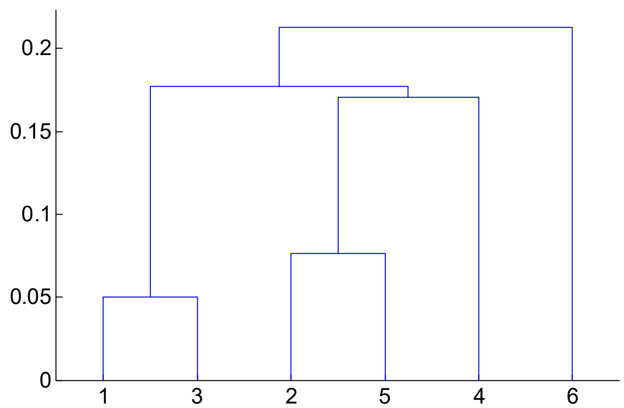
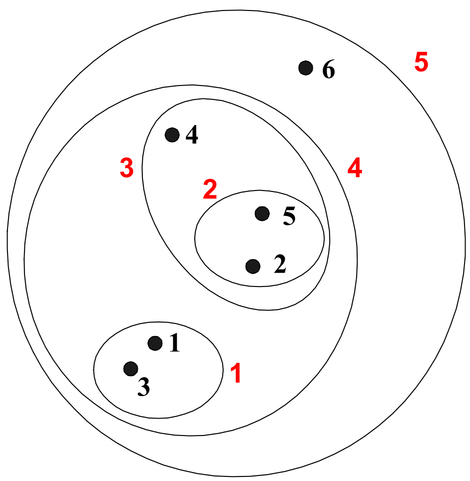
Hierarchical Clustering

- 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

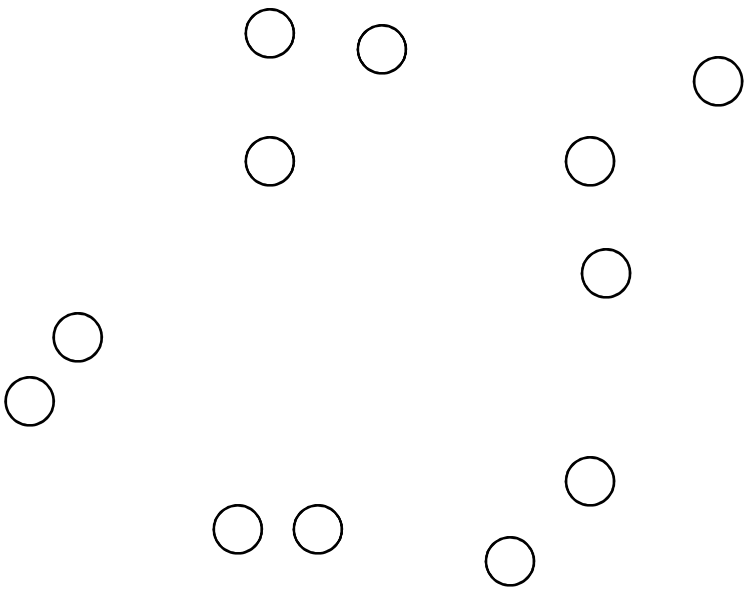
- Two main types of hierarchical clustering
  - Agglomerative:
    - Start with the points as individual clusters
    - At each step, merge the closest pair of clusters until only one cluster (or k clusters) left
  - Divisive:
    - Start with one, all-inclusive cluster
    - At each step, split a cluster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

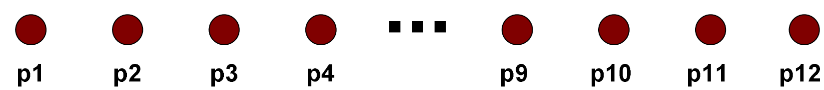
Starting Situation

- Start with clusters of individual points and a proximity matrix



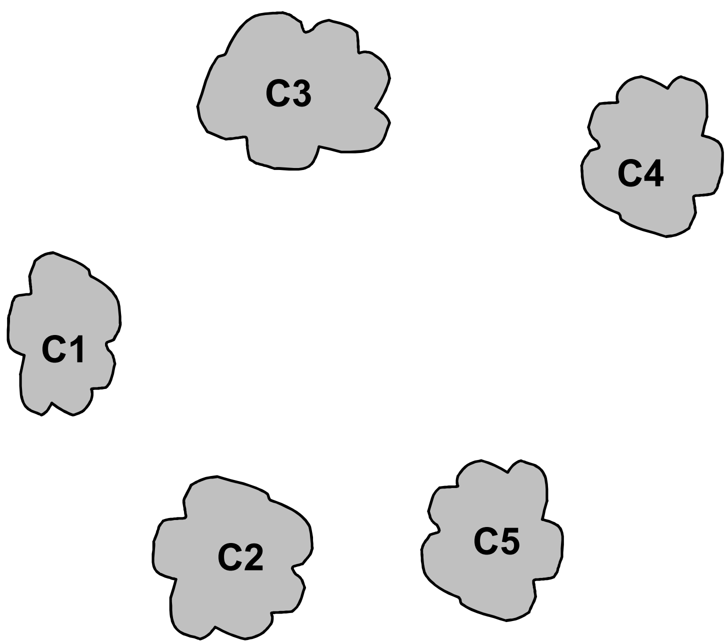
	p1	p2	p3	p4	p5	. . .
p1						
p2						
p3						
p4						
p5						
.						
.						
.						

Proximity Matrix



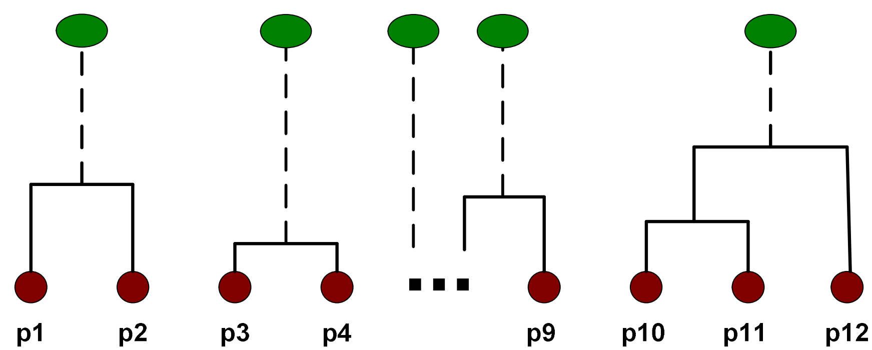
Intermediate Situation

- After some merging steps, we have some clusters



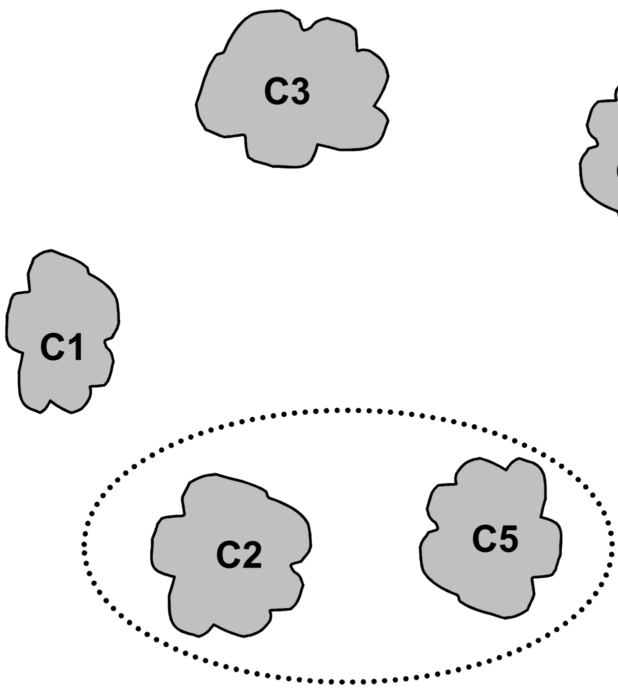
	C1	C2	C3	C4	C5
C1					
C2					
C3					
C4					
C5					

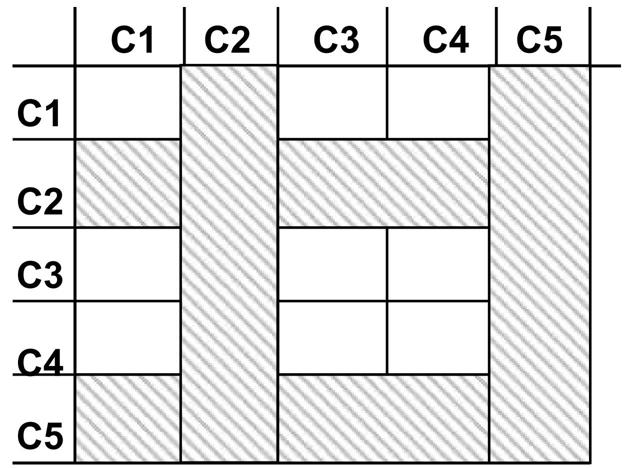
Proximity Matrix



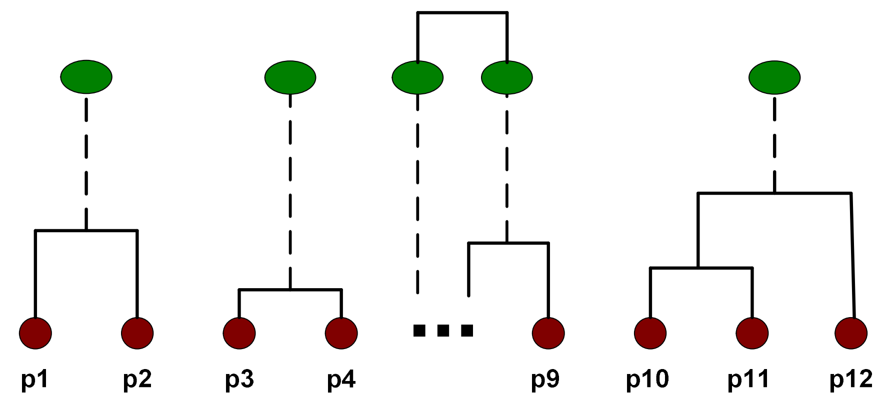
Intermediate Situation

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



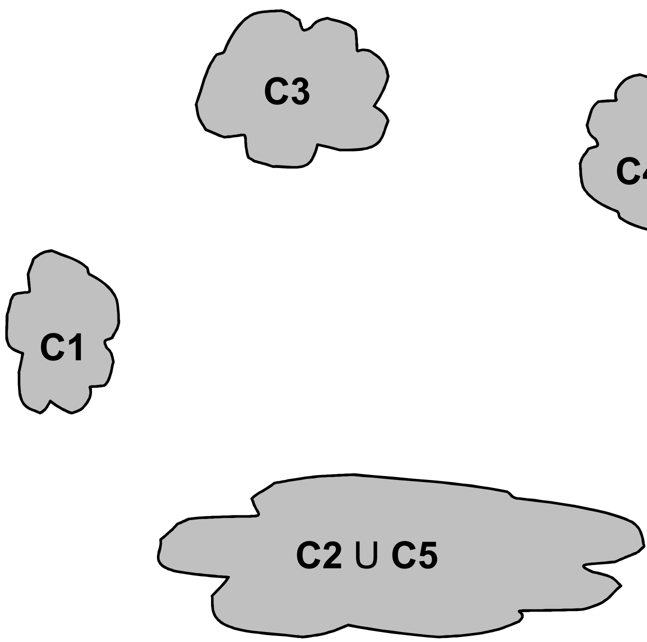


Proximity Matrix



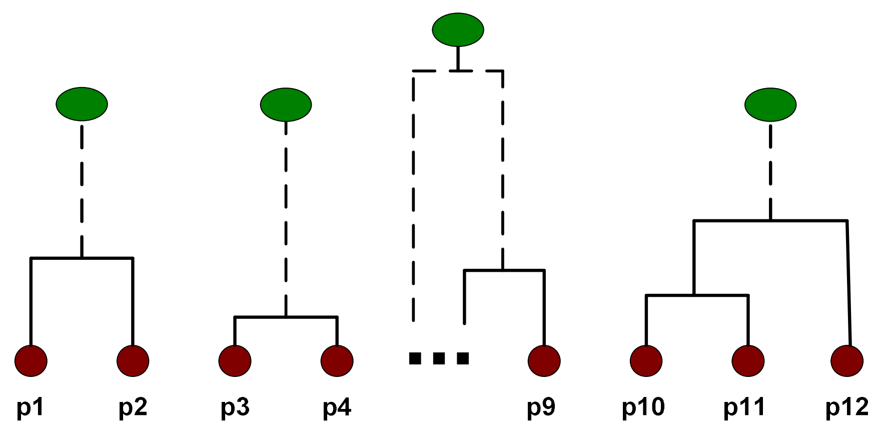
After Merging

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

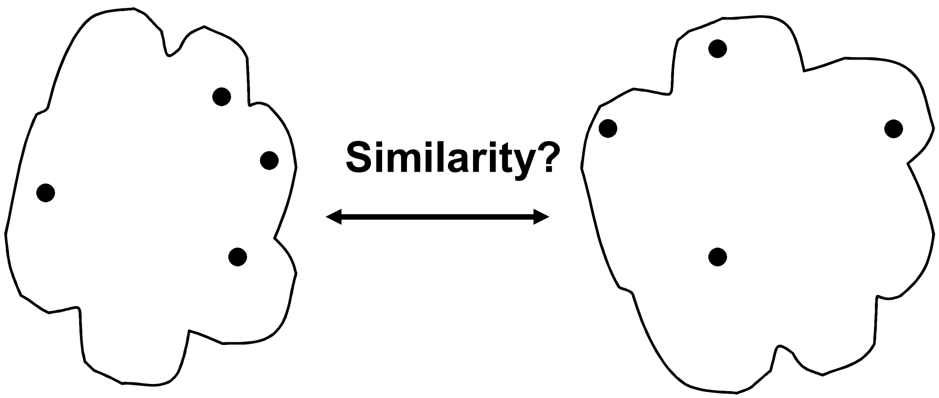


	C1	C2 U C5	C3	C4
C1		?		
C2 U C5	?	?	?	?
C3		?		
C4		?		

Proximity Matrix



How to Define Inter-Cluster Distance

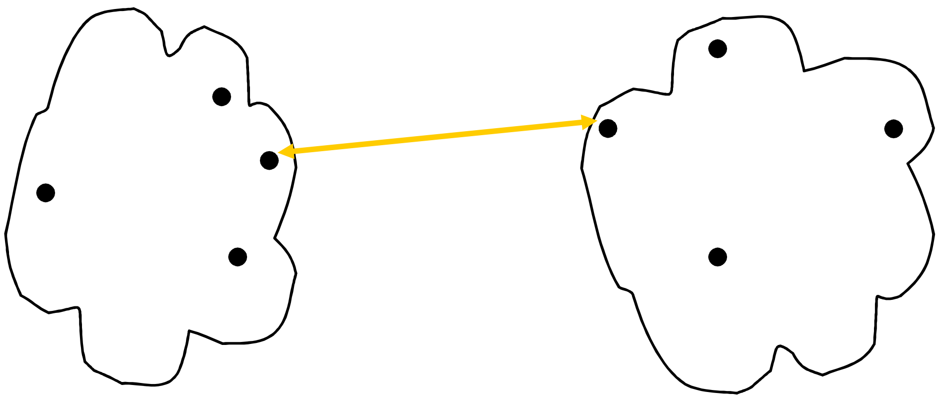


	p1	p2	p3	p4	p5	. . .
p1						
p2						
p3						
p4						
p5						
.						
.						
.						

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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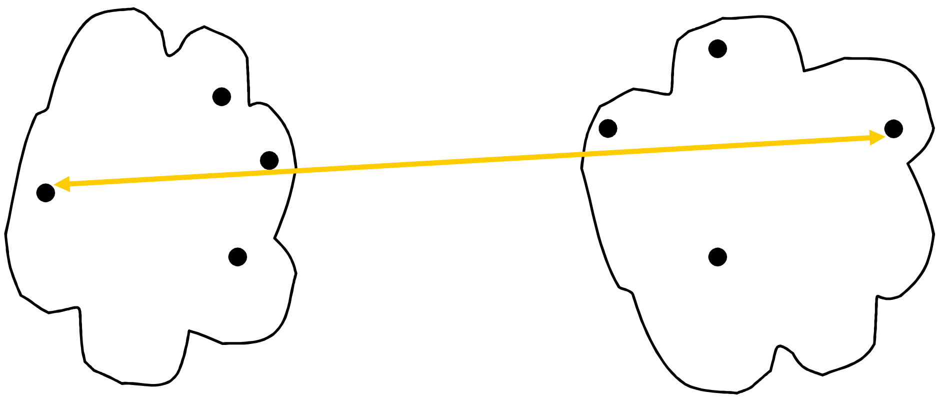
How to Define Inter-Cluster Similarity



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

Proximity Matrix

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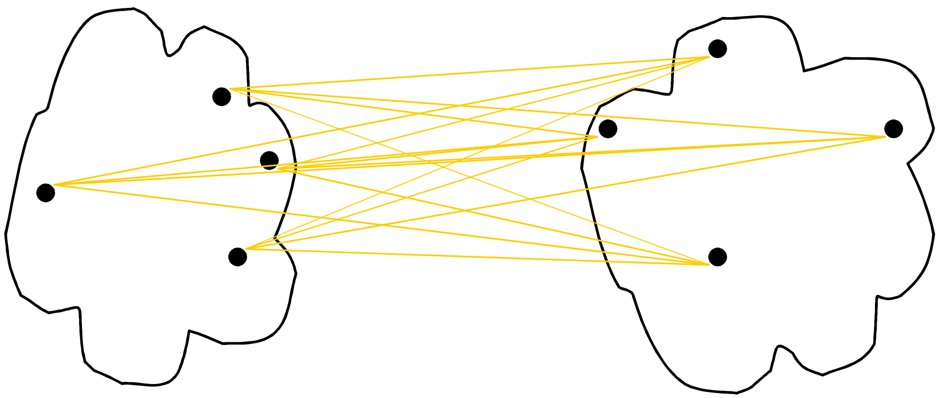
How to Define Inter-Cluster Similarity



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

Proximity Matrix

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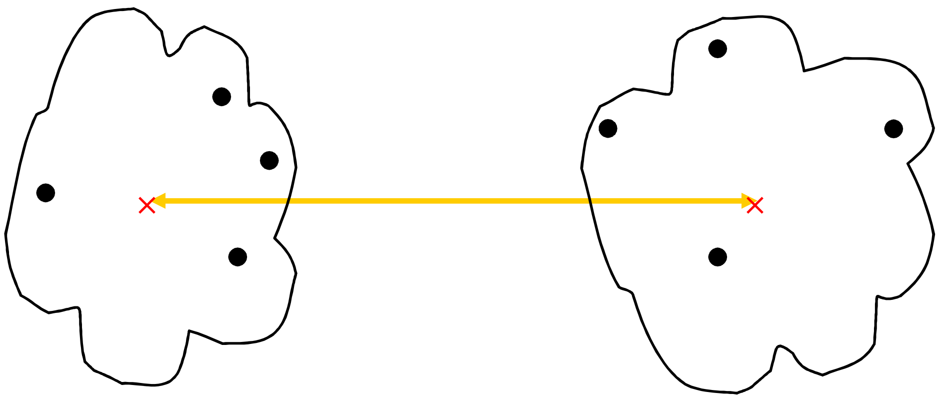
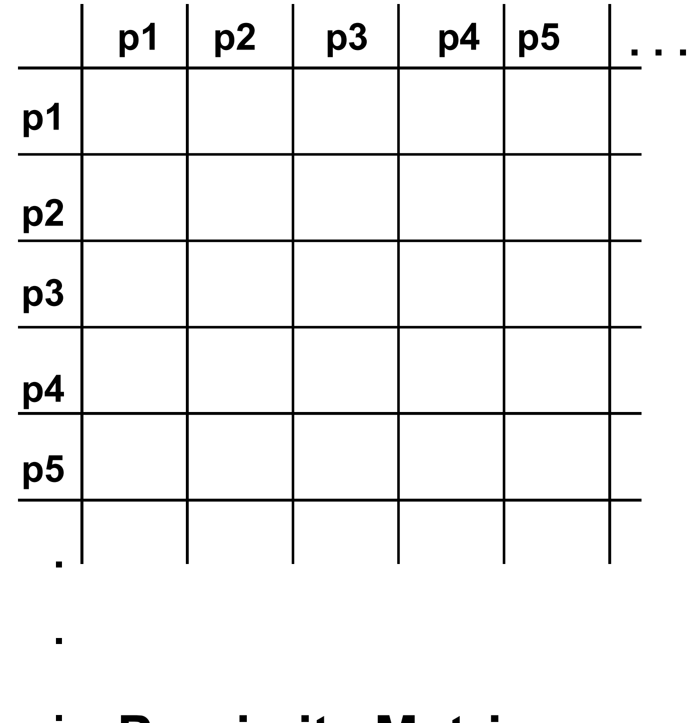
How to Define Inter-Cluster Similarity



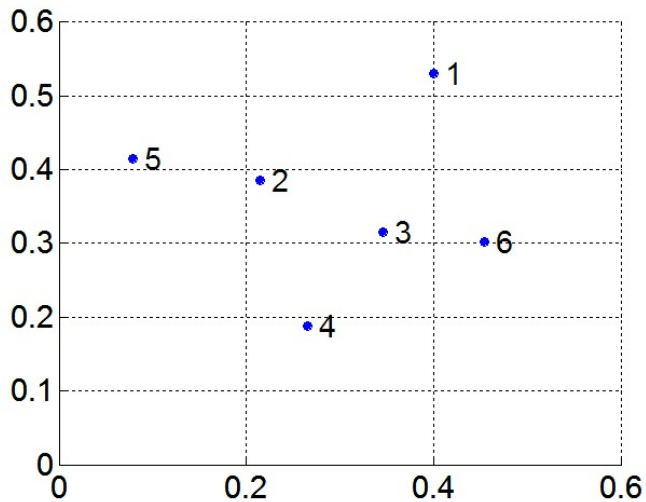


Proximity Matrix

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

MIN or Single Link

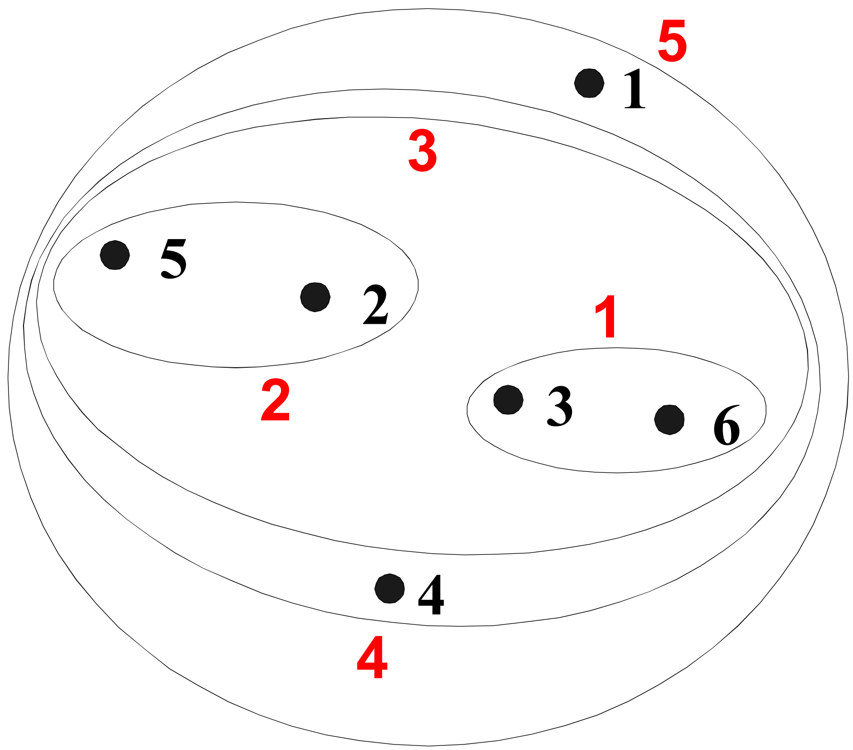
- Proximity of two clusters is based on the two closest points in the different clusters
  - Determined by one pair of points, i.e., by one link in the proximity graph
- Example:

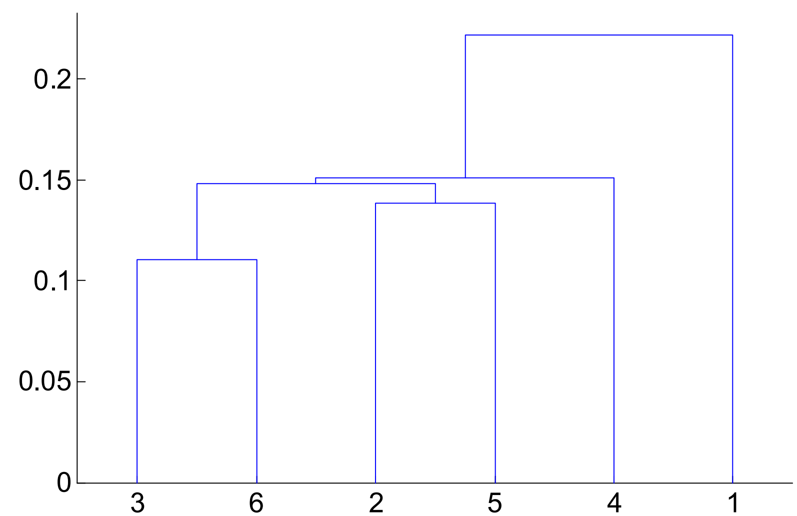


Distance Matrix:

	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

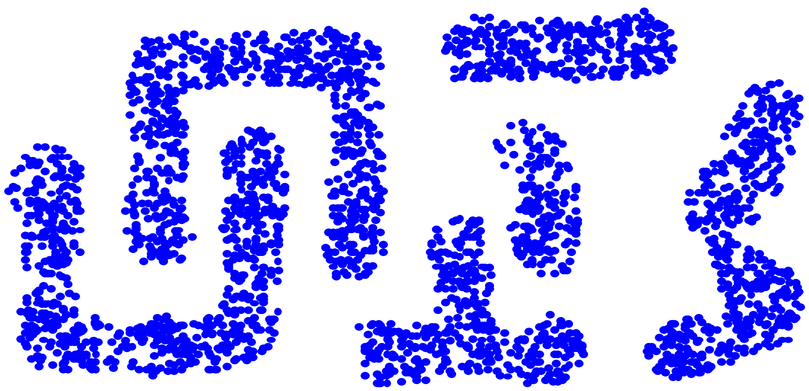




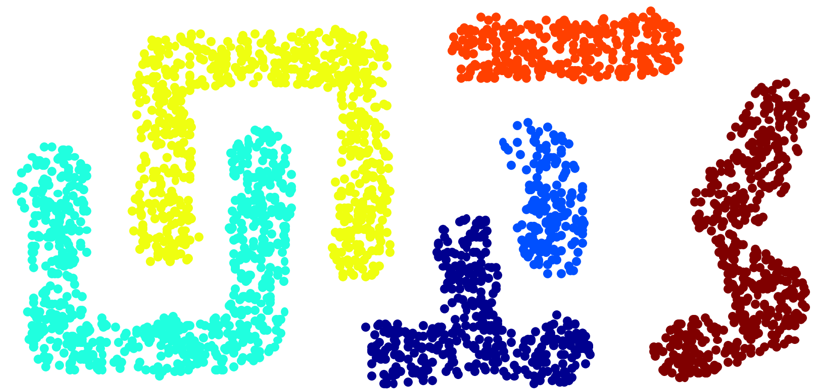
Nested Clusters

Dendrogram

Strength of MIN



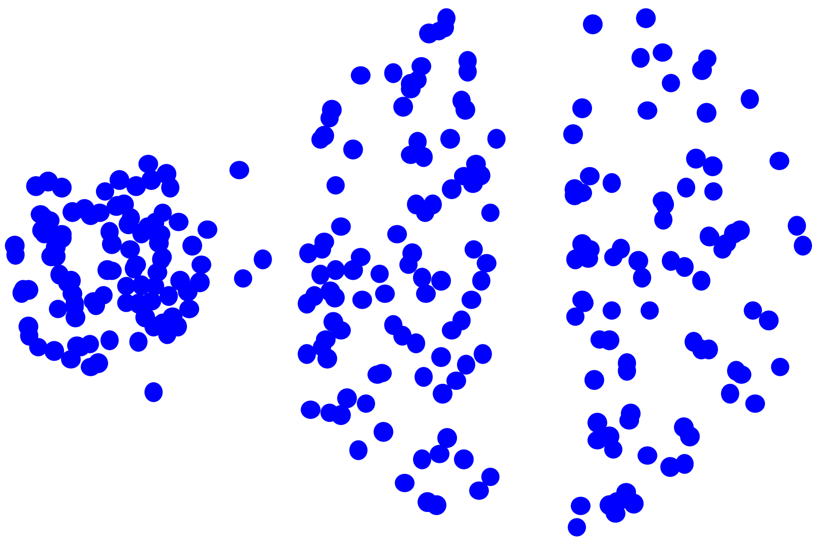
Original Points



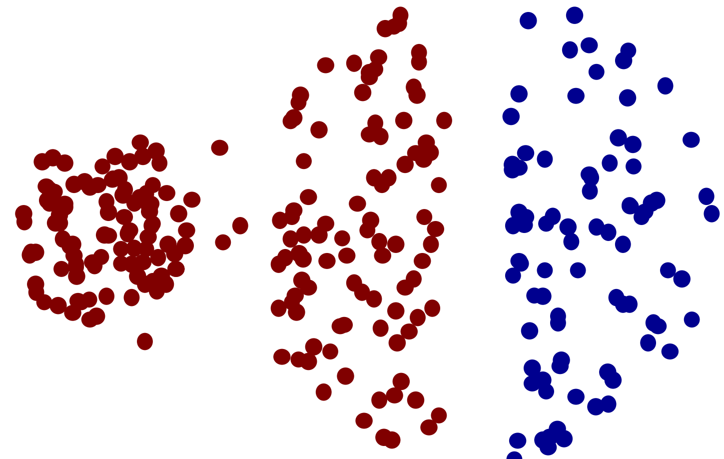
Six Clusters

- Can handle non-elliptical shapes

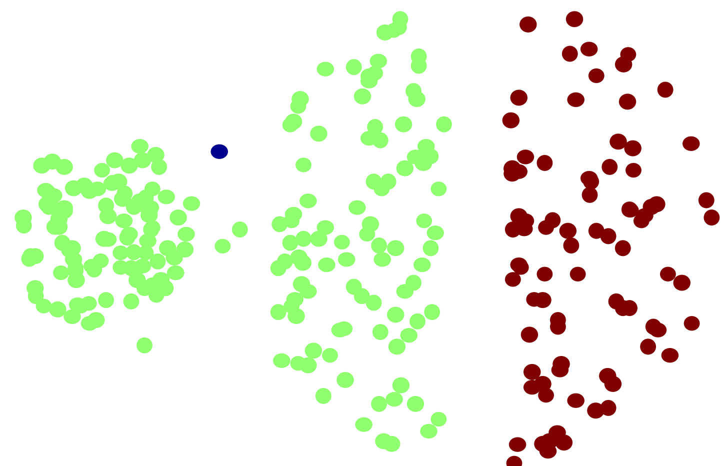
Limitations of MIN



Original Points



Two Clusters

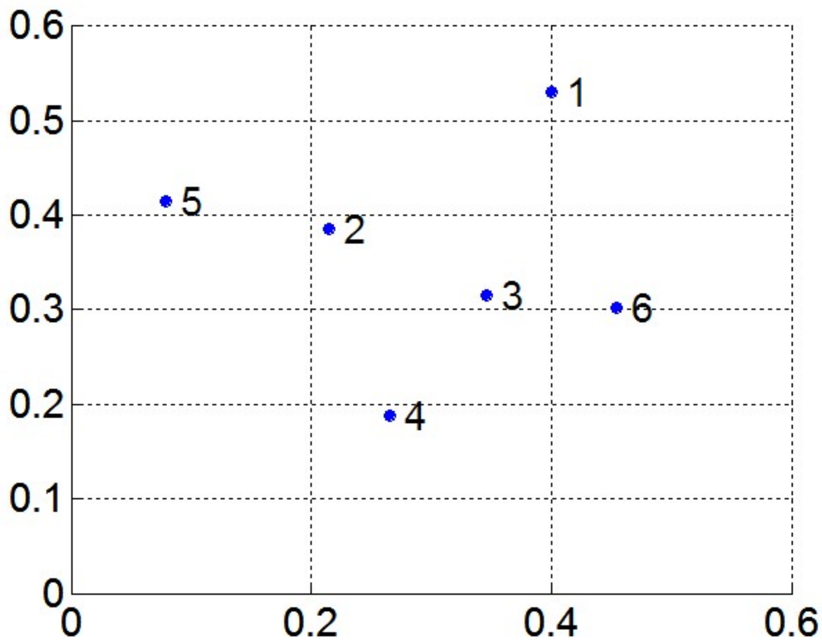


Three Clusters

• Sensitive to noise and outliers

MAX or Complete Linkage

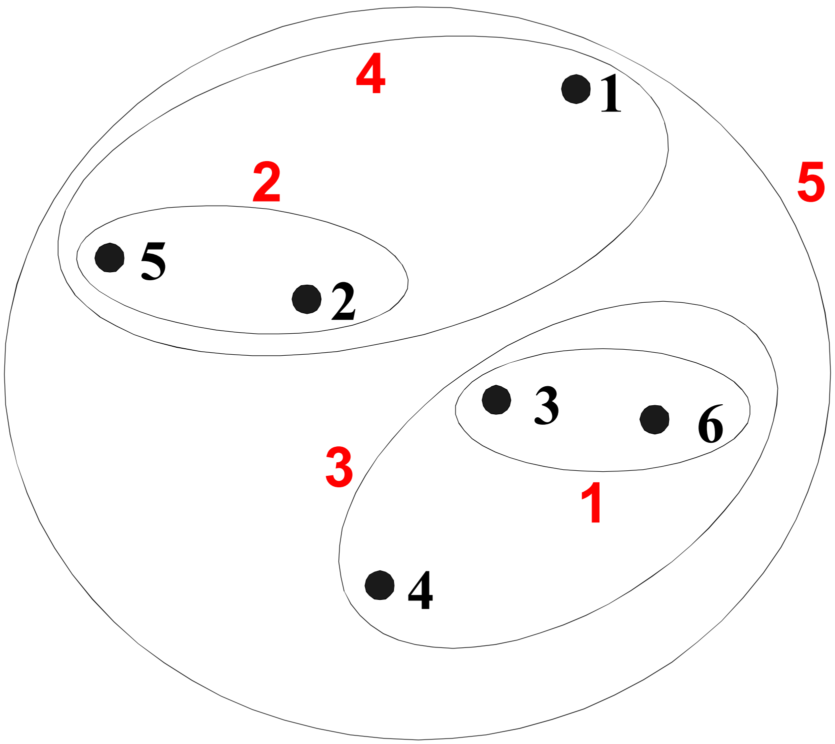
- Proximity of two clusters is based on the two most distant points in the different clusters
  - Determined by all pairs of points in the two clusters



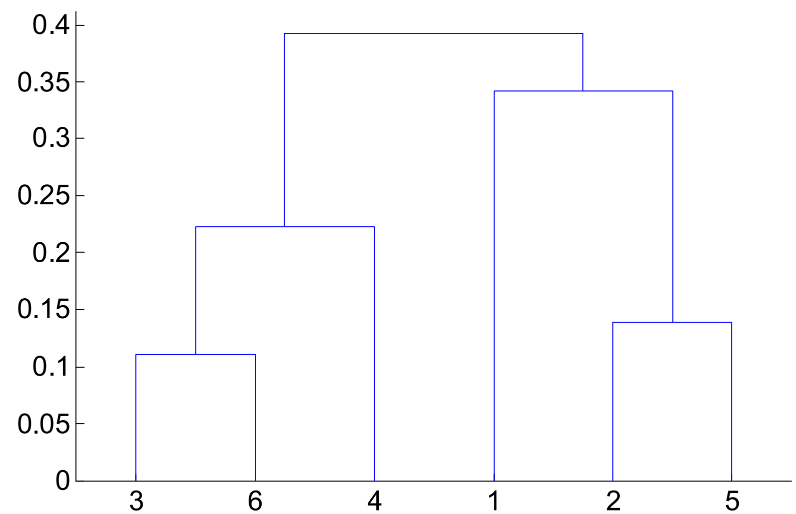
Distance Matrix:

	p1	p2	p3	p4	p5	p6
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

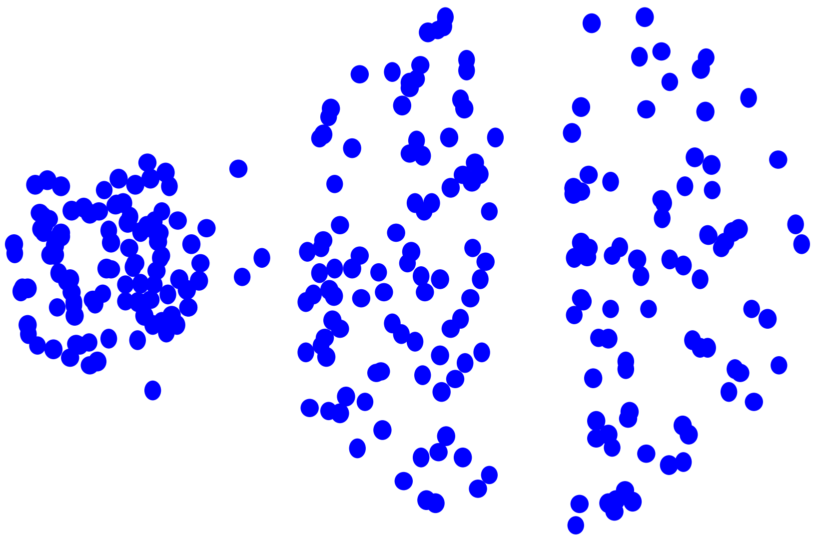


Nested Clusters

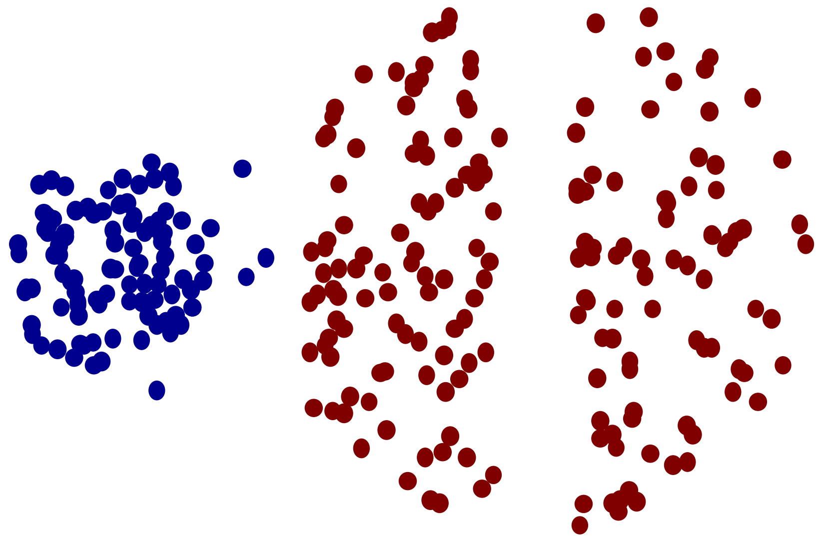


Dendrogram

Strength of MAX



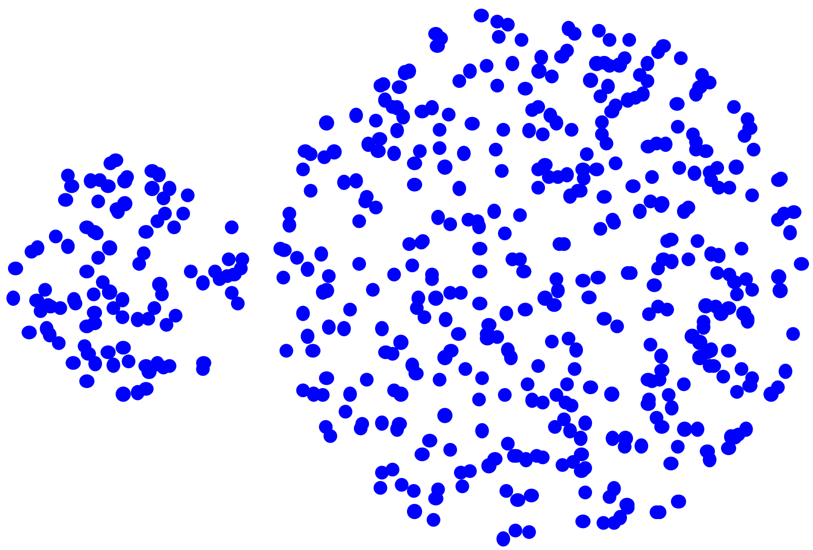
Original Points



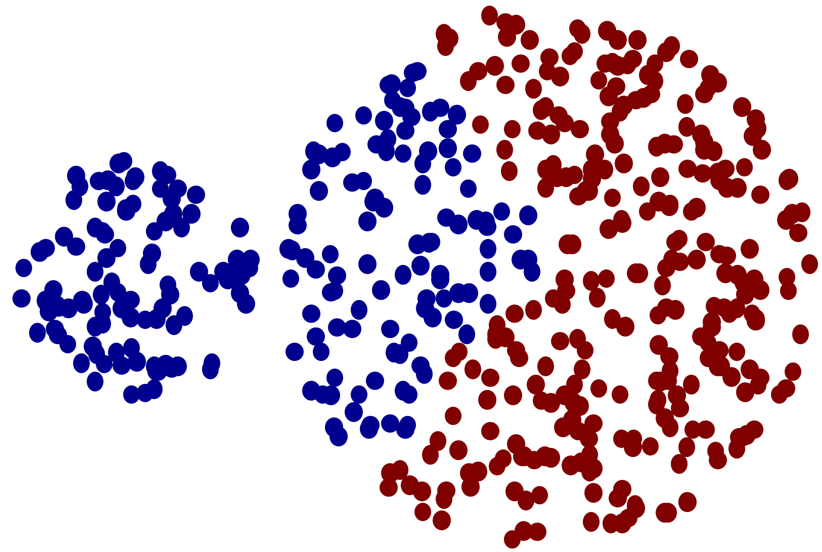
Two Clusters

- Less susceptible to noise and outliers

Limitations of MAX



Original Points



Two Clusters

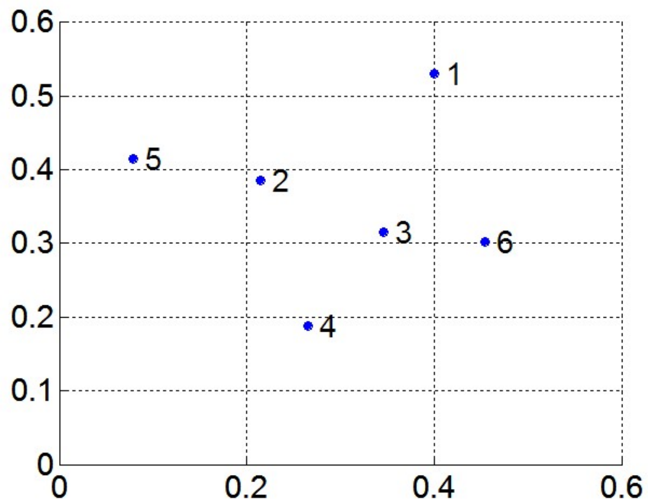
- Tends to break large clusters
- Biased towards globular clusters

Group Average

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

$$\mathbf{proximity}(\mathbf{Cluster_i},\mathbf{Cluster_j}) = \frac{\sum\limits_{\substack{p_i \in Cluster_i \\ p_j \in Cluster_j}} \mathbf{proximity}(\mathbf{p_i},\mathbf{p_j})}{|\mathbf{Cluster_i}| \times |\mathbf{Cluster_j}|}$$

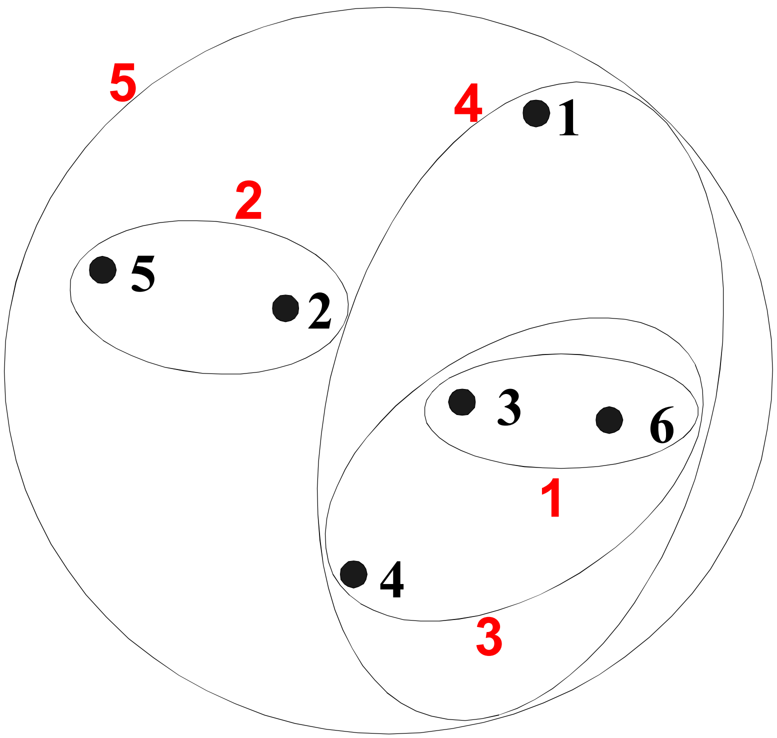
- Need to use average connectivity for scalability since total proximity favors large clusters



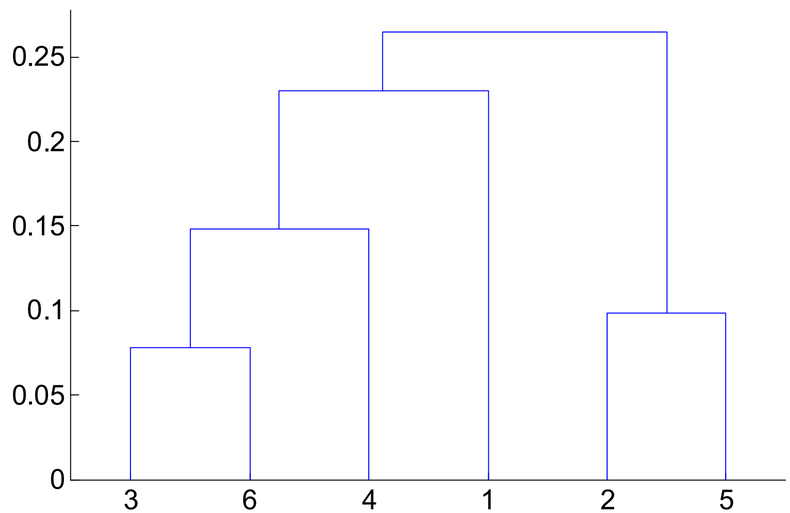
Distance Matrix:

	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: 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

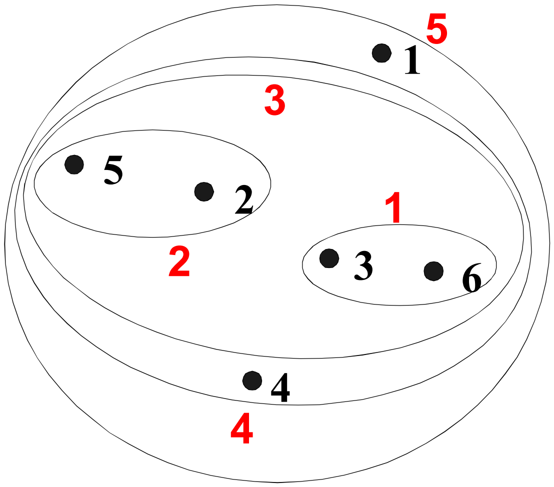
- Similarity of two clusters is based on the increase in squared error when two clusters are merged
  - Similar to group average if distance between points is distance squared

- Less susceptible to noise and outliers

- Biased towards globular clusters

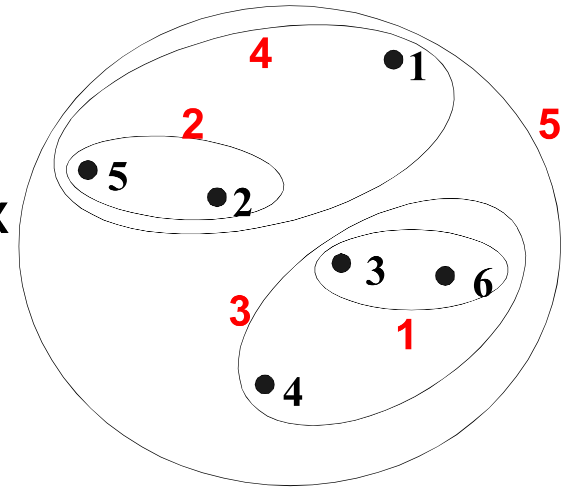
- Hierarchical analogue of K-means
  - Can be used to initialize K-means

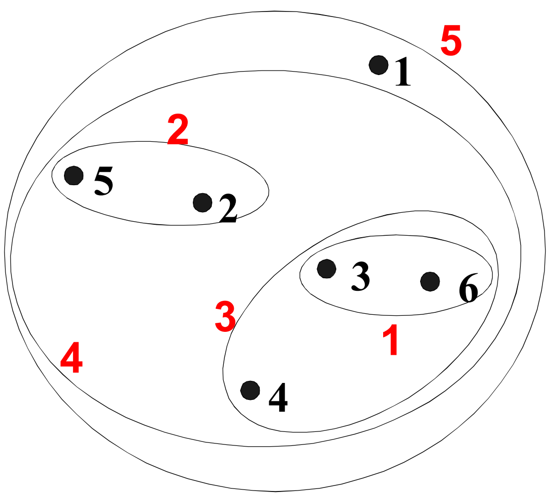
Hierarchical Clustering: Comparison



MIN

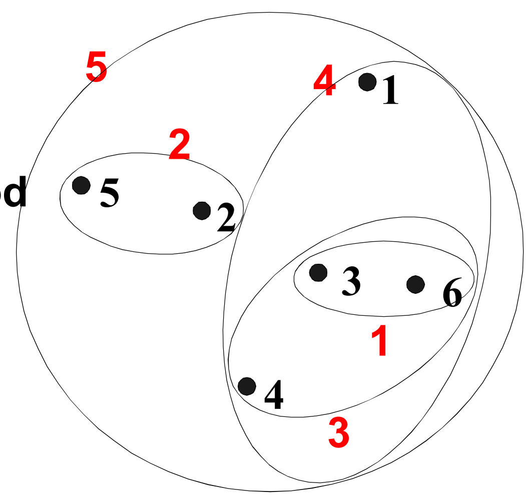
MAX





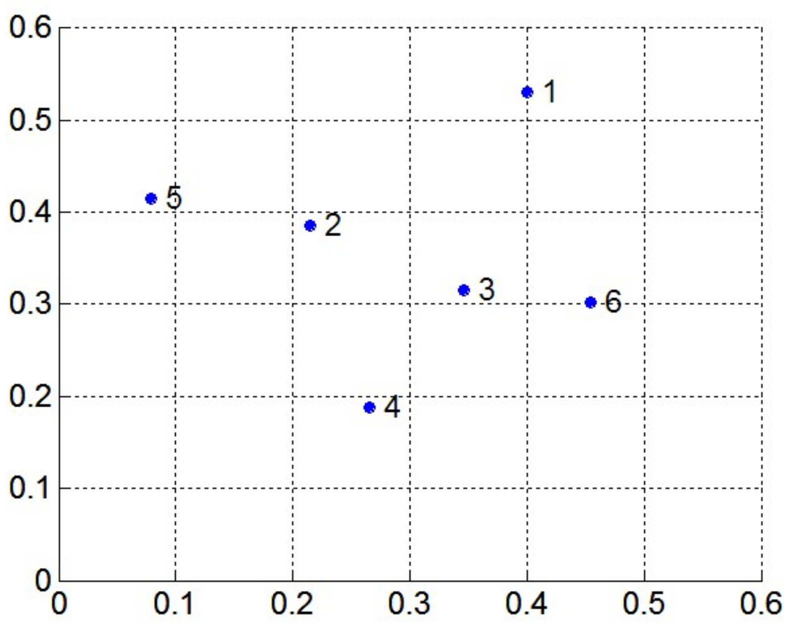
Group Average

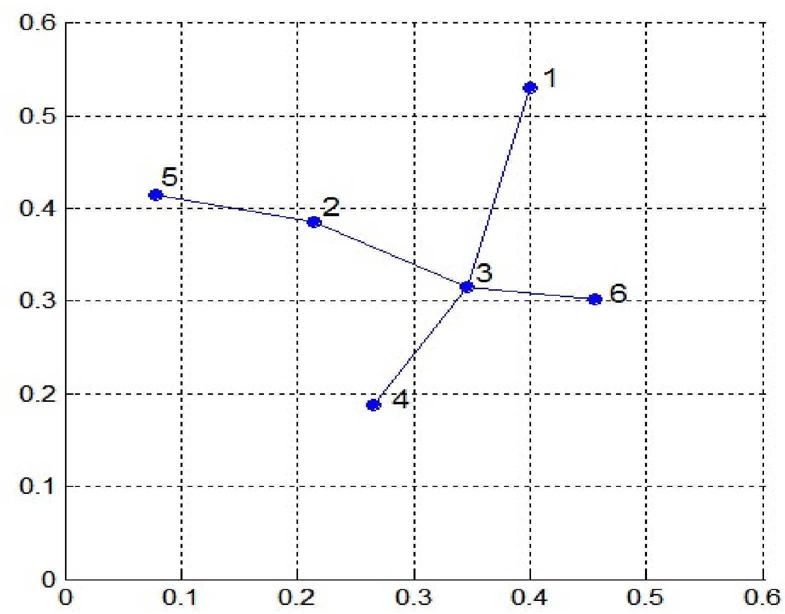
Ward's Method



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

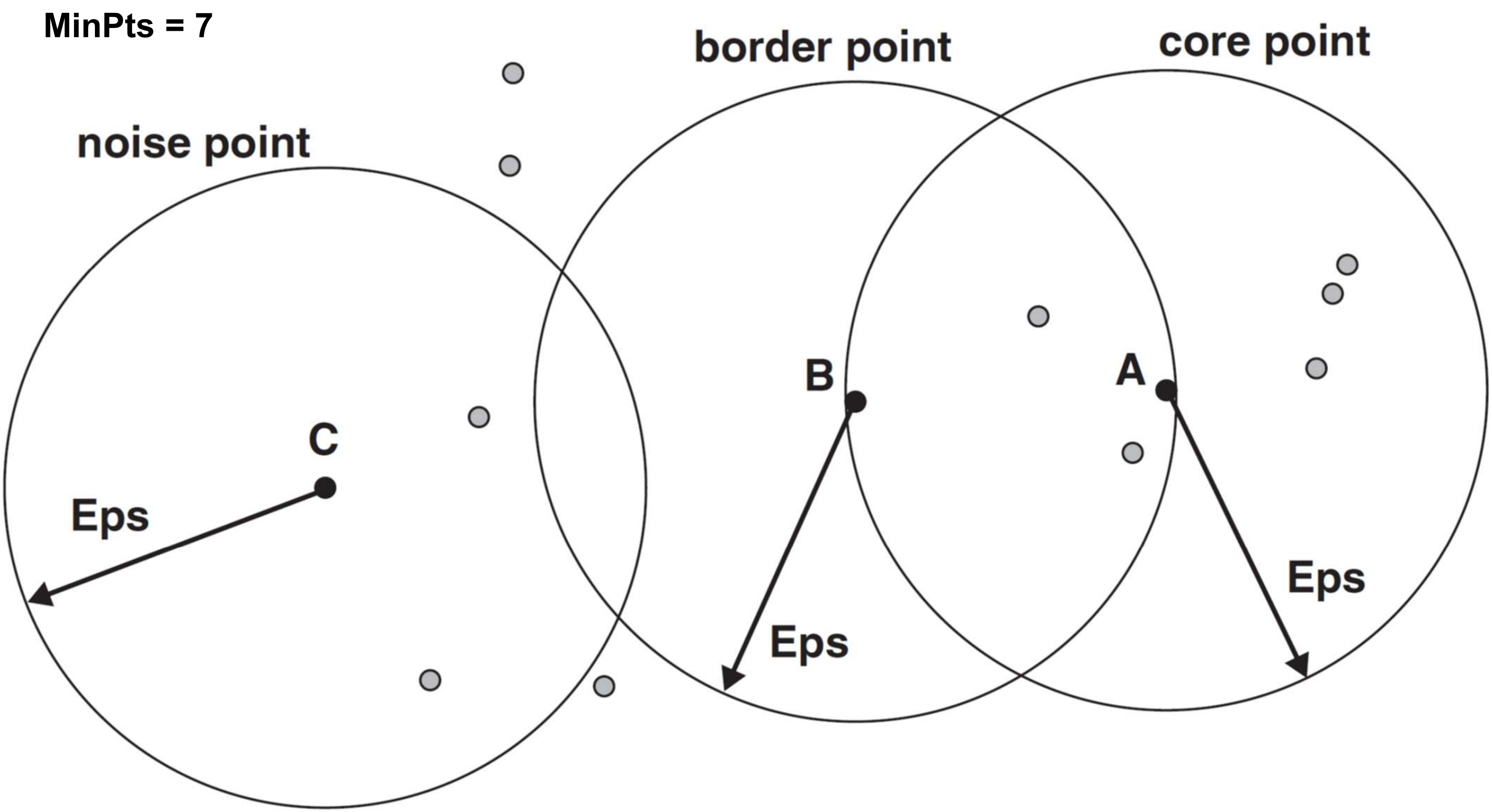
- No global objective function is directly minimized

- 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

DBSCAN

- DBSCAN (Density-based spatial clustering of applications with noise) is a density-based clustering algorithm.
  - Density = number of points within a specified radius (Eps)
  - A point is a core point if it has at least a specified number of points (MinPts) within Eps
    - These are points that are at the interior of a cluster
    - Counts the point itself
  - A border point is not a core point, but is in the neighborhood of a core point
  - A noise point is any point that is not a core point or a border point

DBSCAN: Core, Border, and Noise Points



DBSCAN Algorithm

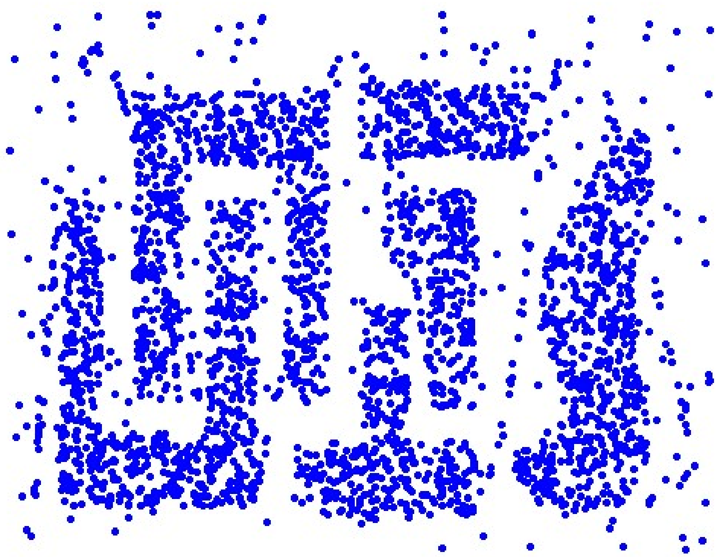
- Eliminate noise points
- Perform clustering on the remaining points

$current\_cluster\_label \leftarrow 1$
for all core points **do**
  if the core point has no cluster label **then**
    $current\_cluster\_label \leftarrow current\_cluster\_label + 1$
    Label the current core point with cluster label $current\_cluster\_label$
  end if
  for all points in the Eps-neighborhood, except i^{th} the point itself **do**
    if the point does not have a cluster label **then**
      Label the point with cluster label $current\_cluster\_label$
    end if
  end for
end for

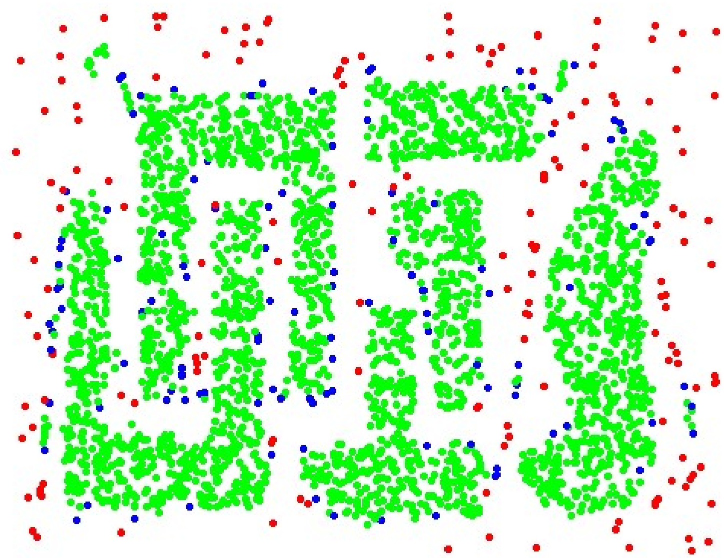
DBSCAN Algorithm

- Starts with an arbitrary point ‘p’ that has not been visited.
- If $|Eps_p|$ >= MinPts, start a cluster otherwise ‘p’ is labeled as noise. (‘p’ might later be found in a sufficiently sized ε-environment of a different point and hence be made part of a cluster.)
- Add all points which are density reachable from ‘p’ to this cluster
- Repeat unless all points are visited.

DBSCAN: Core, Border and Noise Points



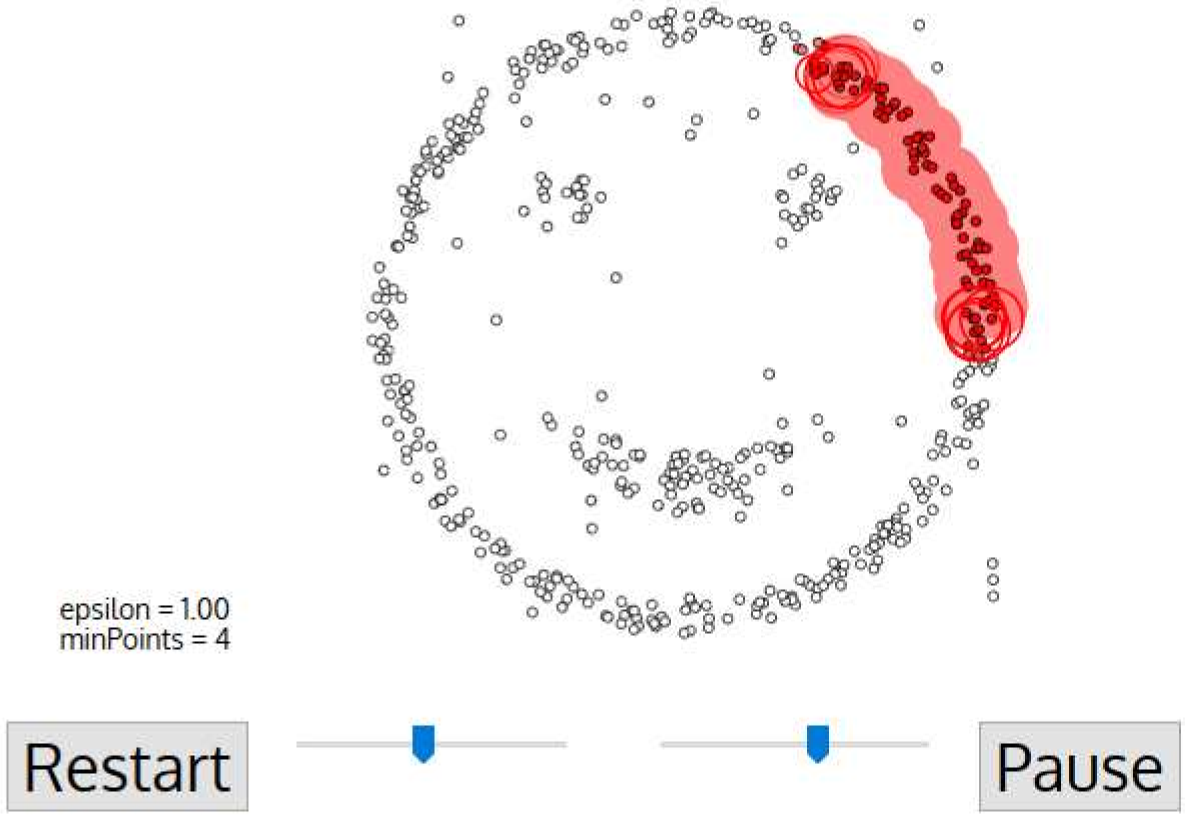
Original Points



Point types: core, border and noise

Eps = 10, MinPts = 4

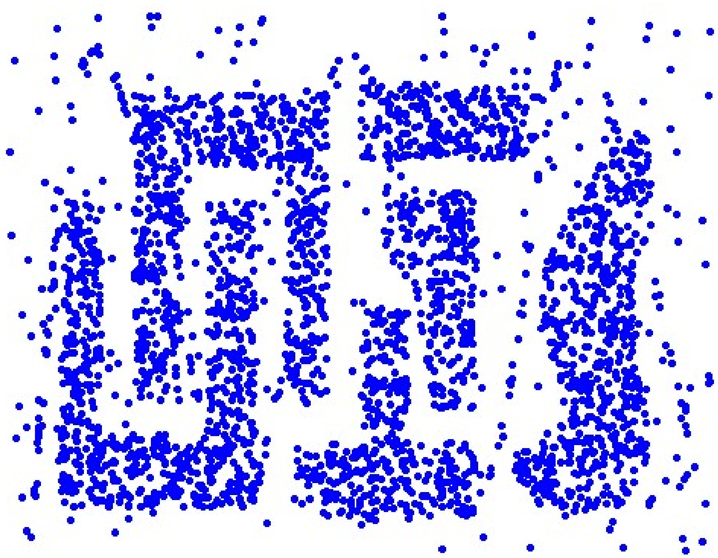
Working of DBSCAN – Sample data



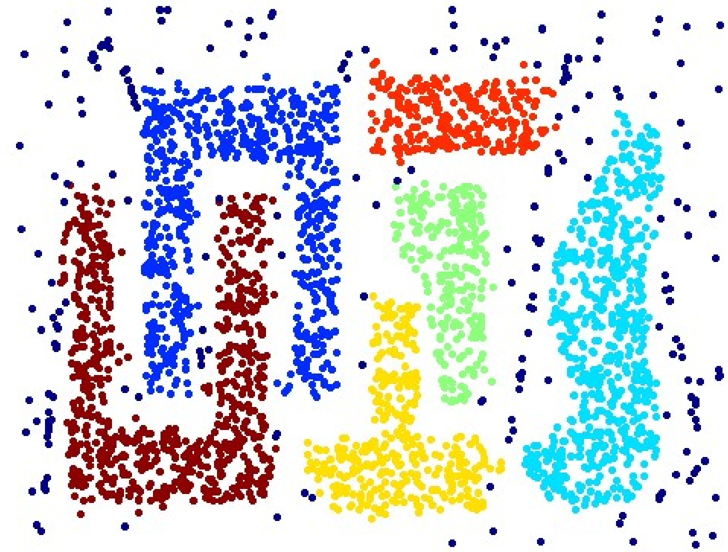
Definitions

- **Directly density reachable**
  - An object (or instance) q is directly density reachable from object p if q is within the ε-Neighborhood of p and p is a core object.
- **Density reachable**
  - An object q is density-reachable from p w.r.t ε and MinPts if there is a chain of objects q_1, q_2…, q_n, with $q_1=p$, $q_n=q$ such that q_{i+1} is directly density-reachable from q_i w.r.t ε and MinPts for all 1 <= i <= n.
- **Density connectivity**
  - Object q is density-connected to object p w.r.t ε and MinPts if there is an object o such that both p and q are density-reachable from o w.r.t ε and MinPts.

When DBSCAN Works Well



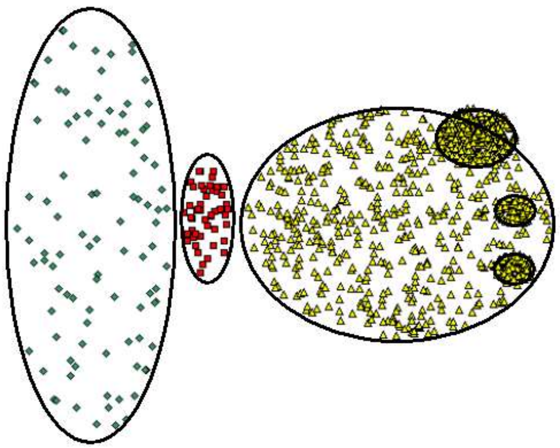
Original Points



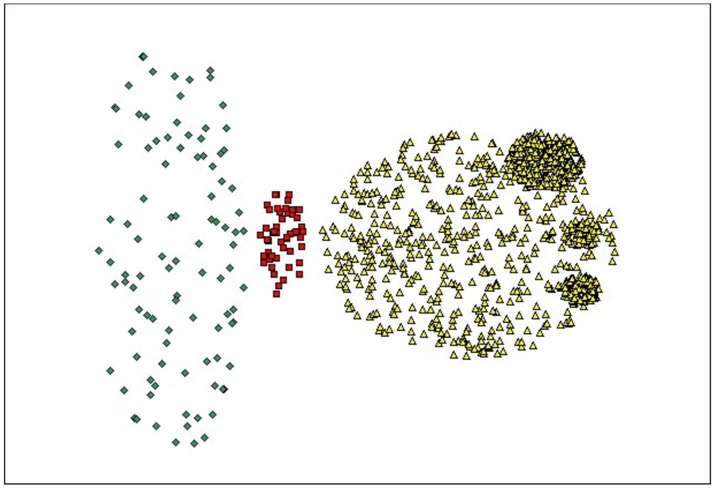
Clusters

- Resistant to Noise
- Can handle clusters of different shapes and sizes

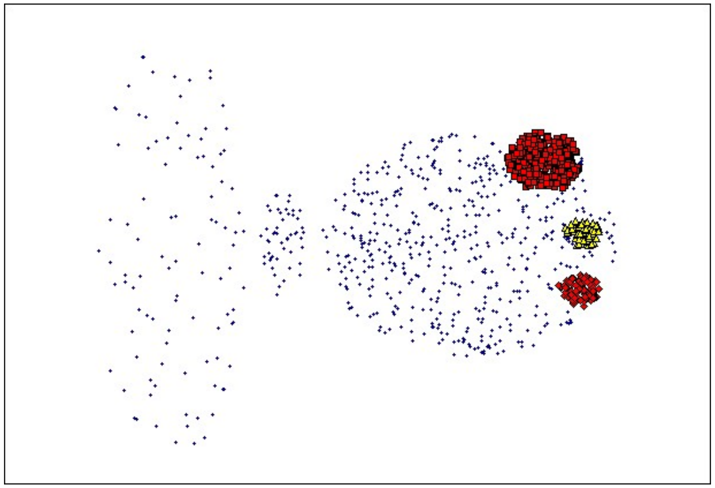
When DBSCAN Does NOT Work Well



Original Points



(MinPts=4, Eps=9.75).



(MinPts=4, Eps=9.92)

- **Varying densities**
- **High-dimensional data**

DBSCAN: Determining EPS and MinPts

- Idea is that for points in a cluster, their k^{th} nearest neighbors are at roughly the same distance
- Noise points have the k^{th} nearest neighbor at farther distance
- So, plot sorted distance of every point to its k^{th} nearest neighbor