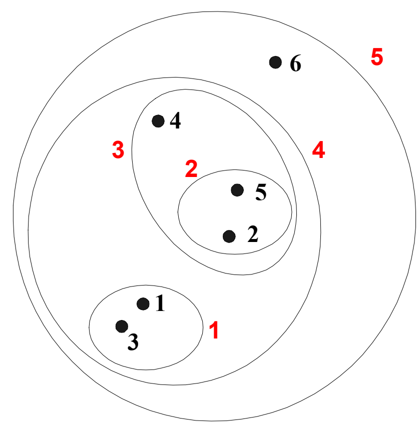
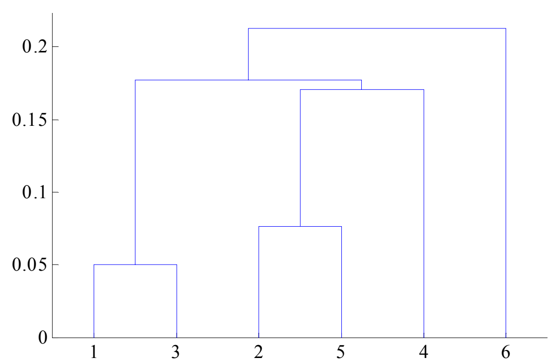
Hierarchical Clustering

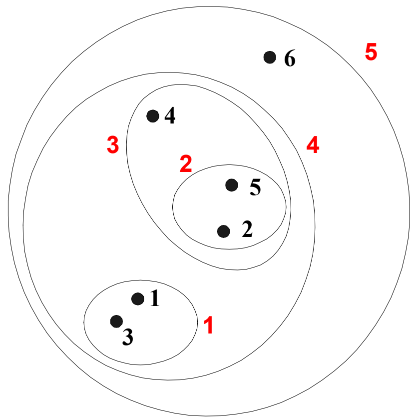
- Produces a set of nested clusters organized as a hierarchical tree



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

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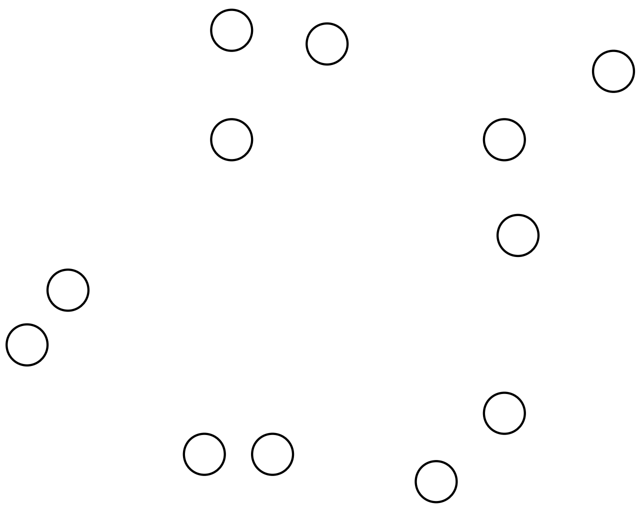
- Traditional hierarchical algorithms use a similarity or distance matrix
  - Merge or split one cluster at a time

Agglomerative Clustering

- 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

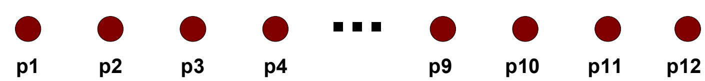
Agglomerative Clustering: Initially

- Start with clusters of individual points and a proximity matrix



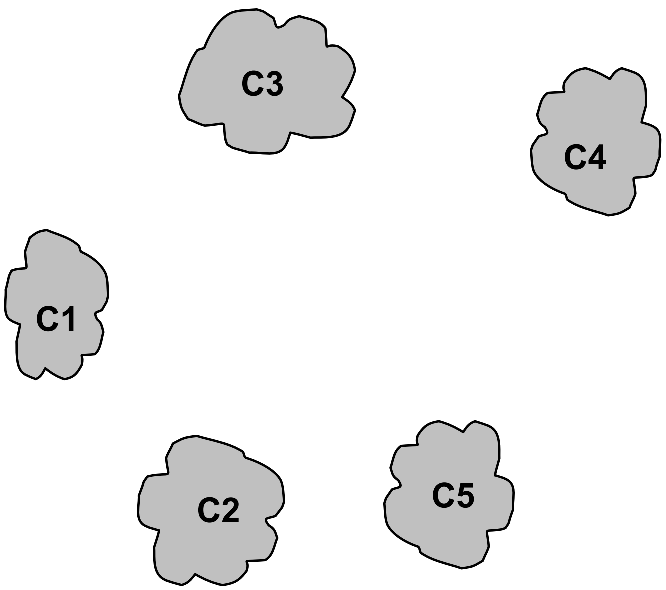
	p1	p2	p3	p4	p5	. . .
p1						
p2						
p3						
p4						
p5						
.						
.						
.						

Proximity Matrix



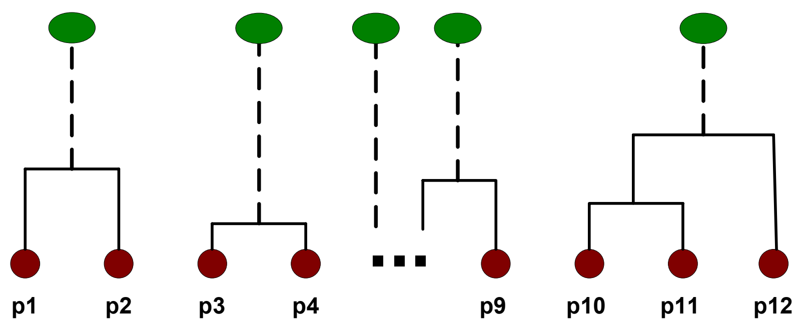
Agglomerative Clustering: Middle

- After some merging steps, we have some clusters



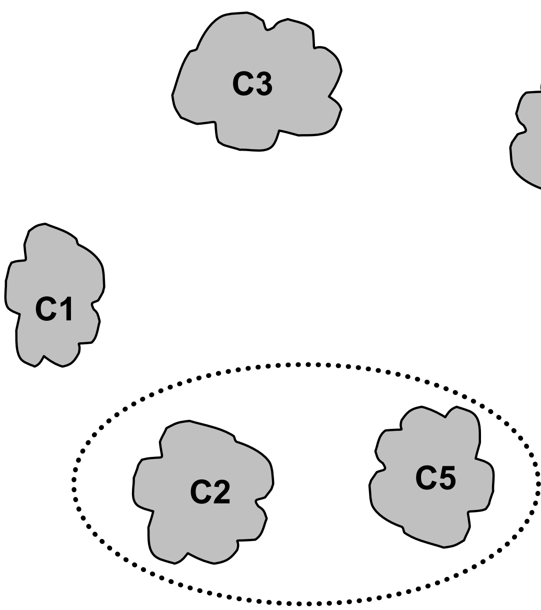
	C1	C2	C3	C4	C5
C1					
C2					
C3					
C4					
C5					

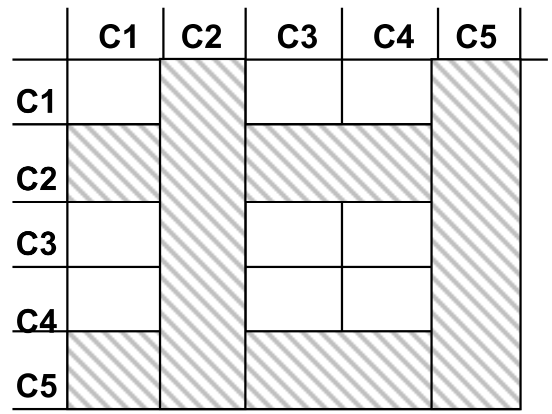
Proximity Matrix



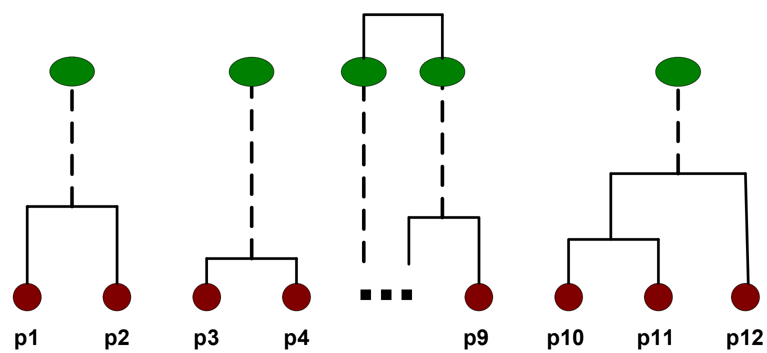
Agglomerative Clustering: Middle

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



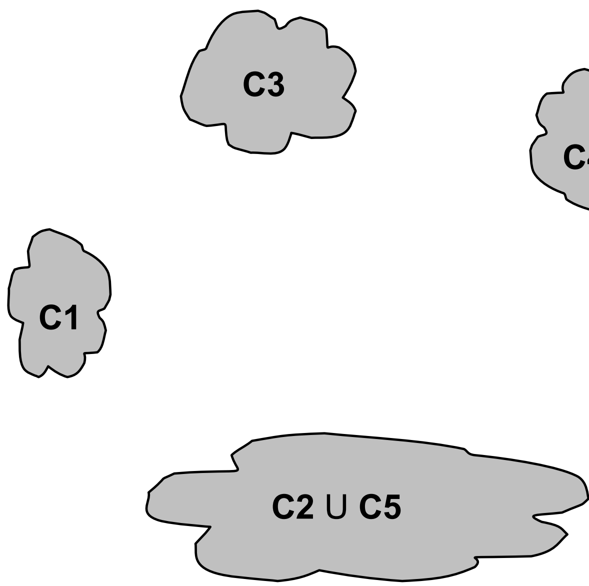


Proximity Matrix



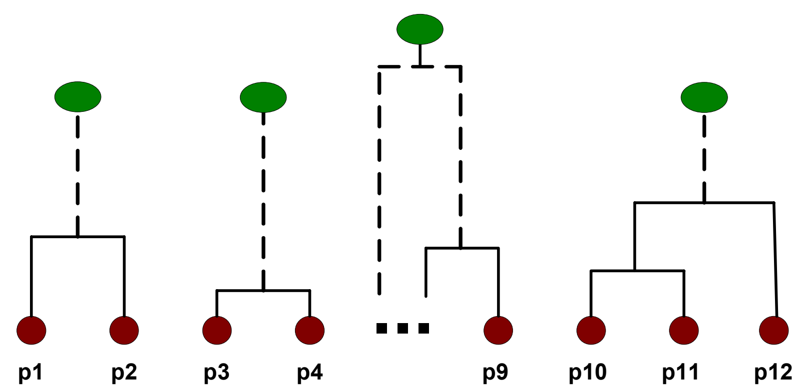
Agglomerative Clustering: After Merging

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

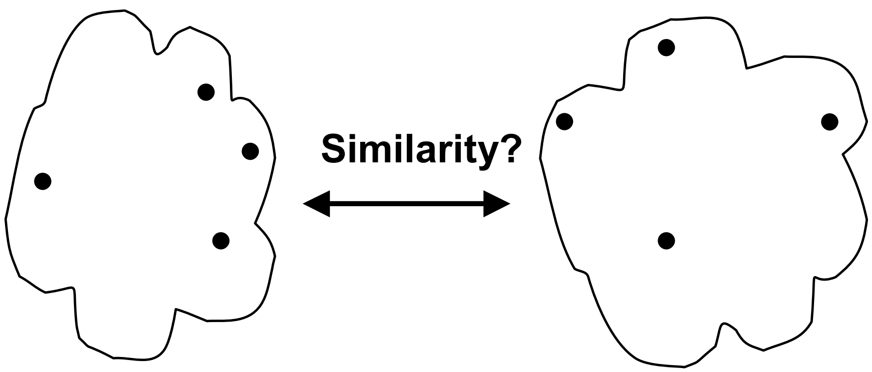


	C1	C2 U C5	C3	C4
C1		?		
C2 U C5	?	?	?	?
C3		?		
C4		?		

Proximity Matrix



How to define Inter-cluster similarity



- MIN
- MAX
- Group Average
- Distance Between Centroids

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

Proximity Matrix

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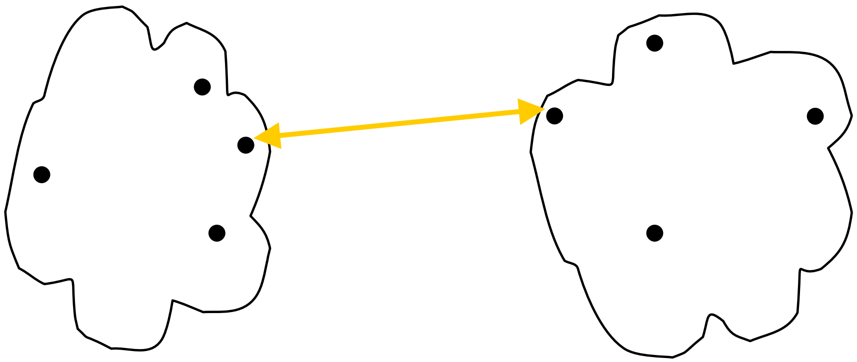

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Proximity Matrix

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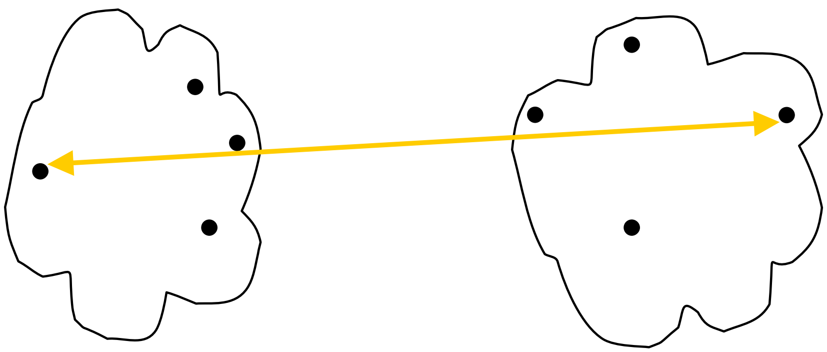

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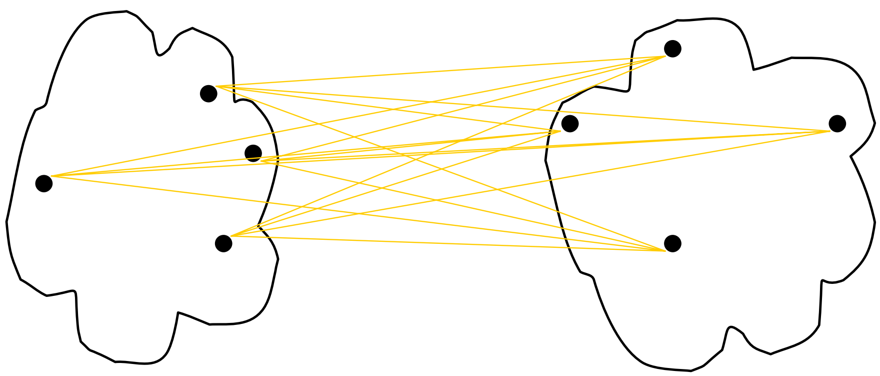

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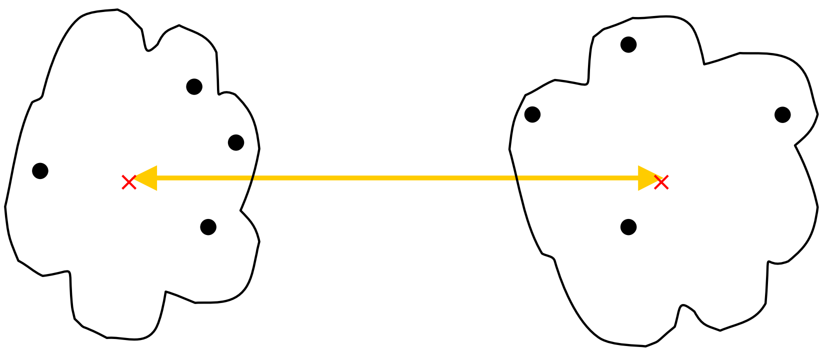

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Proximity Matrix

- MIN
- MAX
- Group Average
- Distance Between Centroids

Cluster Similarity: MIN ("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.

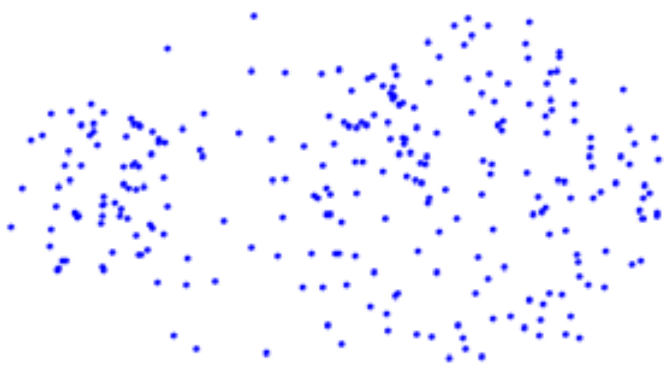
Hierarchical Clustering, MIN: Strengths

Original Points

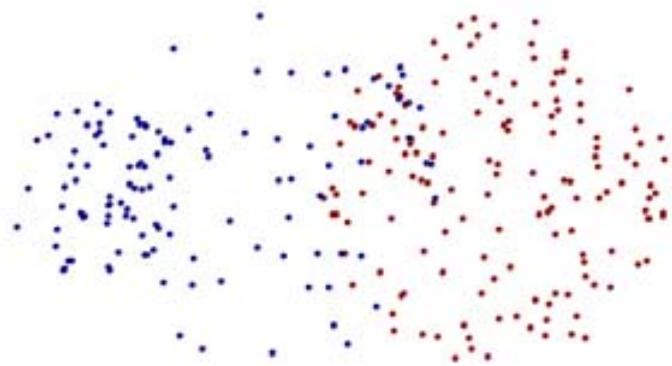
Two Clusters

- **Can handle non-elliptical shapes**

Hierarchical Clustering, MIN: Limitations



Original Points



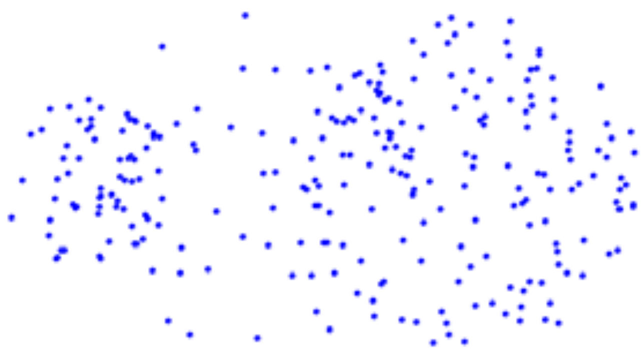
Two Clusters

- **Sensitive to noise and outliers**

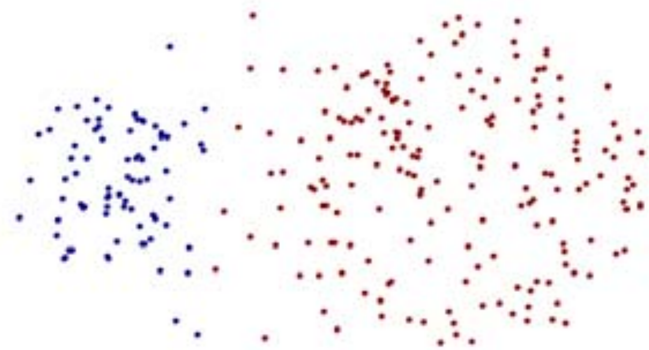
Cluster Similarity: MAX (“Complete Link”)

- 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

Hierarchical Clustering, MAX: Strengths



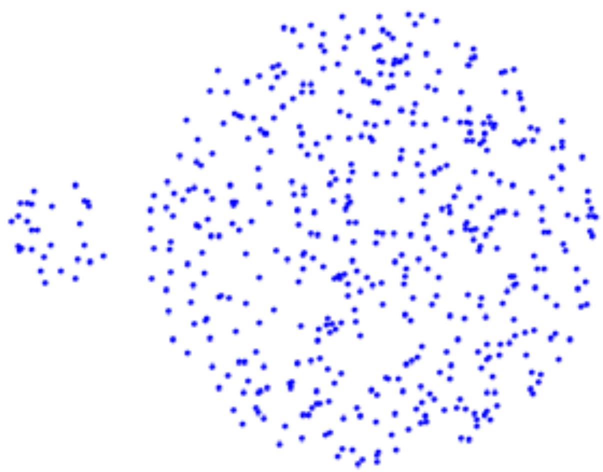
Original Points



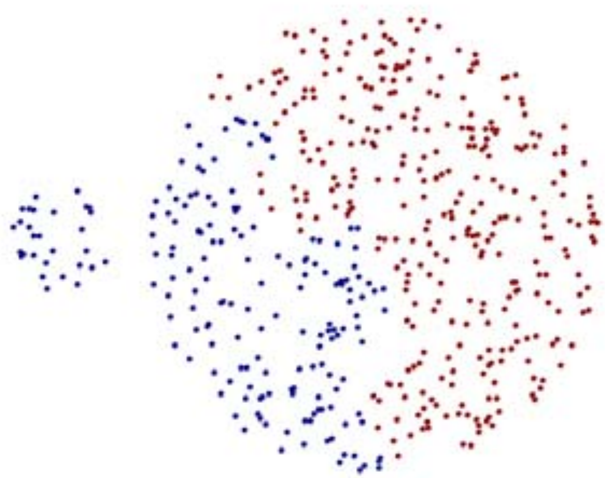
Two Clusters

- **Less susceptible to noise and outliers**

Hierarchical Clustering, MAX: Limitations



Original Points



Two Clusters

•**Tends to break large clusters**

Cluster Similarity: Group Average

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

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

- Compromise between Single and Complete Link

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

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