Data Mining
Cluster Analysis: Basic Concepts and Algorithms

Lecture Notes for Chapter 7

Introduction to Data Mining, 2nd Edition

by

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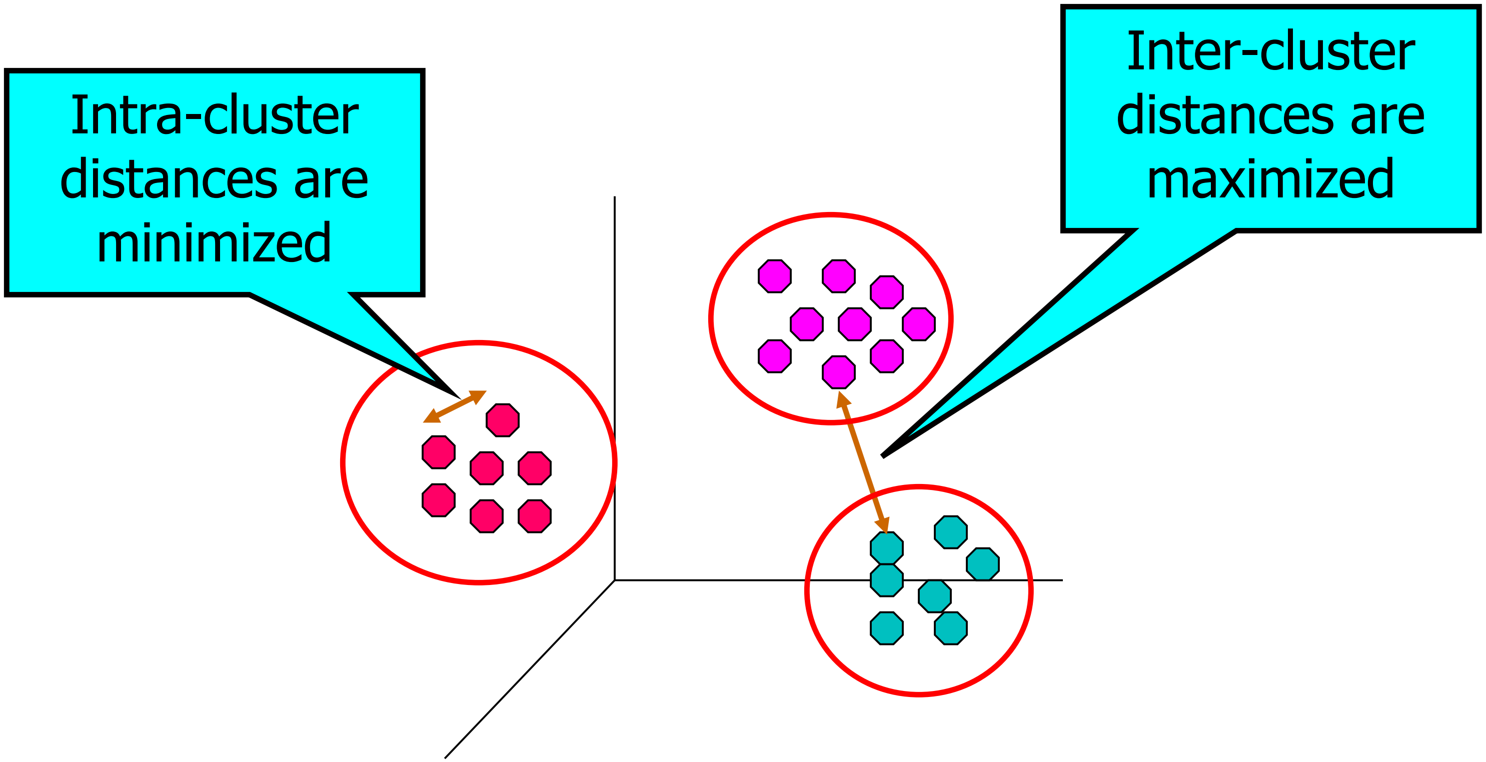
Clustering

What is Cluster Analysis?

- Finding groups of objects such that the objects in a group will be similar (or related) to one another and different from (or unrelated to) the objects in other groups



Applications of Cluster Analysis

- **Understanding**
  - Group related documents for browsing, group genes and proteins that have similar functionality, or group stocks with similar price fluctuations

- **Summarization**
  - Reduce the size of large data sets

What is not Cluster Analysis?

- Simple segmentation
  - Dividing students into different registration groups alphabetically, by last name
- Results of a query
  - Groupings are a result of an external specification
  - Clustering is a grouping of objects based on the data
- Supervised classification
  - Have class label information
- Association Analysis
  - Local vs. global connections

Notion of a Cluster can be Ambiguous

How many clusters?

Six Clusters

Two Clusters

Four Clusters

Types of Clusterings

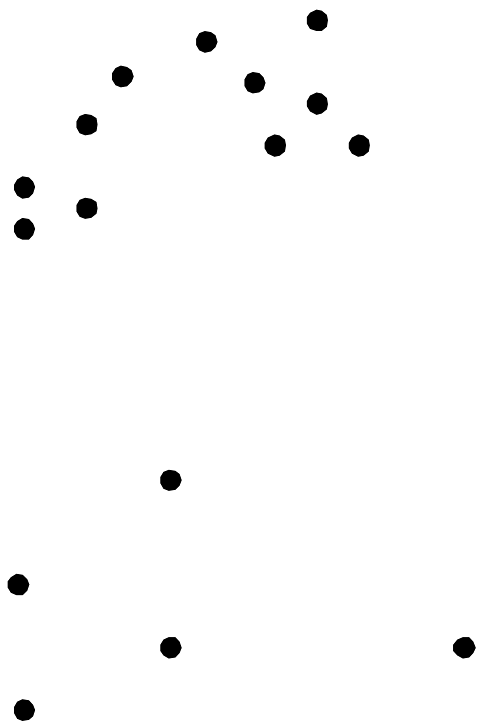
- A clustering is a set of clusters

- Important distinction between hierarchical and partitional sets of clusters

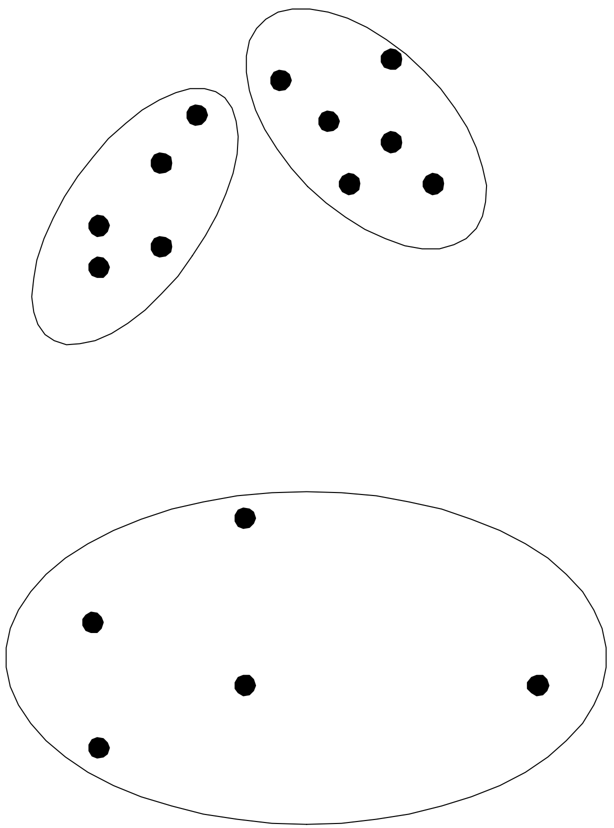
- Partitional Clustering
  - A division of data objects into non-overlapping subsets (clusters) such that each data object is in exactly one subset

- Hierarchical clustering
  - A set of nested clusters organized as a hierarchical tree

Partitional Clustering

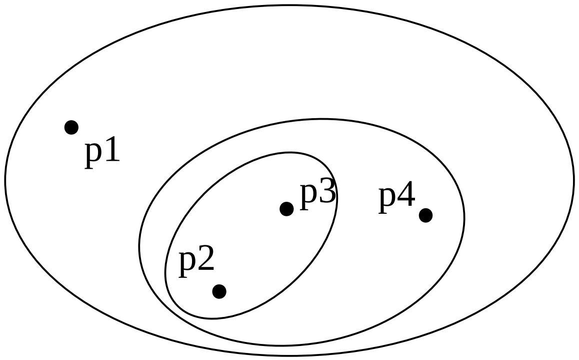


Original Points

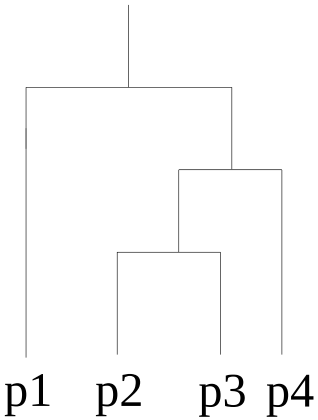


A Partitional Clustering

Hierarchical Clustering



Traditional Hierarchical Clustering



Traditional Dendrogram

Clustering Algorithms

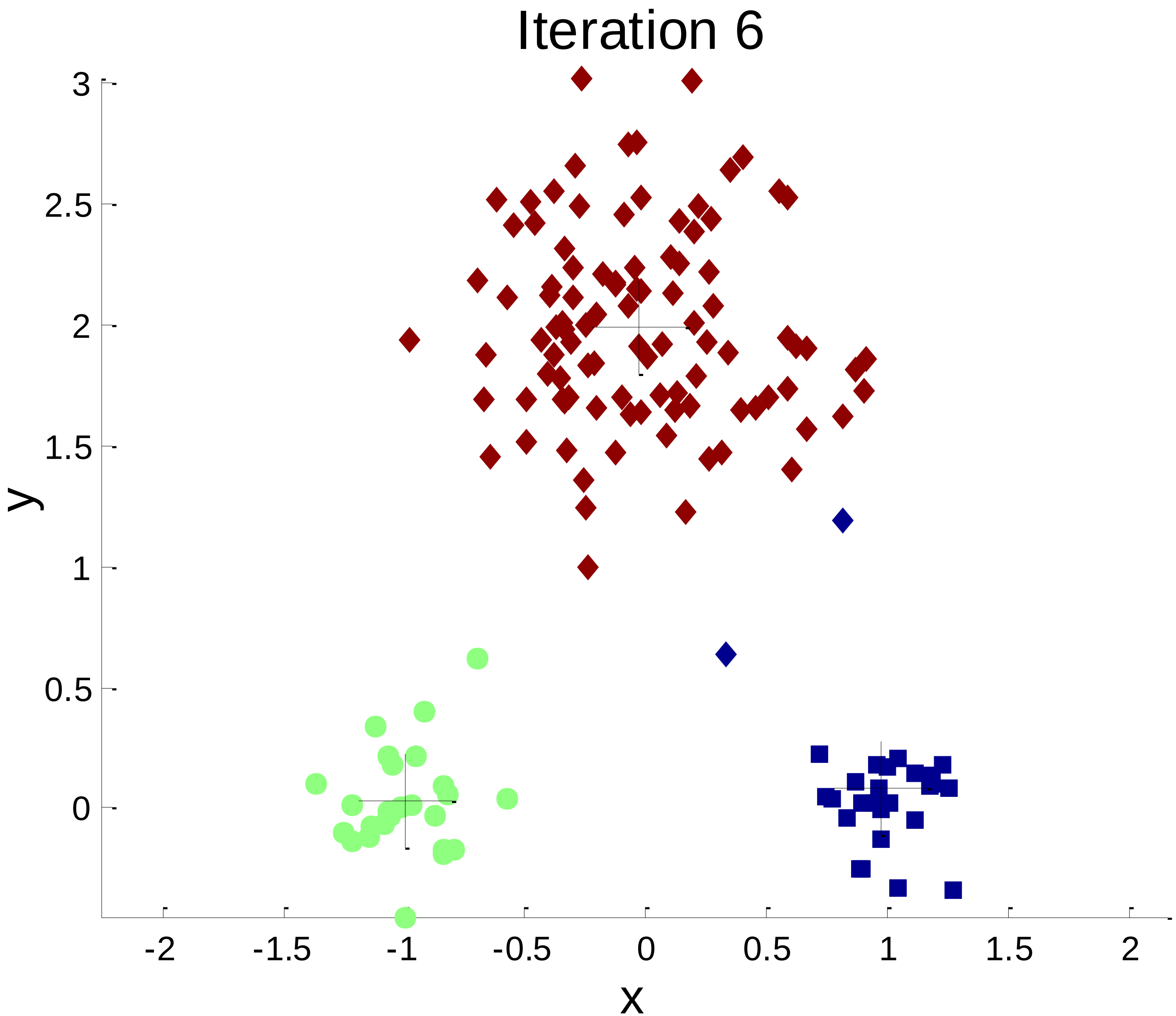
- K-means
- Hierarchical clustering
- Density-based clustering

K-means Clustering

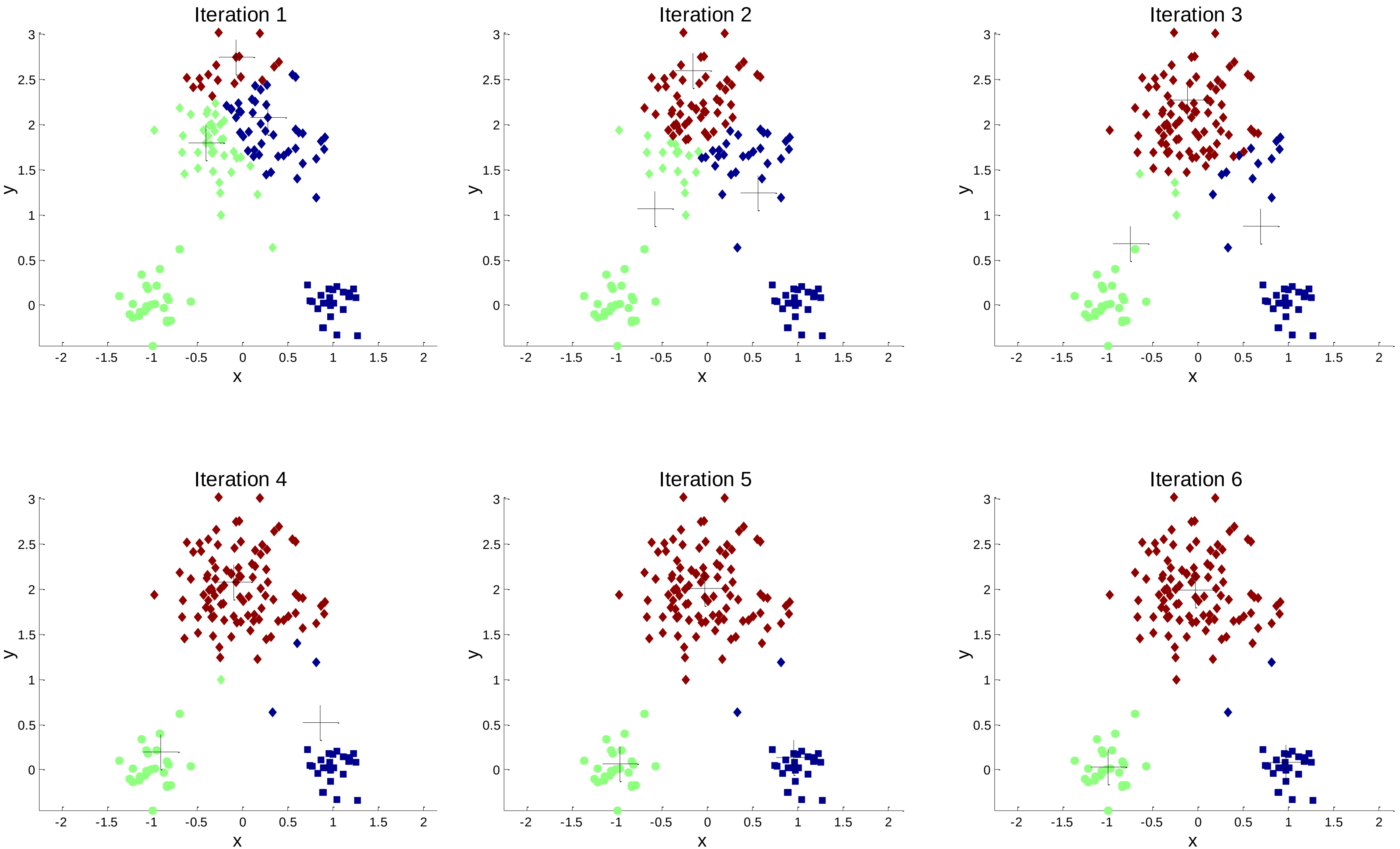
- Partitional clustering approach
- Number of clusters, K, must be specified
- Each cluster is associated with a centroid (center point)
- Each point is assigned to the cluster with the closest centroid
- The basic algorithm is very simple

Select K points as the initial centroids.
repeat
    Form K clusters by assigning all points to the closest centroid.
    Recompute the centroid of each cluster.
until The centroids don't change

Example of K-means Clustering



Example of K-means Clustering



K-means Clustering – Details

- Initial centroids are often chosen randomly.
  - Clusters produced vary from one run to another.

- The centroid is (typically) the mean of the points in the cluster.

- 'Closeness' is measured by Euclidean distance, cosine similarity, correlation, etc.

- K-means will converge for common similarity measures mentioned above.

- Most of the convergence happens in the first few iterations.
  - Often the stopping condition is changed to 'Until relatively few points change clusters'

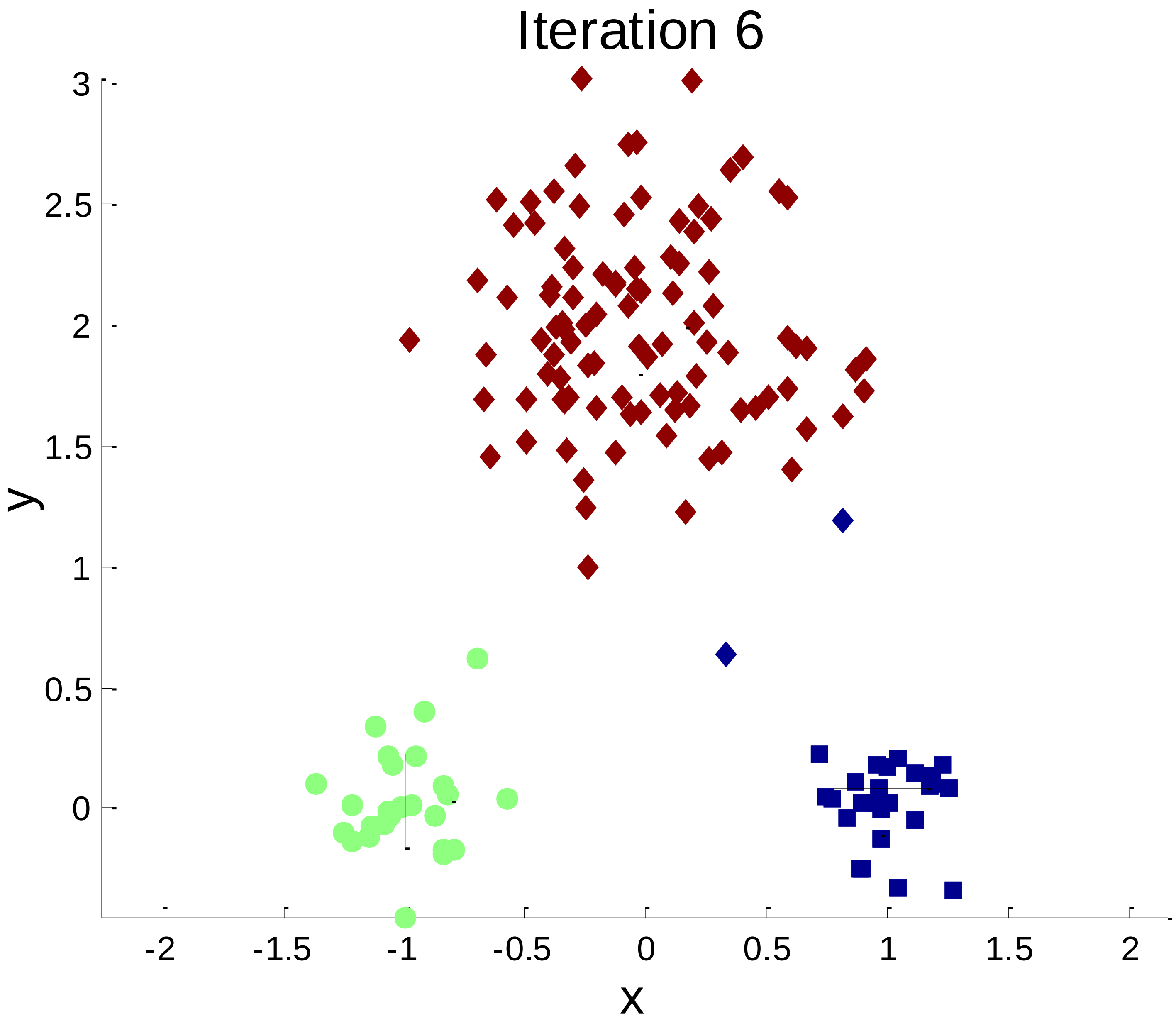
Evaluating K-means Clusters

- Most common measure is Sum of Squared Error (SSE)
  - For each point, the error is the distance to the nearest cluster
  - To get SSE, we square these errors and sum them.

$$SSE = \sum_{i=1}^{K} \sum_{x \in C_i} dist^2(m_i, x)$$

  - x is a data point in cluster C_i and m_i is the representative point for cluster C_i
    - can show that m_i corresponds to the center (mean) of the cluster
  - Given two sets of clusters, we prefer the one with the smallest error

Importance of Choosing Initial Centroids



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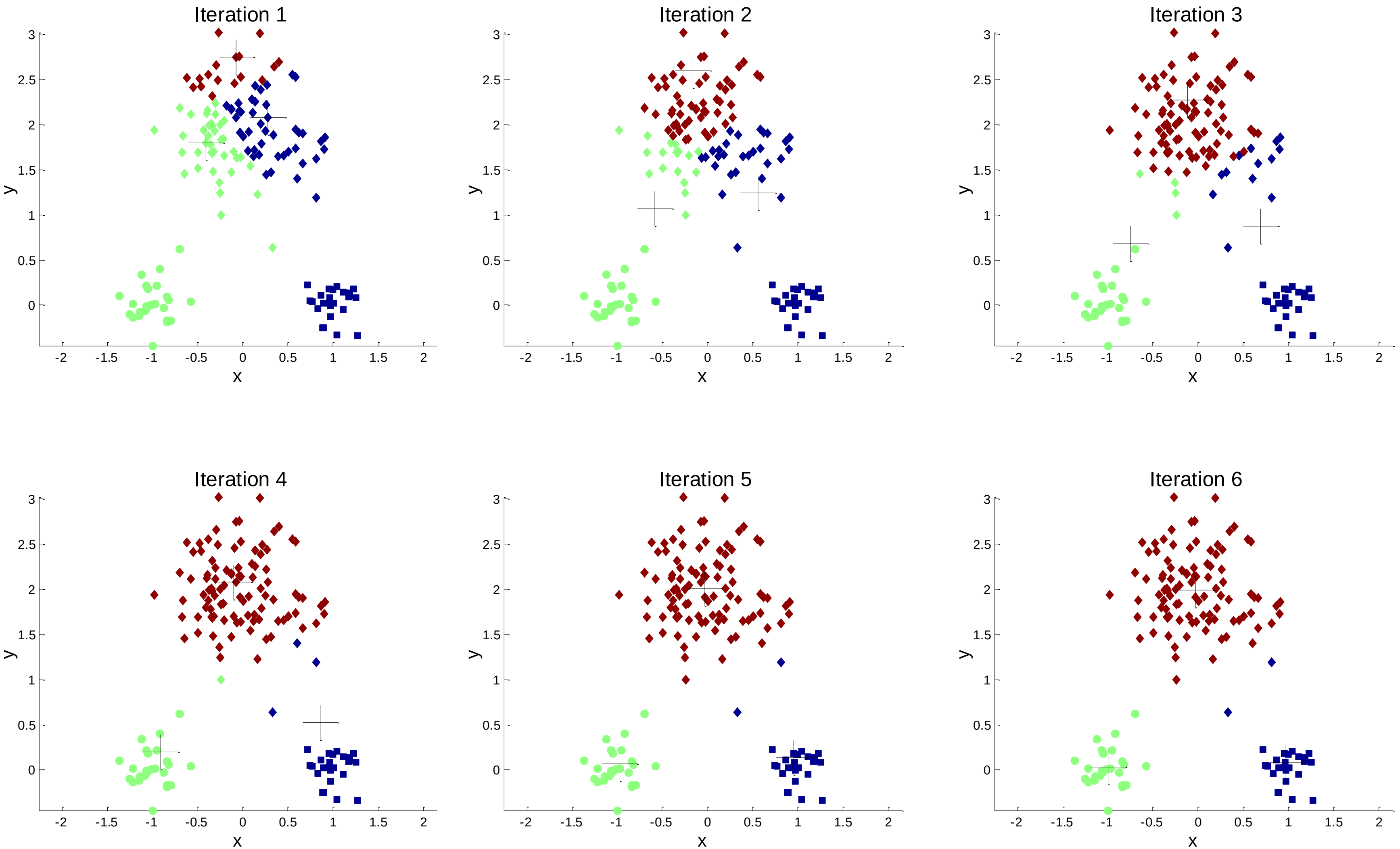

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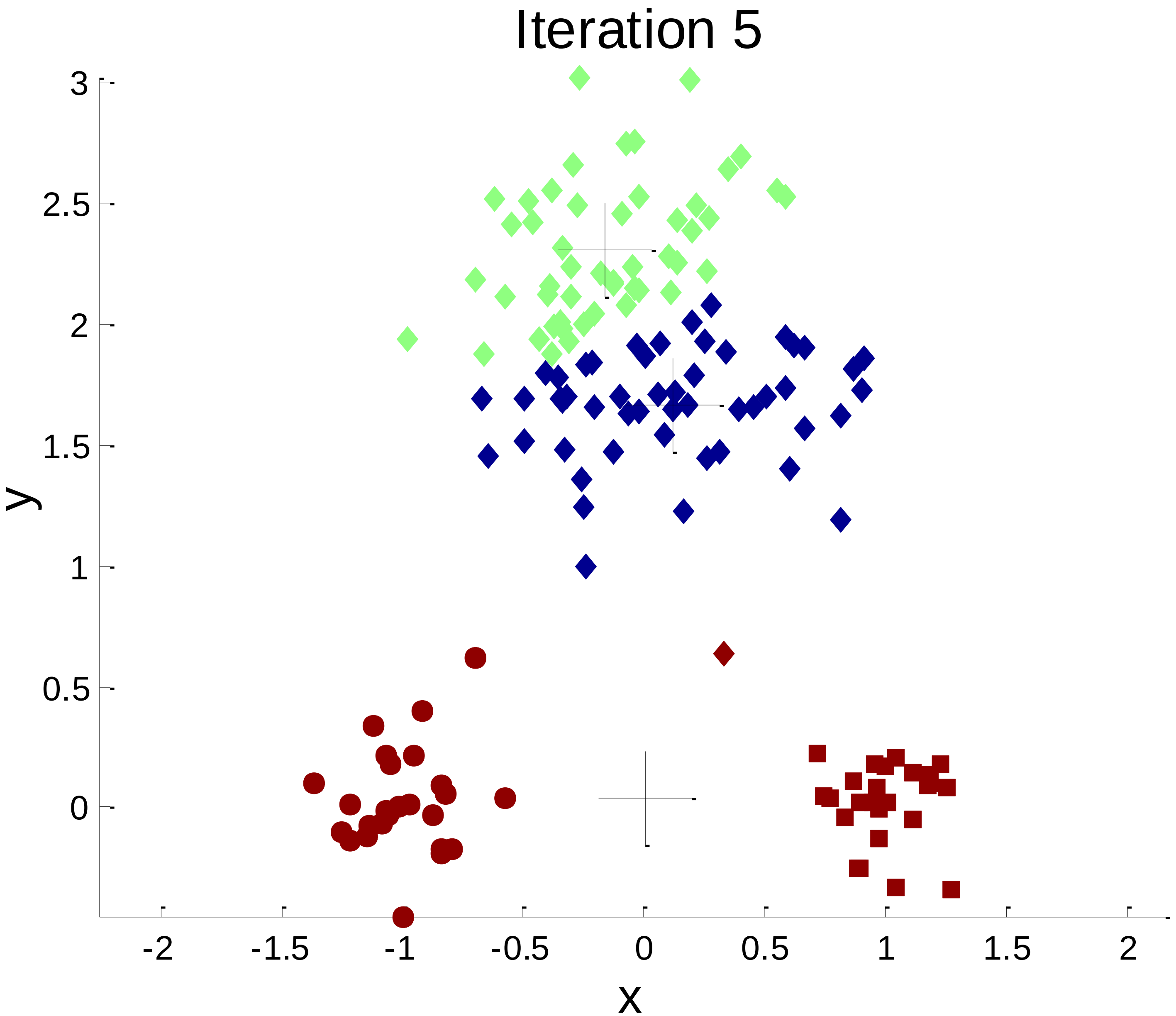

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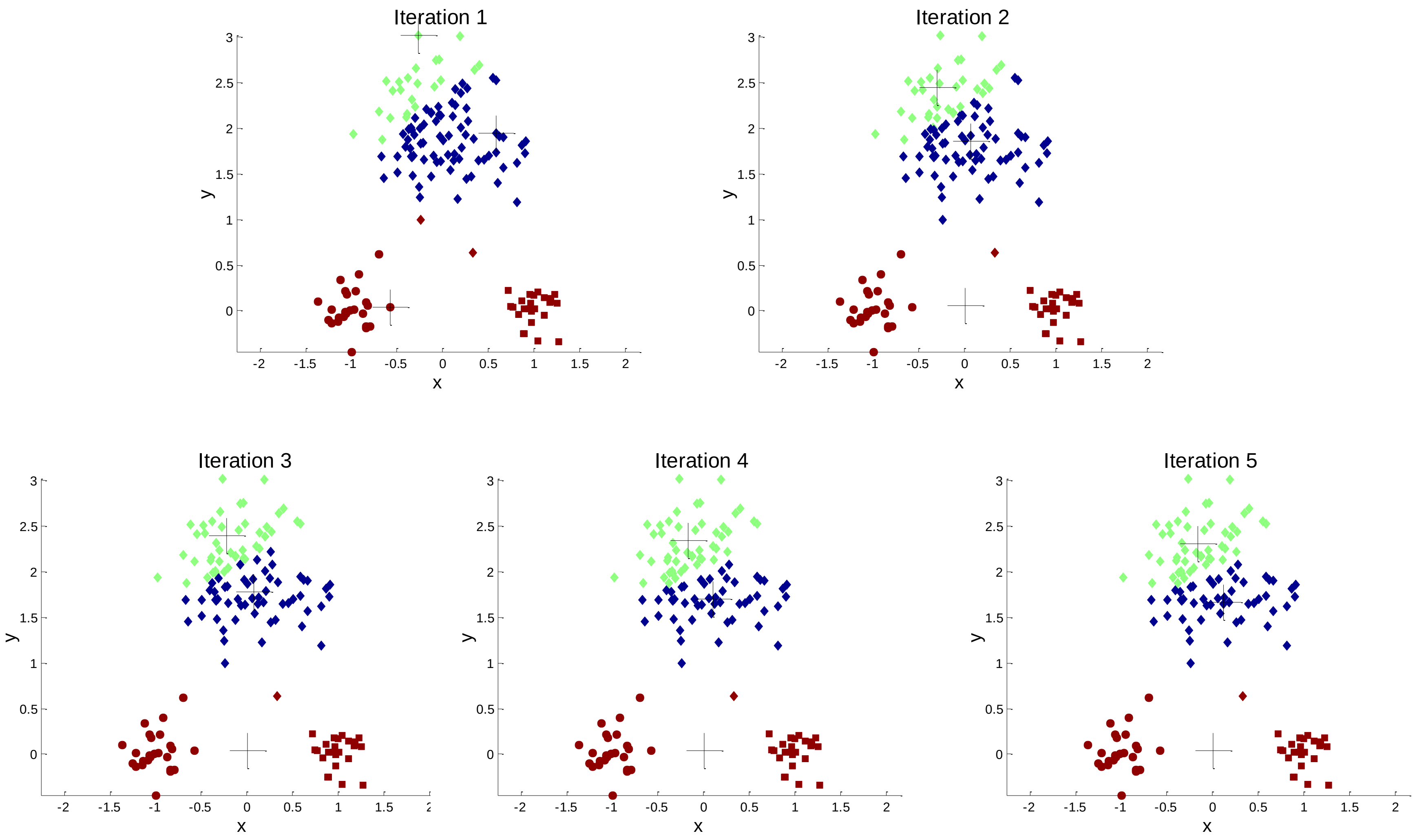
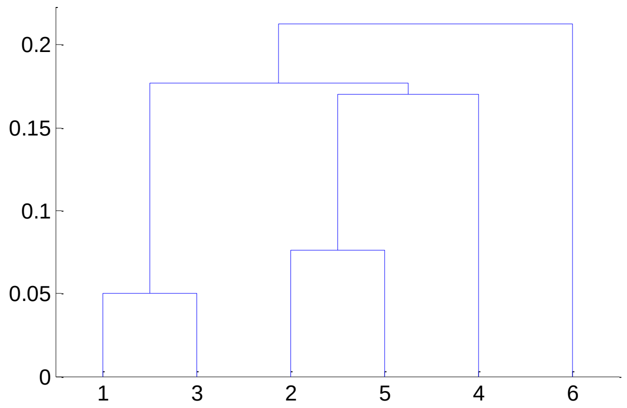
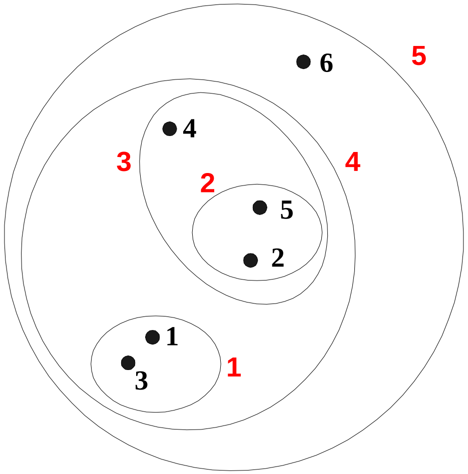


Hierarchical Clustering

- 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

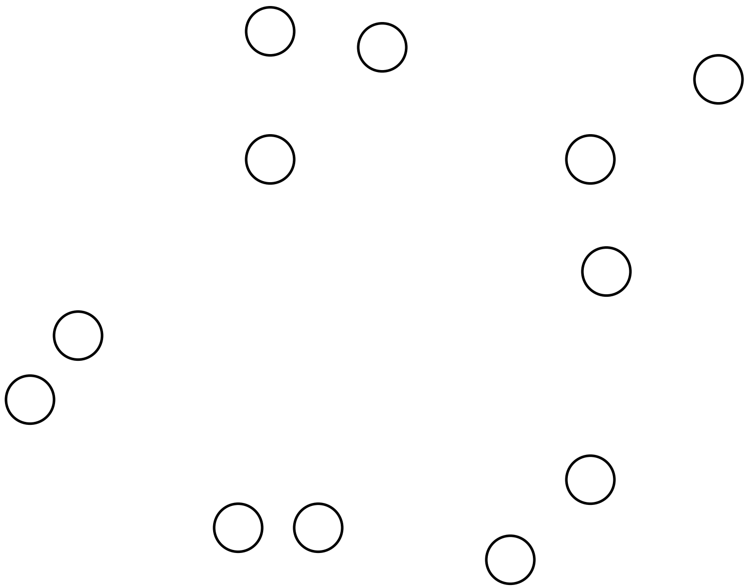
- Two main types of hierarchical clustering
  - Agglomerative:
    - Start with the points as individual clusters
    - At each step, merge the closest pair of clusters until only one cluster (or k clusters) left
  - Divisive:
    - Start with one, all-inclusive cluster
    - At each step, split a cluster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

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

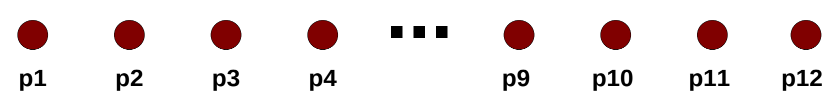
Starting Situation

- Start with clusters of individual points and a proximity matrix



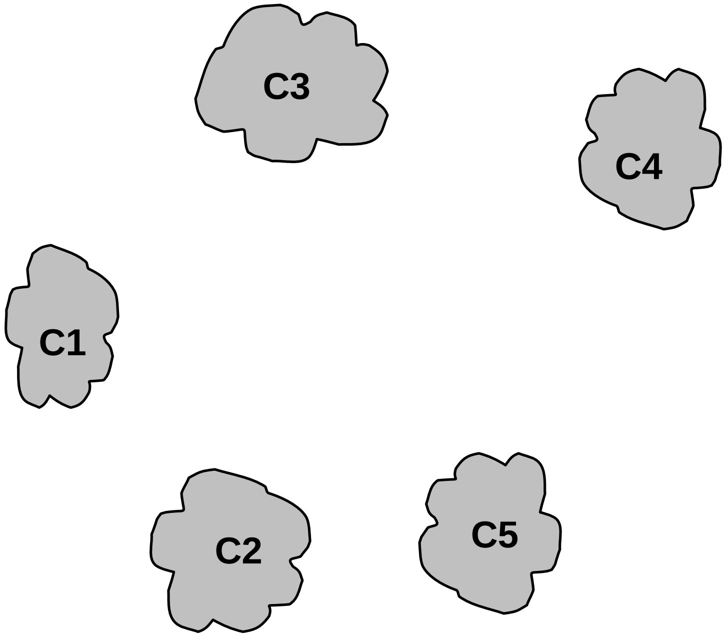
	p1	p2	p3	p4	p5	. . .
p1						
p2						
p3						
p4						
p5						
.						
.						
.						

Proximity Matrix



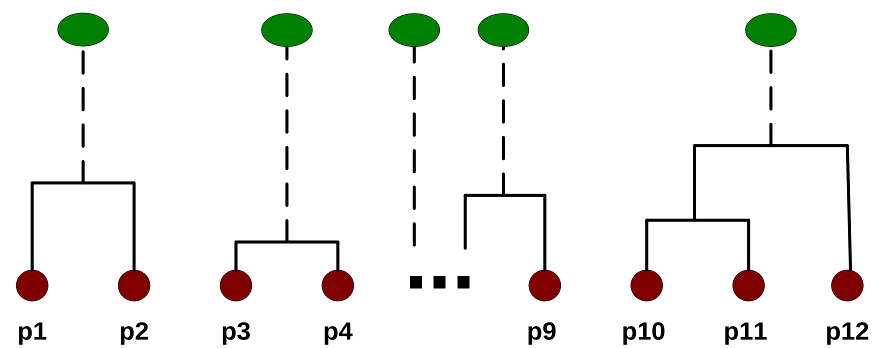
Intermediate Situation

- After some merging steps, we have some clusters



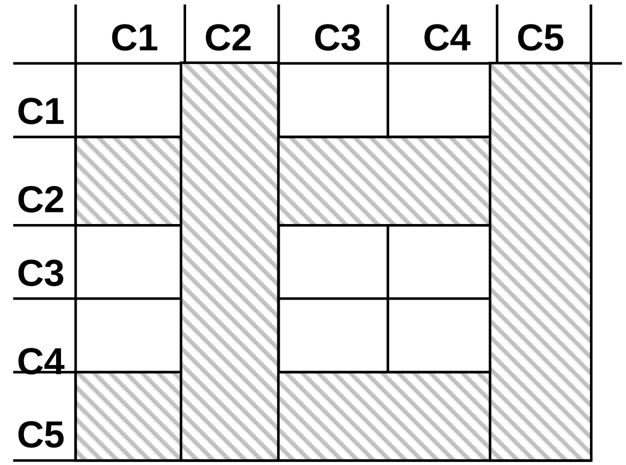
	C1	C2	C3	C4	C5
C1					
C2					
C3					
C4					
C5					

Proximity Matrix

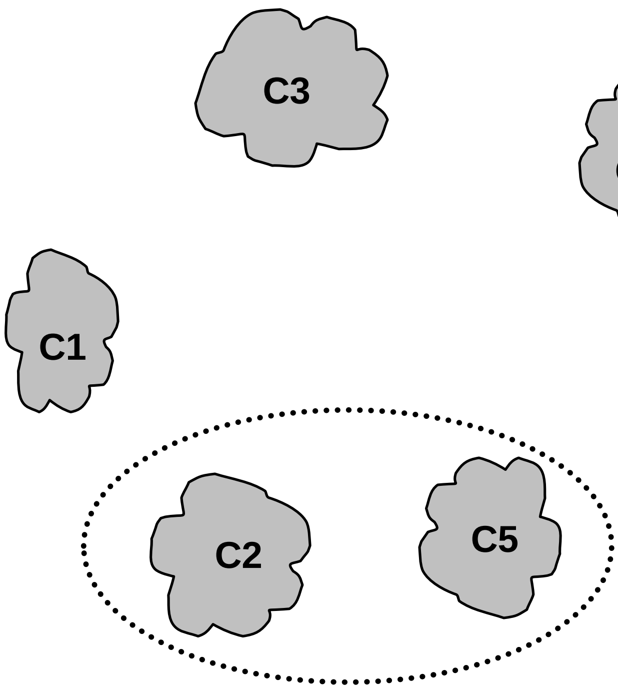


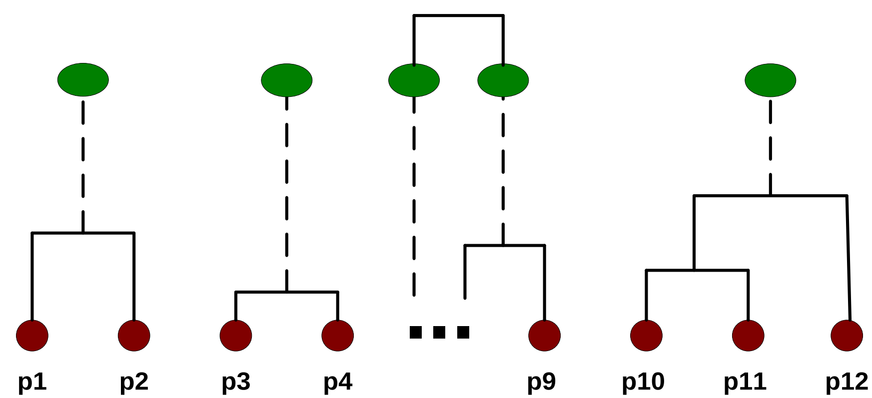
Intermediate Situation

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



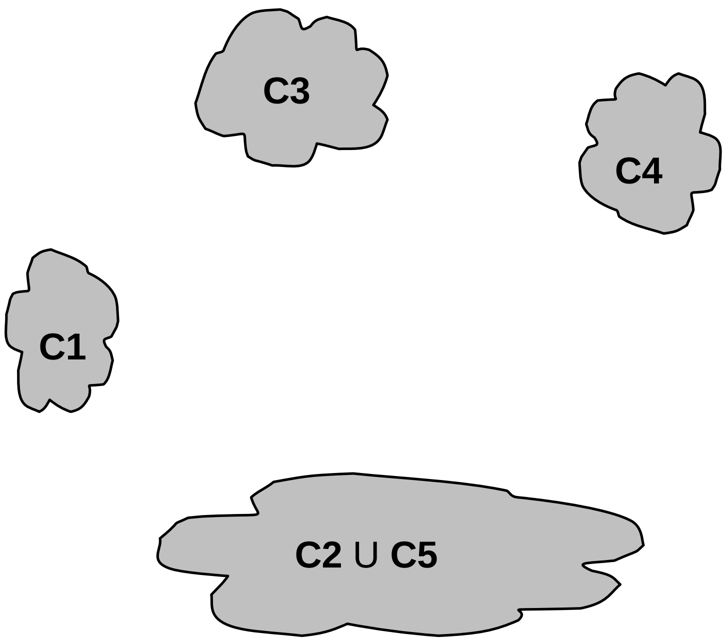
Proximity Matrix





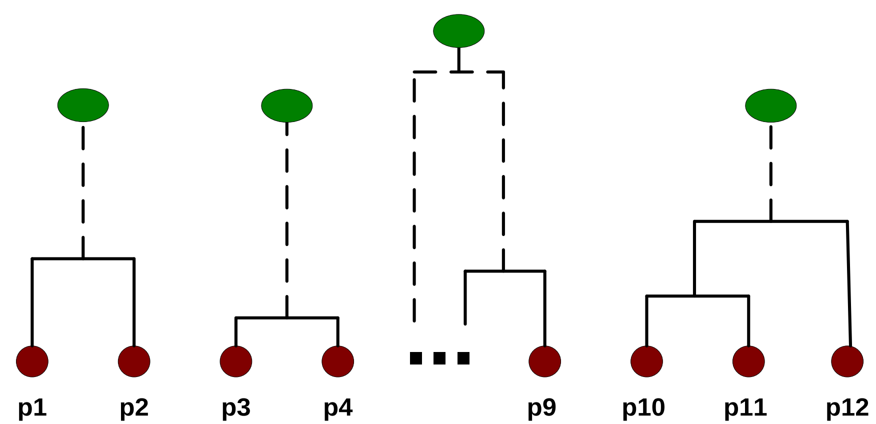
After Merging

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

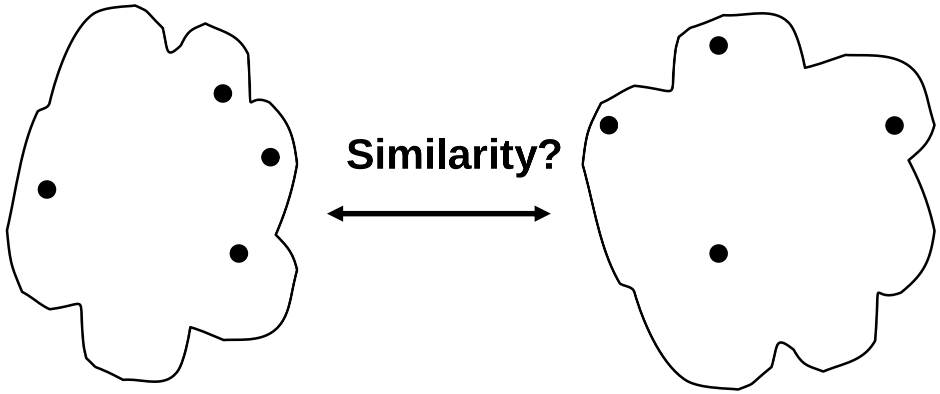


	C1	C2 U C5	C3	C4
C1		?		
C2 U C5	?	?	?	?
C3		?		
C4		?		

Proximity Matrix



How to Define Inter-Cluster Distance

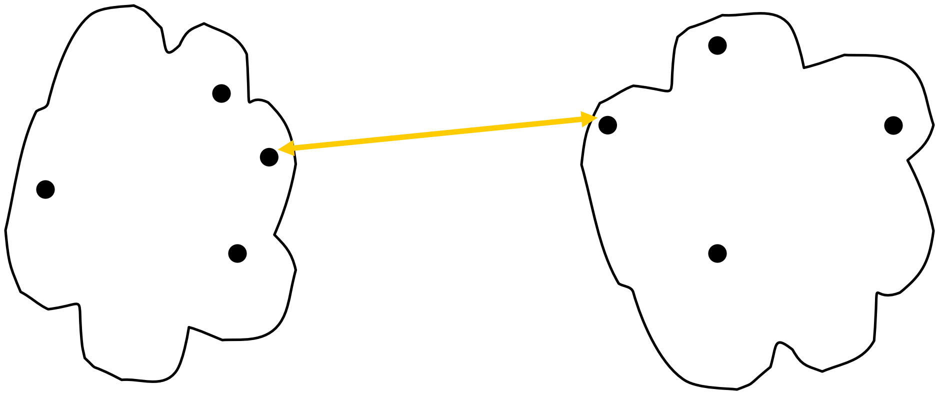


	p1	p2	p3	p4	p5	. . .
p1						
p2						
p3						
p4						
p5						
.						
.						
.						

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



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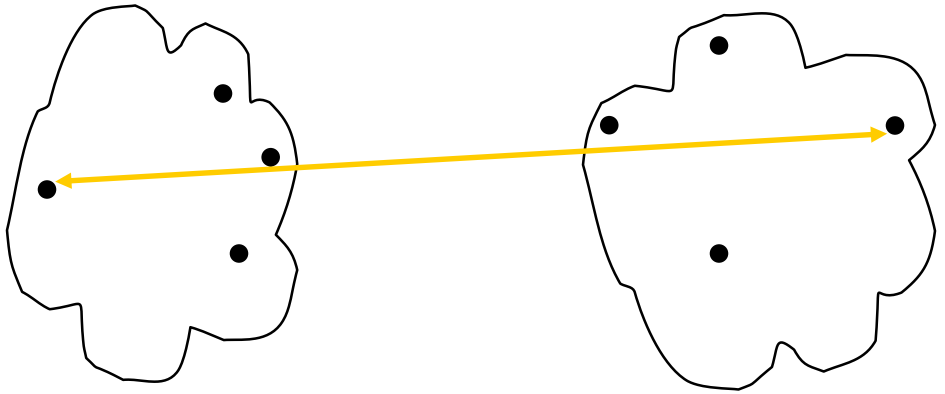

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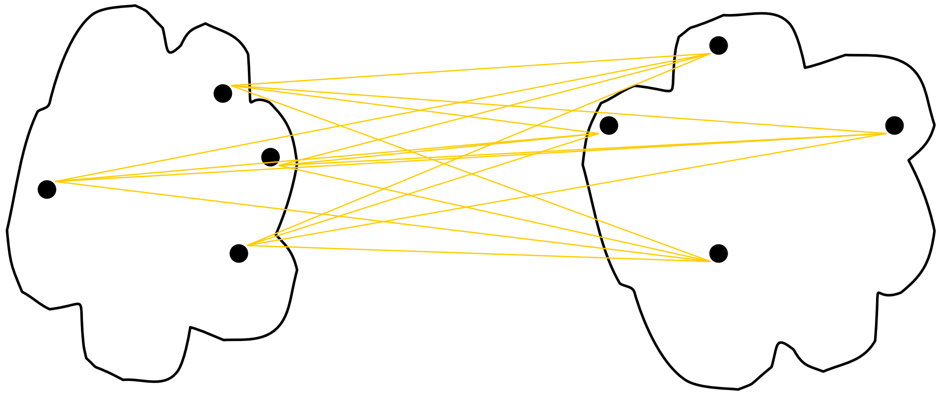

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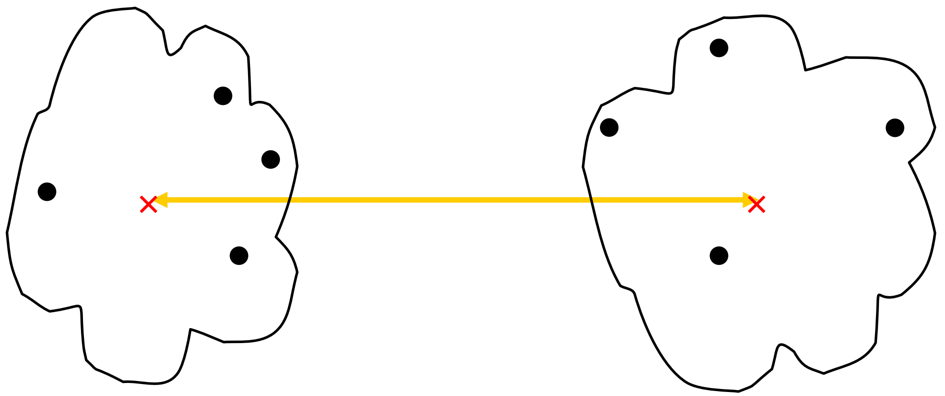

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p4						
p5						
.						
.						
.						

Proximity Matrix

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- MAX
- Group Average
- Distance Between Centroids
- Other methods driven by an objective function
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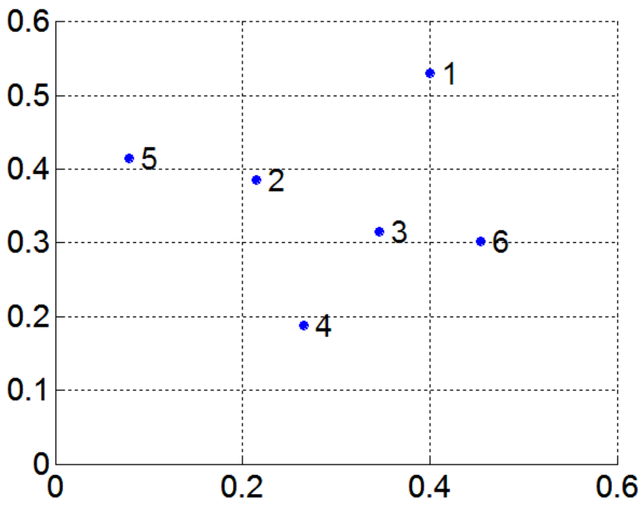
MIN or Single Link

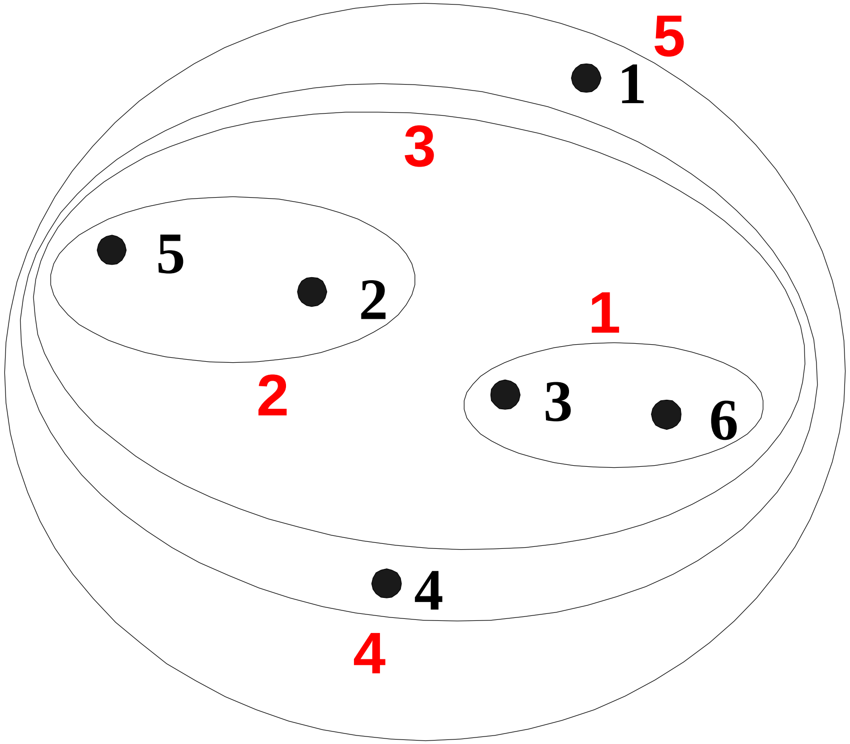
- Proximity of two clusters is based on the two closest points in the different clusters
  - Determined by one pair of points, i.e., by one link in the proximity graph
- Example:



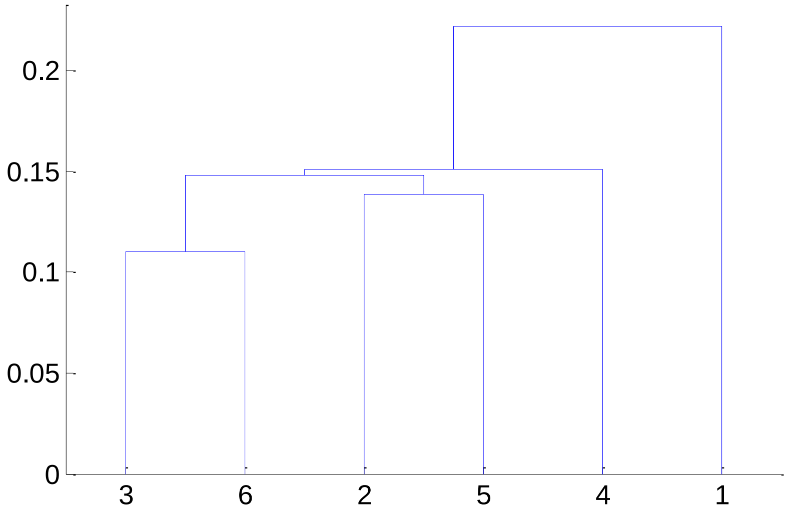
Distance Matrix:

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

Hierarchical Clustering: MIN

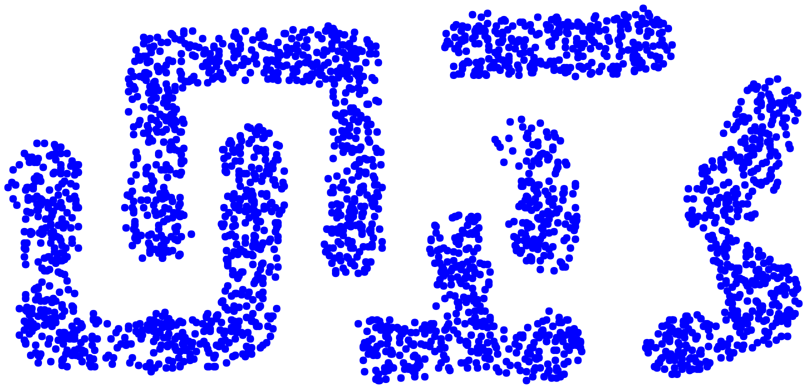


Nested Clusters

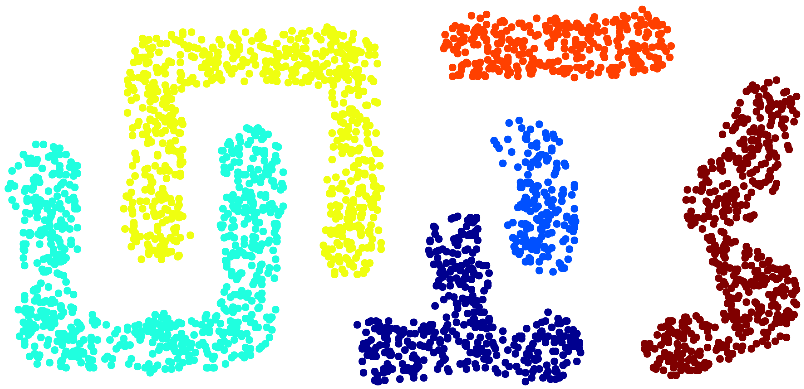


Dendrogram

Strength of MIN



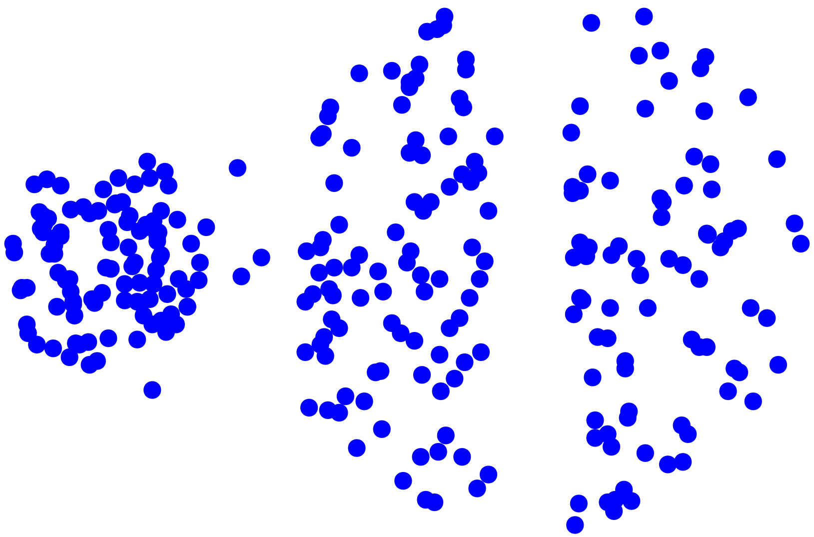
Original Points



Six Clusters

- **Can handle non-elliptical shapes**

Limitations of MIN



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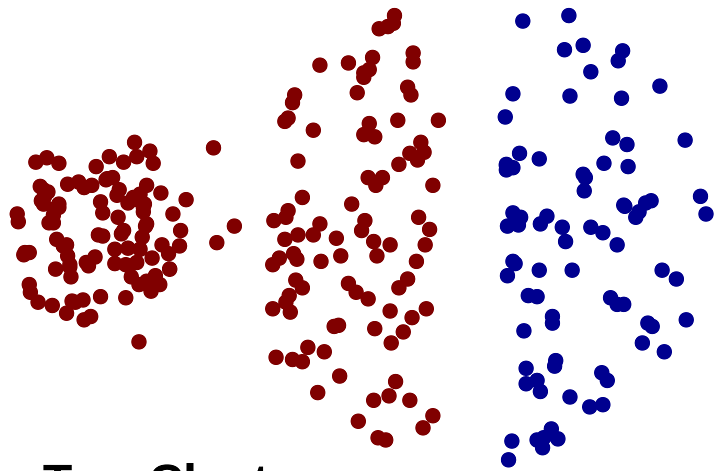
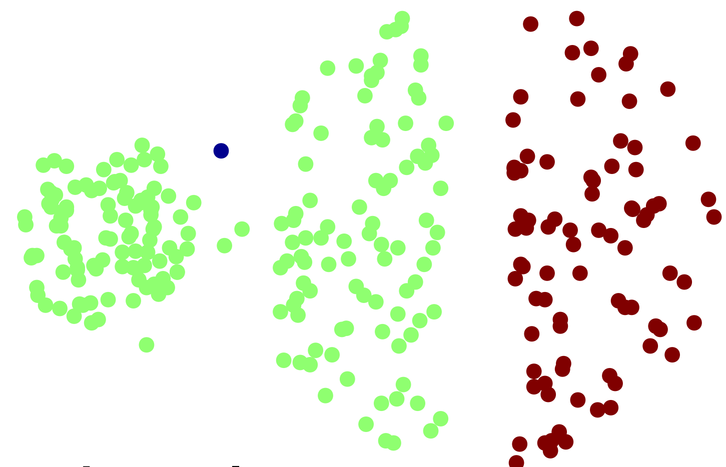


Two Clusters

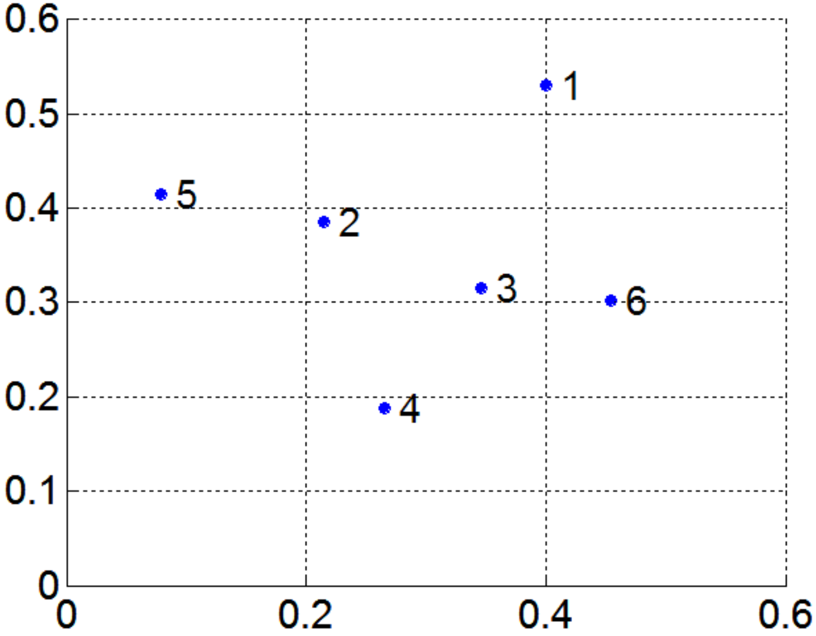


Three Clusters

- 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



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p5	0.34	0.14	0.28	0.29	0.00	
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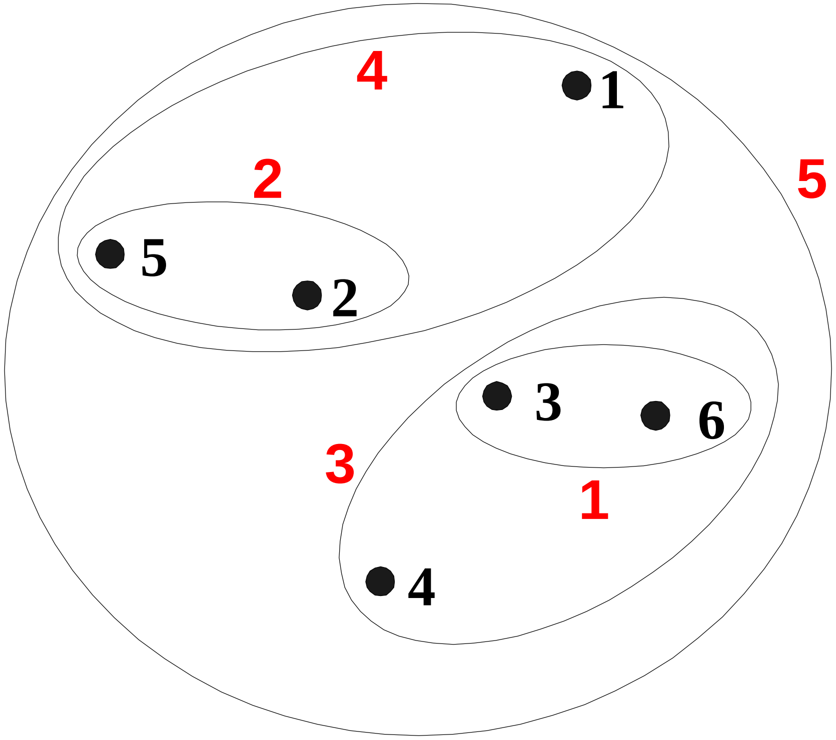
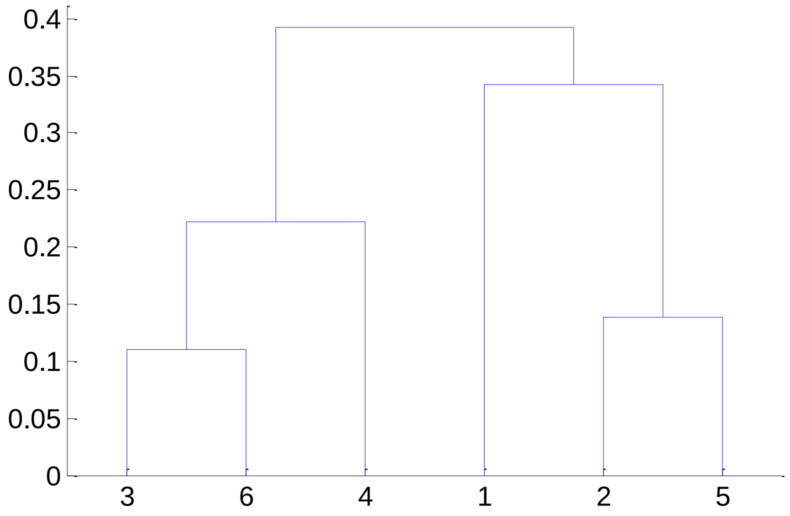
Hierarchical Clustering: MAX

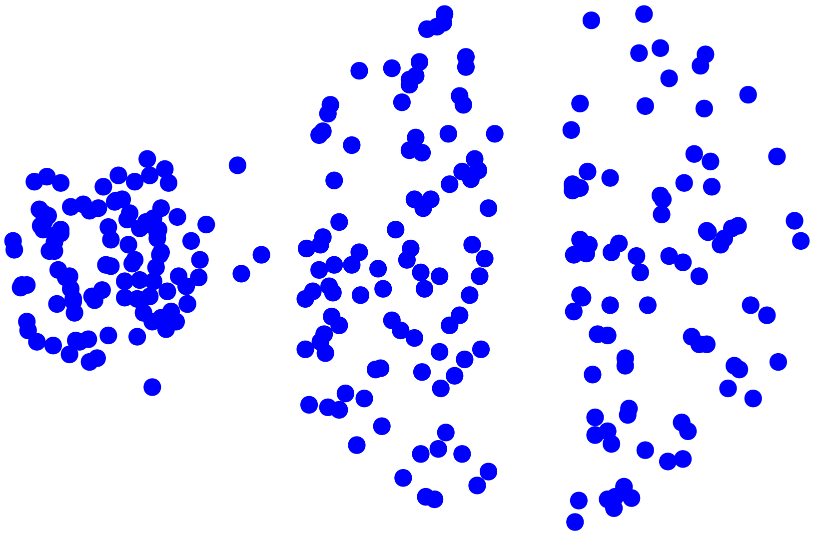


Nested Clusters

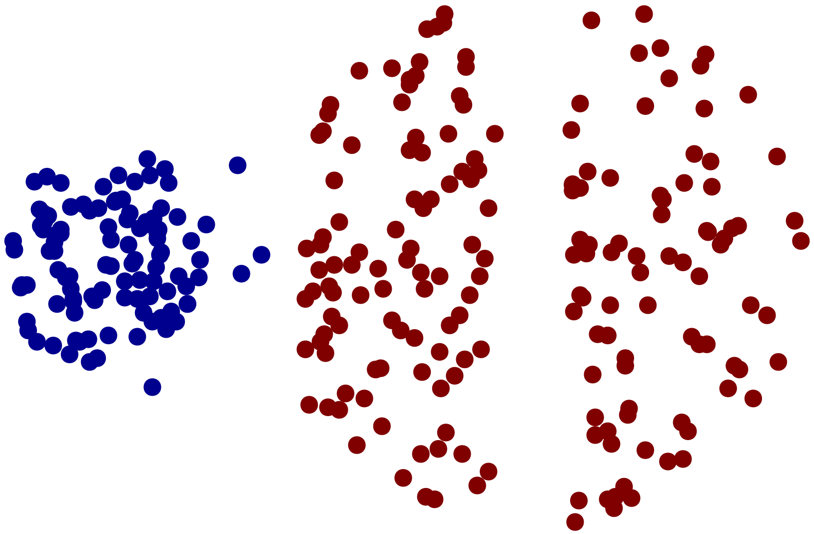


Dendrogram

Strength of MAX



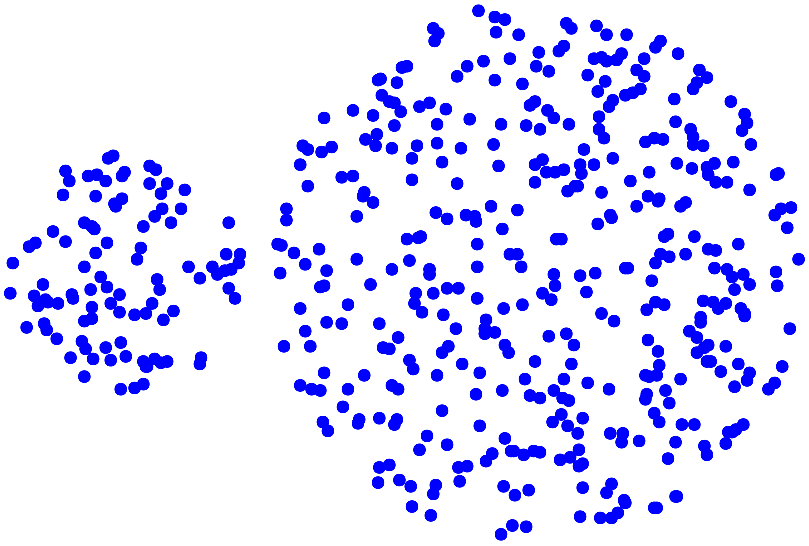
Original Points



Two Clusters

- Less susceptible to noise and outliers

Limitations of MAX



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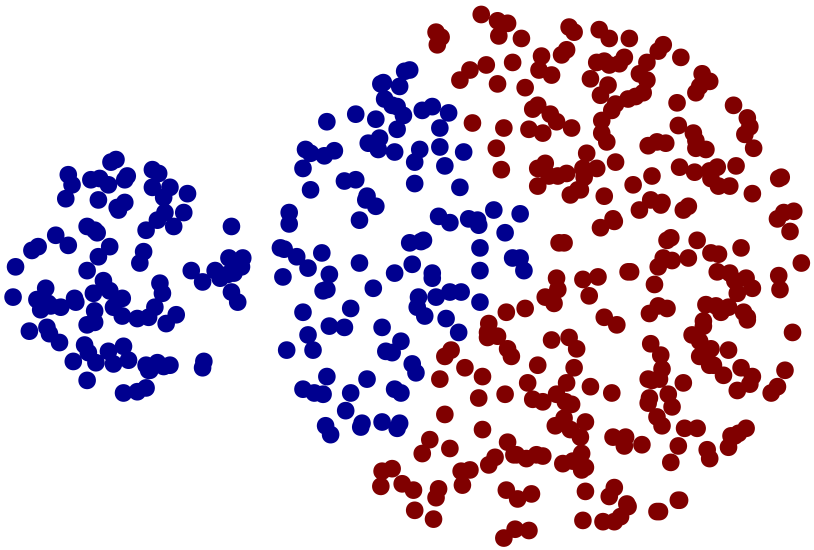


Two Clusters

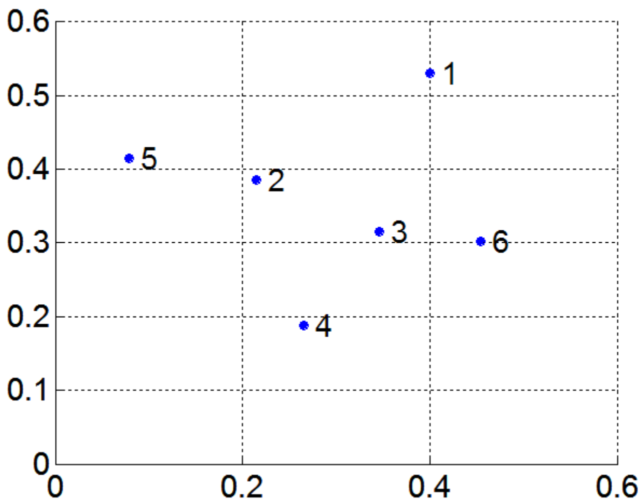
- Tends to break large clusters
- Biased towards globular clusters

Group Average

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

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

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



Distance Matrix:

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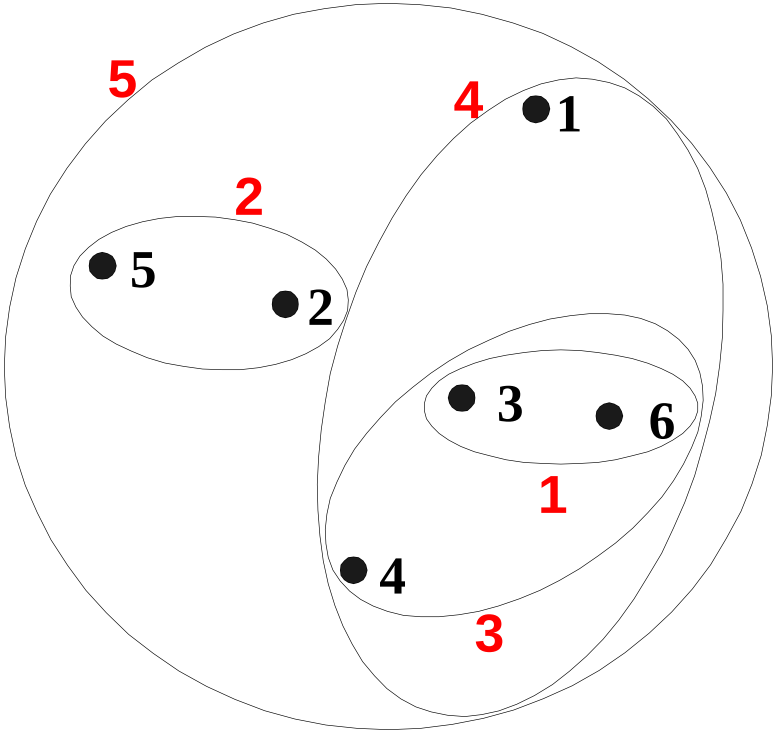
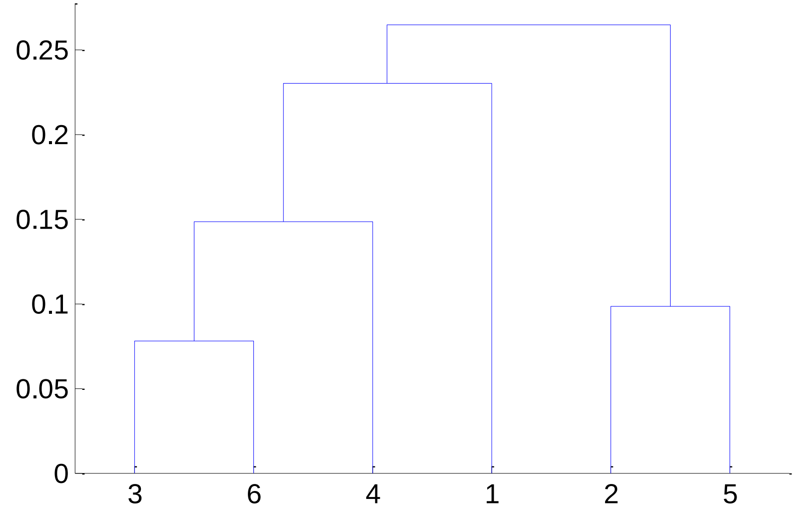
p2	0.24	0.00				
p3	0.22	0.15	0.00			
p4	0.37	0.20	0.15	0.00		
p5	0.34	0.14	0.28	0.29	0.00	
p6	0.23	0.25	0.11	0.22	0.39	0.00

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

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

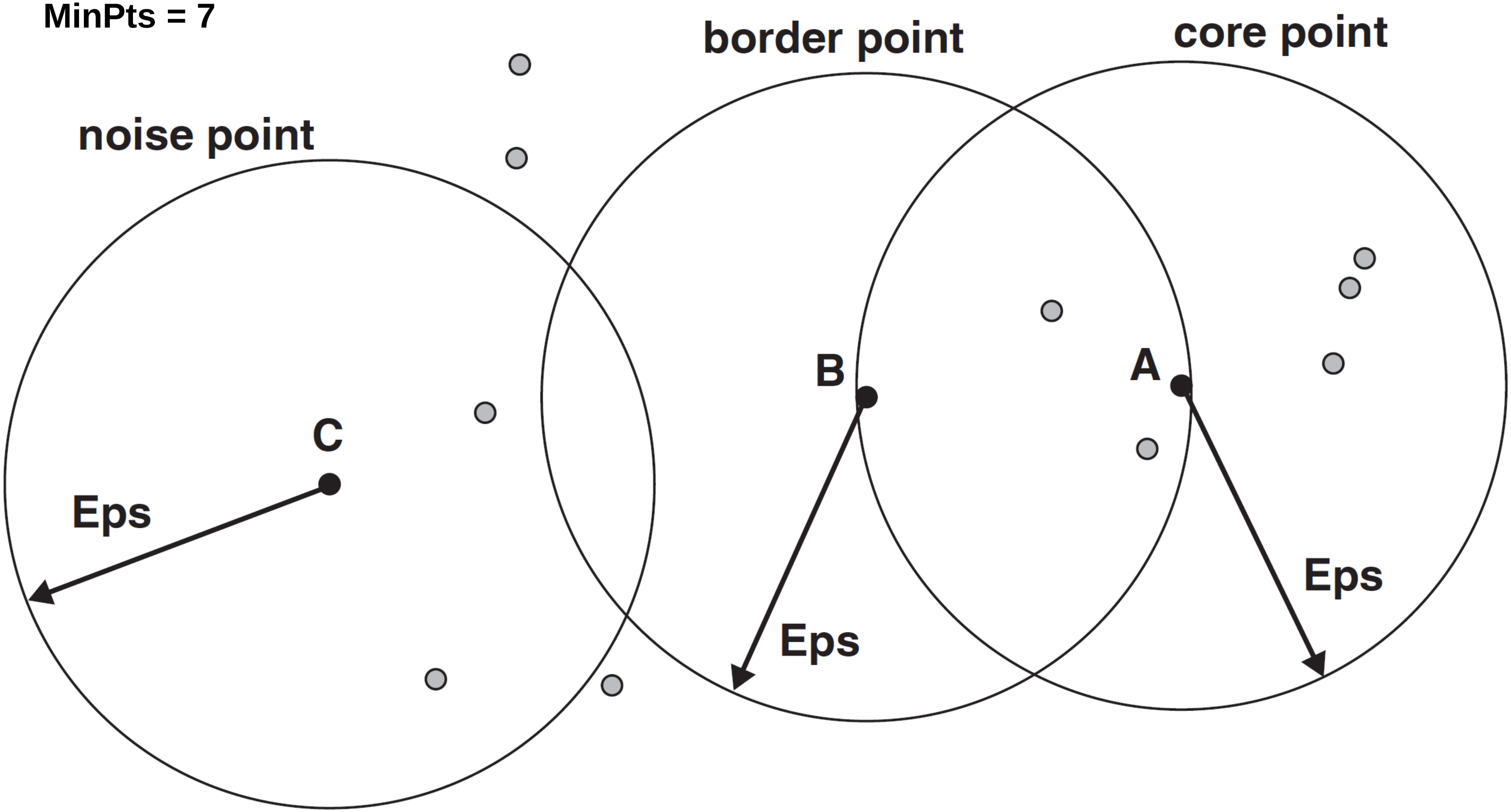
- Different schemes have problems with one or more of the following:
  - Sensitivity to noise and outliers
  - Difficulty handling clusters of different sizes and non-globular shapes
  - Breaking large clusters

DBSCAN

- DBSCAN is a density-based 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

MinPts = 7



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 $current\_cluster\_label$

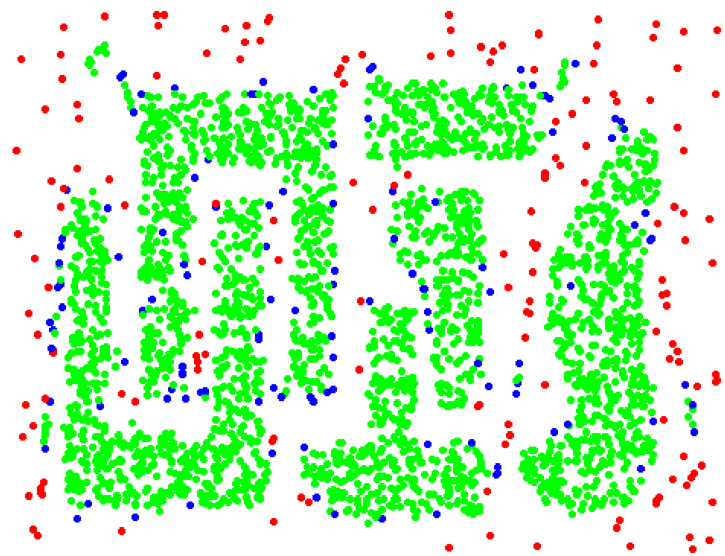
    end if

  end for

end for

DBSCAN: Core, Border and Noise Points

Original Points

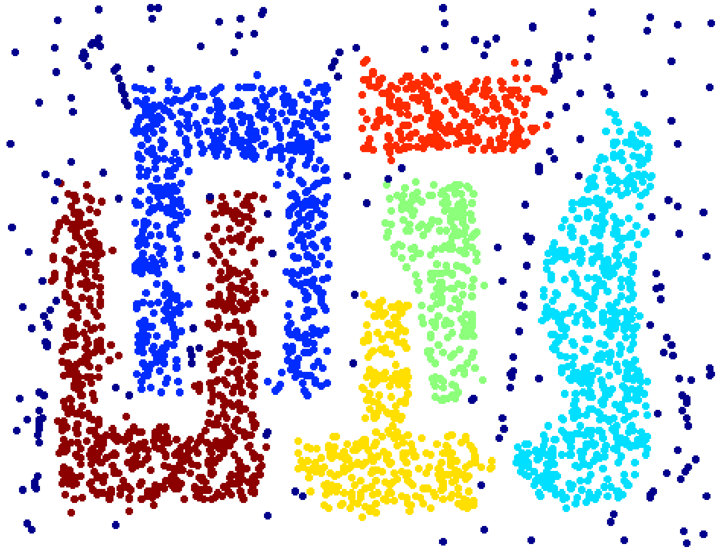


Point types: core, border and noise

Eps = 10, MinPts = 4

When DBSCAN Works Well

Original Points



Clusters

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

When DBSCAN Does NOT Work Well

- Widely Varying densities
- High-dimensional data