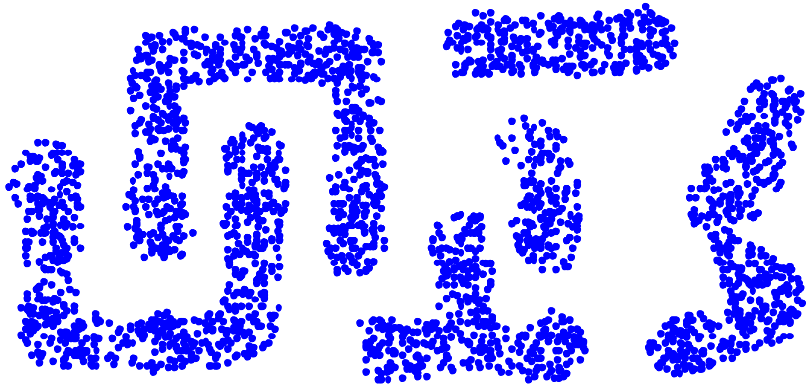


Nested Clusters

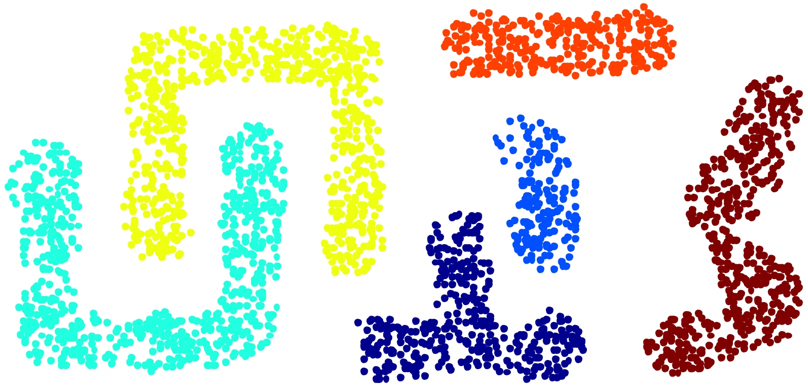


Dendrogram

Strength of MIN



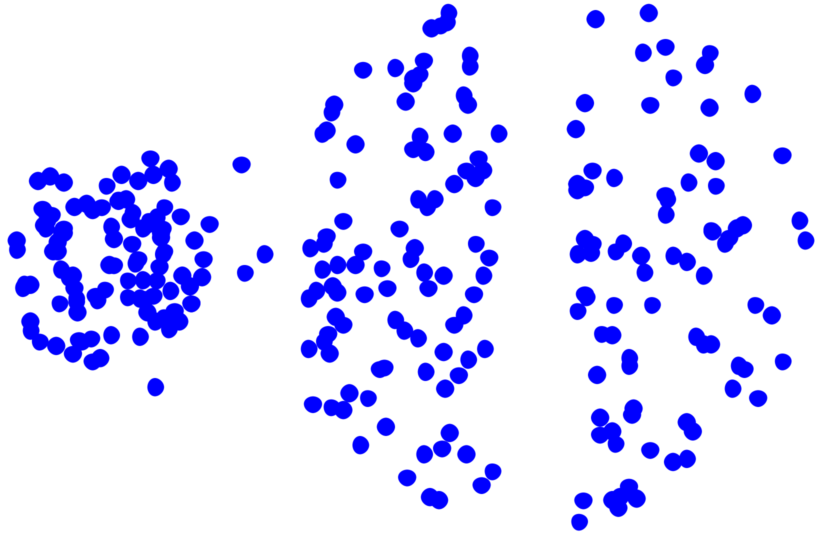
Original Points



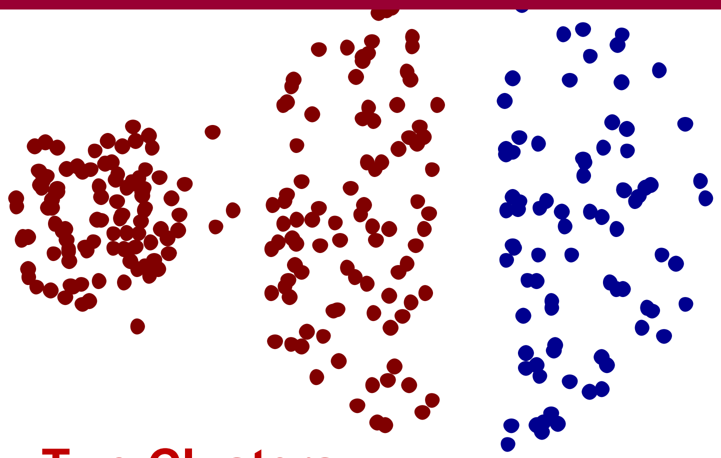
Six Clusters

- Can handle non-elliptical shapes

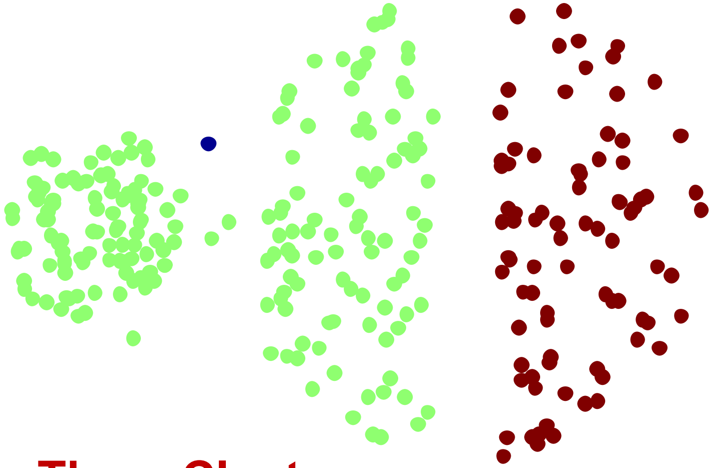
Limitations of MIN



Original Points



Two Clusters

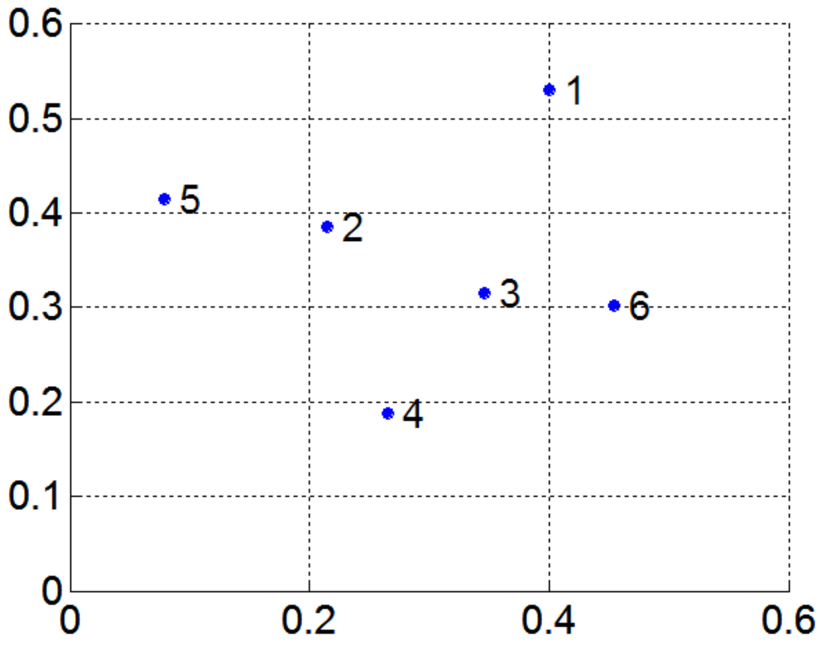


Three Clusters

- Sensitive to noise

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:

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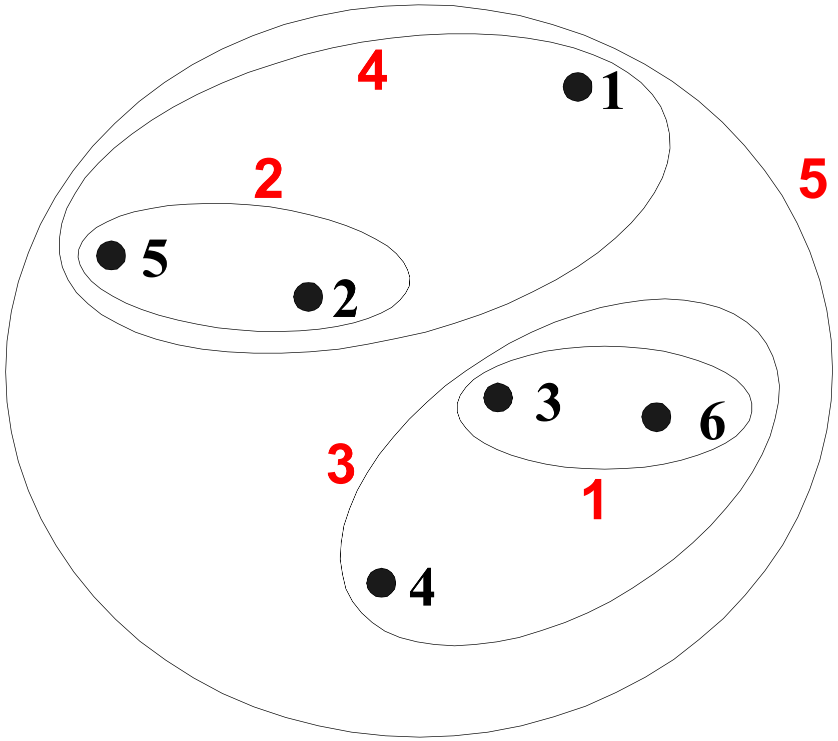
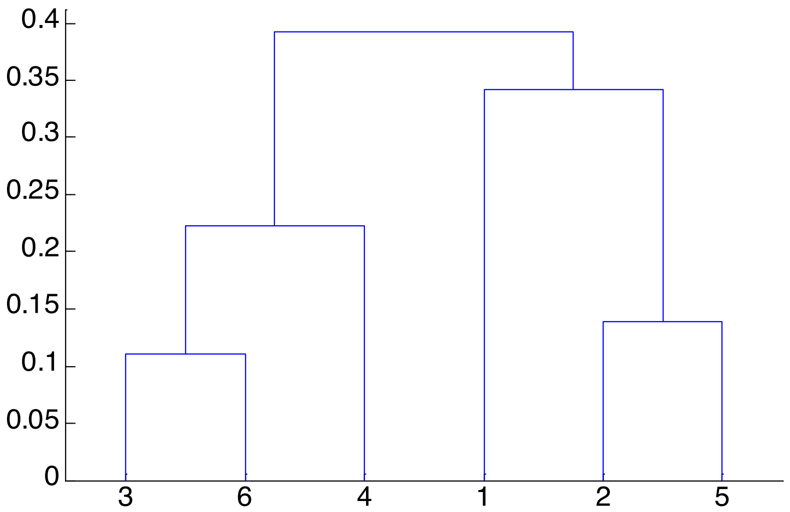
p2	0.24	0.00	0.15	0.20	0.14	0.25
p3	0.22	0.15	0.00	0.15	0.28	0.11
p4	0.37	0.20	0.15	0.00	0.29	0.22
p5	0.34	0.14	0.28	0.29	0.00	0.39
p6	0.23	0.25	0.11	0.22	0.39	0.00

Hierarchical Clustering: MAX

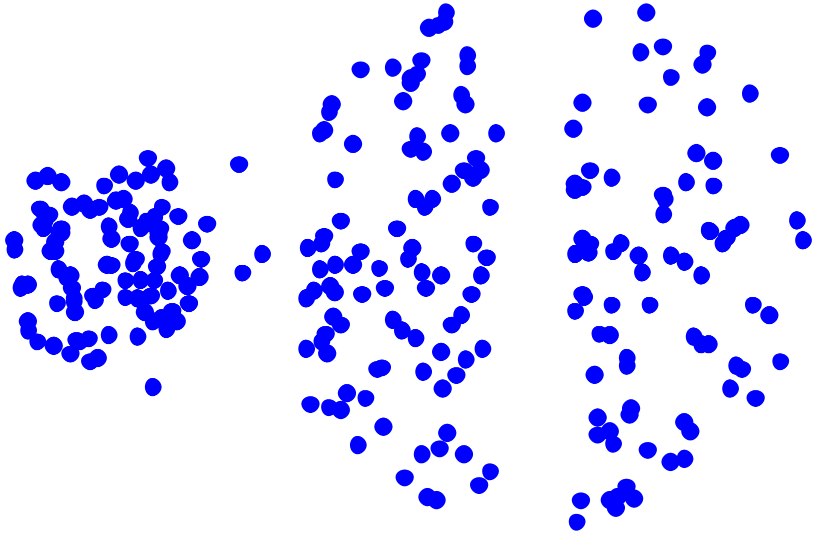


Nested Clusters

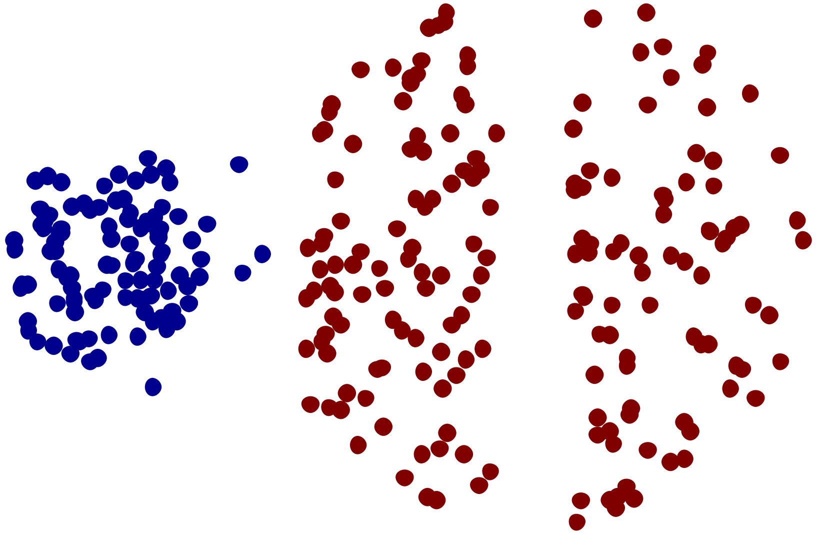


Dendrogram

Strength of MAX



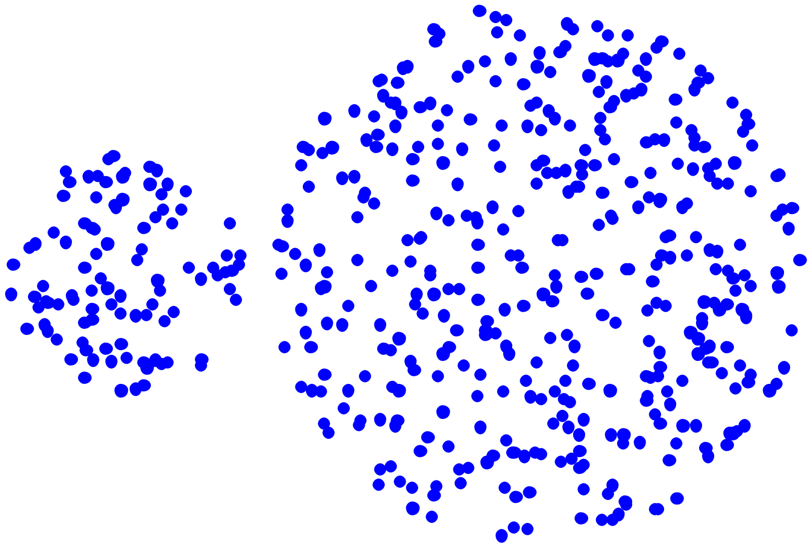
Original Points



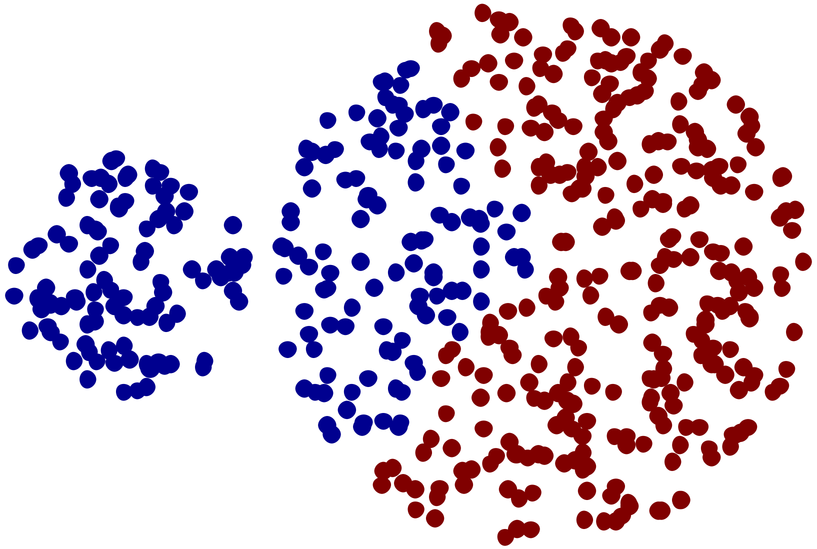
Two Clusters

- Less susceptible to noise

Limitations of MAX



Original Points



Two Clusters

- Tends to break large clusters
- Biased towards globular clusters

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, $O(N^2)$ proximity matrix must be updated and searched.
  - Complexity can be reduced to $O(N^2 \log(N))$ time with some cleverness

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 irregular shapes
  - Breaking large clusters