Week 10
Clustering (Part I)

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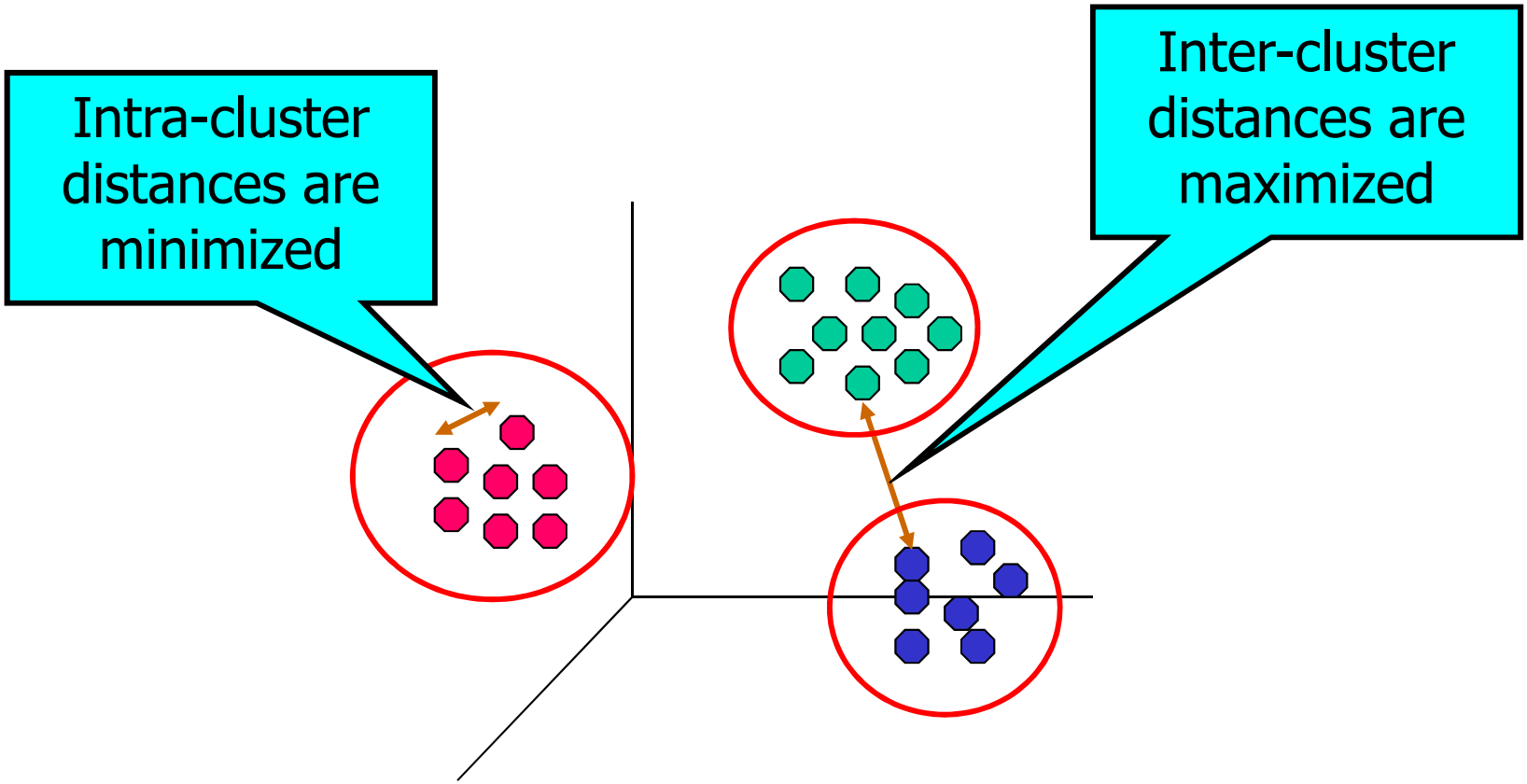
Source: Tan, Kumar, Steinback (2006)

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



Adapted from:
Tan,Steinbach, Kumar - Introduction to Data Mining
Han, Kamber - Data Mining: Concepts and Techniques

General Applications of Clustering

- Pattern Recognition
- Spatial Data Analysis
  - create thematic maps in GIS by clustering feature spaces
  - detect spatial clusters and explain them in spatial data mining
- Image Processing
- Economic Science (especially market research)
- WWW
  - Cluster Weblog data to discover groups of similar access patterns

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Examples of Clustering Applications

- Marketing: Help marketers discover distinct groups in their customer bases, and then use this knowledge to develop targeted marketing programs
- Land use: Identification of areas of similar land use in an earth observation database
- Insurance: Identifying groups of motor insurance policy holders with a high average claim cost
- City-planning: Identifying groups of houses according to their house type, value, and geographical location
- Earthquake studies: Observed earth quake epicenters should be clustered along continent faults

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What Is Good Clustering?

- A good clustering method will produce high quality clusters with
  - high intra-class similarity
  - low inter-class similarity
- The quality of a clustering result depends on both the similarity measure used by the method and its implementation.
- The quality of a clustering method is also measured by its ability to discover some or all of the hidden patterns.

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Requirements of Clustering in Data Mining

- Scalability
- Ability to deal with different types of attributes
- Discovery of clusters with arbitrary shape
- Minimal requirements for domain knowledge to determine input parameters
- Able to deal with noise and outliers
- Insensitive to order of input records
- High dimensionality
- Incorporation of user-specified constraints
- Interpretability and usability

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Notion of a Cluster can be Ambiguous

How many clusters?

Six Clusters

Two Clusters

Four Clusters

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Types of Clusterings

- A clustering is a set of clusters
- Important distinction between hierarchical and partitional sets of clusters
- Partitional Clustering
  - A division 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

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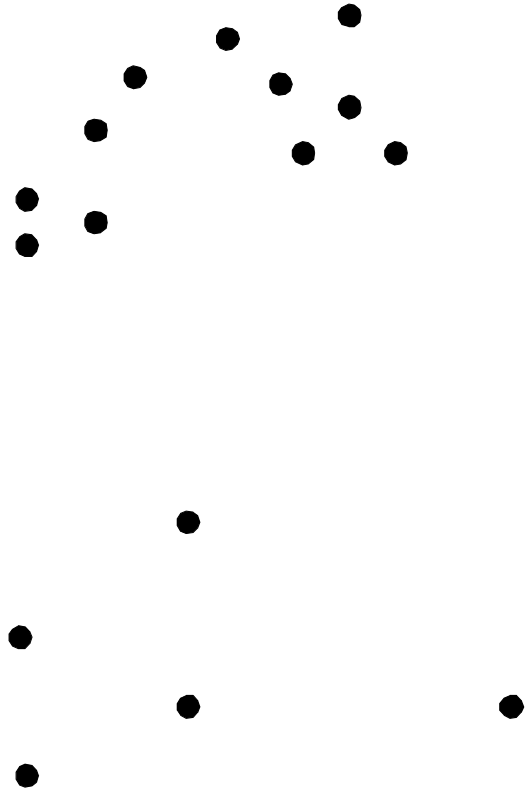
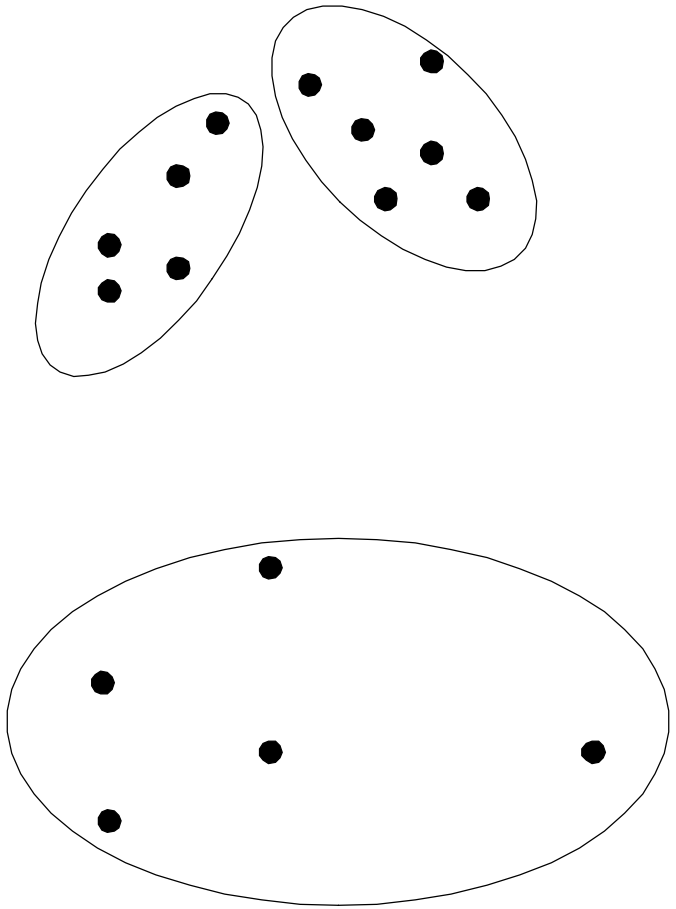
Partitional Clustering



Original Points



A Partitional Clustering

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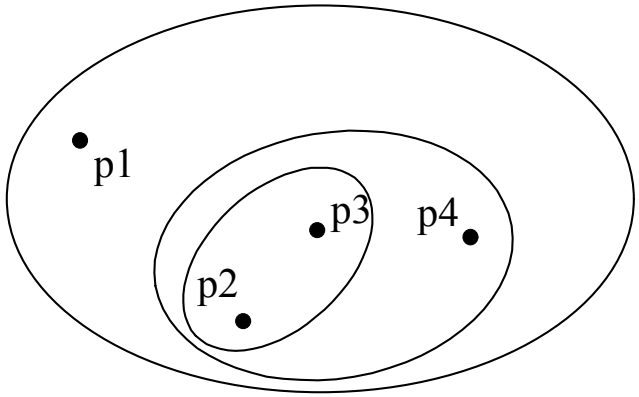
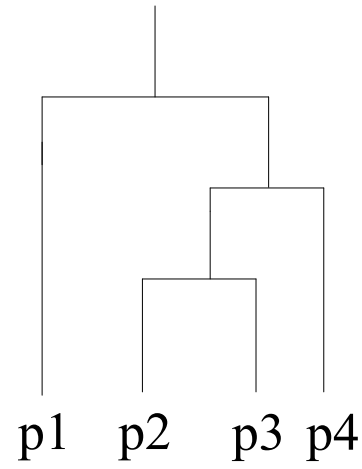
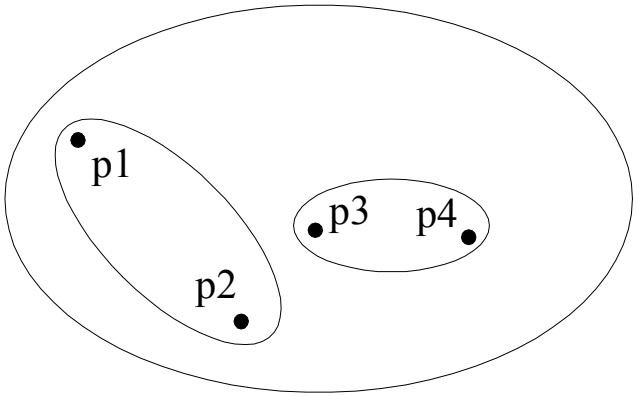
Hierarchical Clustering



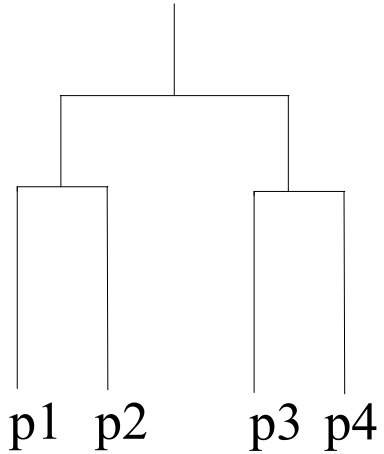
Traditional Hierarchical Clustering



Traditional Dendrogram



Non-traditional Hierarchical Clustering



Non-traditional Dendrogram

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Other Distinctions Between Sets of Clusters

partitional *hierarchical*

- Exclusive versus non-exclusive
  - In non-exclusive clusterings, points may belong to multiple clusters.
  - Can represent multiple classes or 'border' points
- Fuzzy versus non-fuzzy
  - In fuzzy clustering, a point belongs to every cluster with some weight between 0 and 1 *X belongs to A: 98%, B: 2%*
  - Weights must sum to 1
  - Probabilistic clustering has similar characteristics
- Partial versus complete
  - In some cases, we only want to cluster some of the data
- Heterogeneous versus homogeneous
  - Cluster of widely different sizes, shapes, and densities

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Major Clustering Approaches

- Partitioning algorithms: Construct various partitions and then evaluate them by some criterion
- Hierarchy algorithms: Create a hierarchical decomposition of the set of data (or objects) using some criterion
- Density-based: based on connectivity and density functions
- Grid-based: based on a multiple-level granularity structure
- Model-based: A model is hypothesized for each of the clusters and the idea is to find the best fit of that model to each other

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Characteristics of the Input Data Are Important

- Type of proximity or density measure
  - This is a derived measure, but central to clustering
- Sparseness
  - Dictates type of similarity
  - Adds to efficiency
- Attribute type
  - Dictates type of similarity
- Type of Data
  - Dictates type of similarity
  - Other characteristics, e.g., autocorrelation
- Dimensionality
- Noise and Outliers
- Type of Distribution

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K-means Clustering

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

1: Select K points as the initial centroids.
2: **repeat**
3: Form K clusters by assigning all points to the closest centroid.
4: Recompute the centroid of each cluster.
5: **until** The centroids don't change

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K-means Clustering – Details

- Initial centroids are often chosen randomly.
  - Clusters produced may 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.

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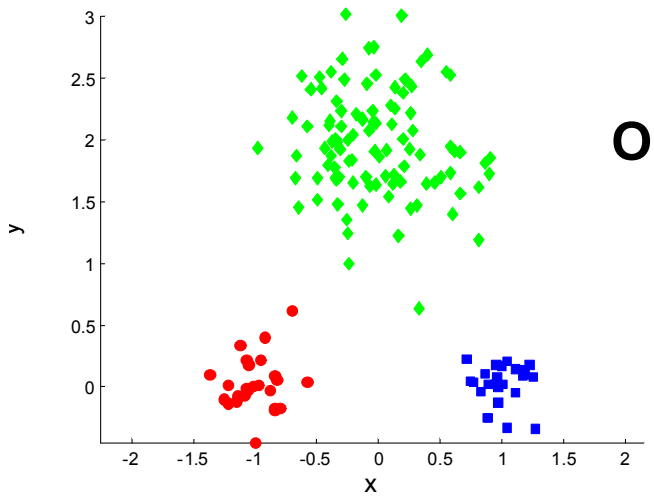
Two different K-means Clusterings



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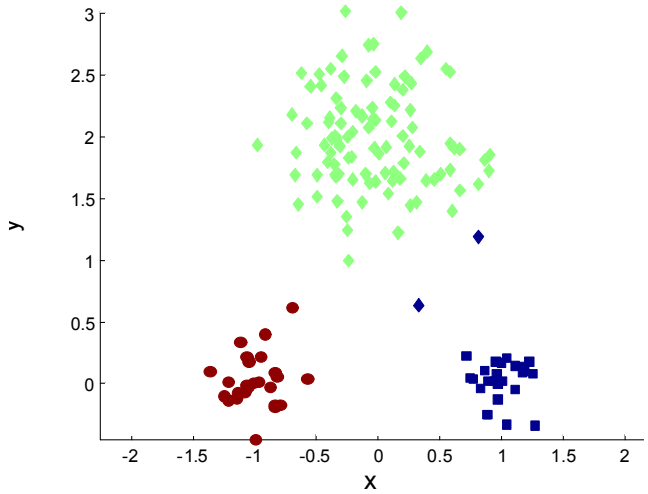
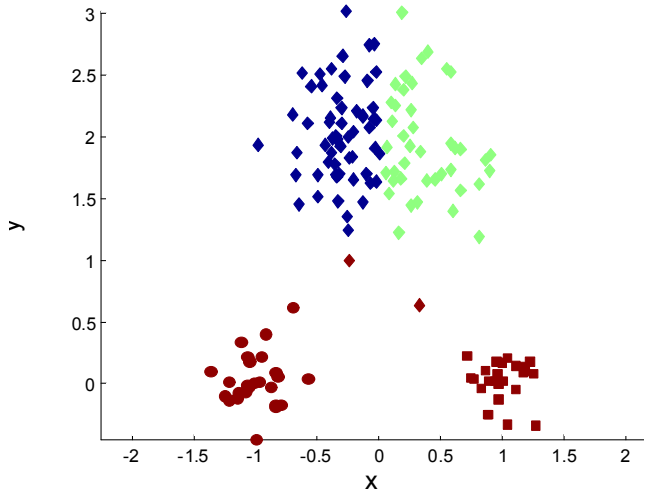


Optimal Clustering



Sub-optimal Clustering

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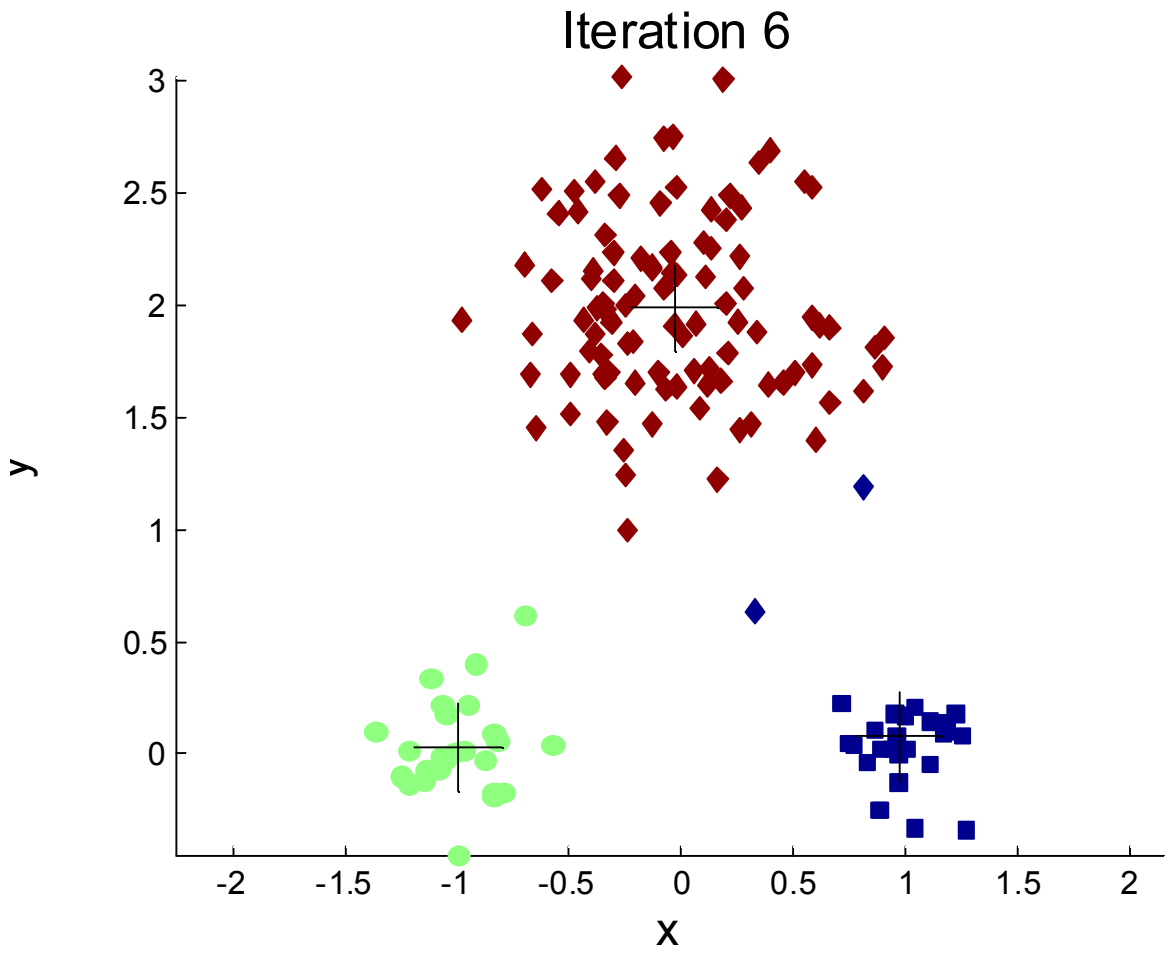
Importance of Choosing Initial Centroids (A)



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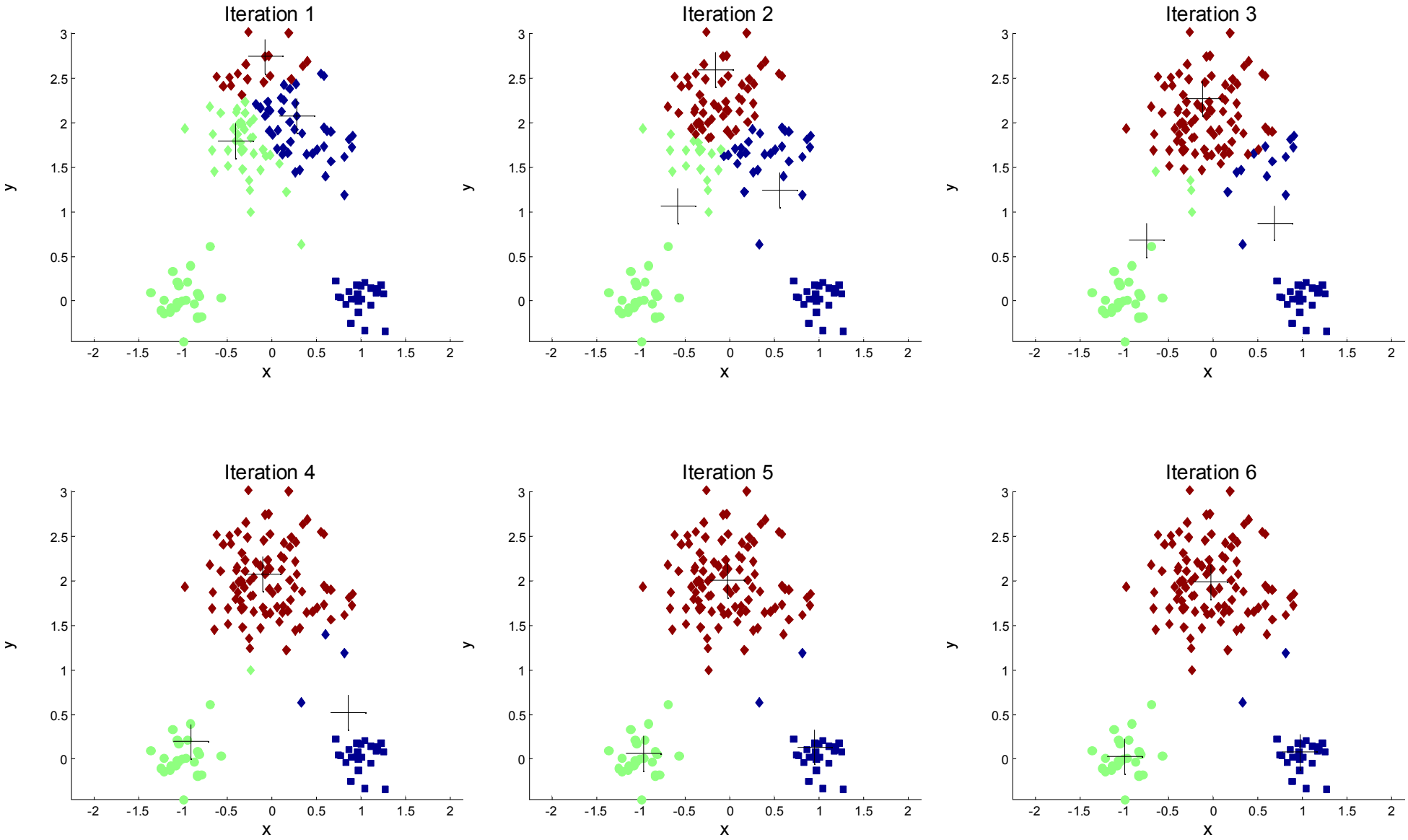

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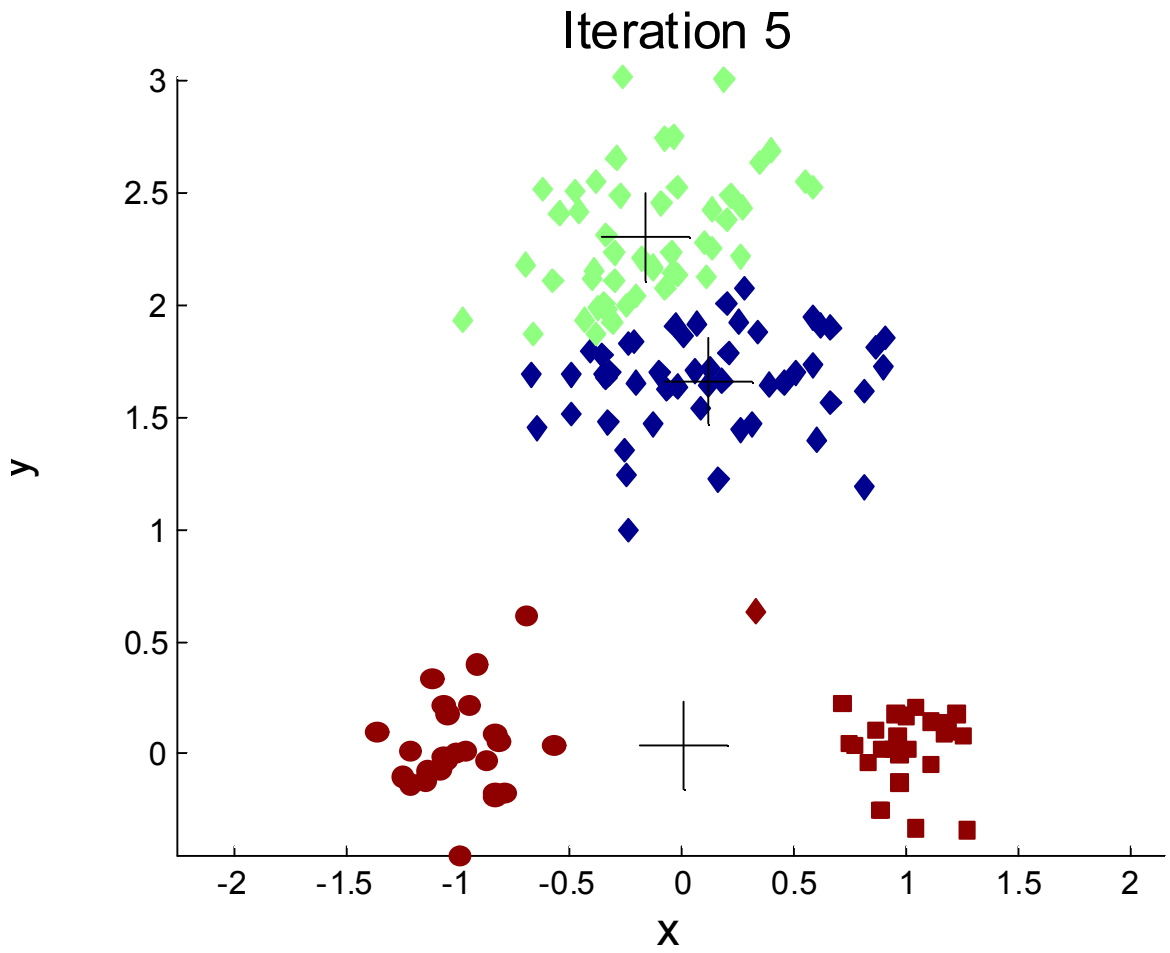
Importance of Choosing Initial Centroids (B)



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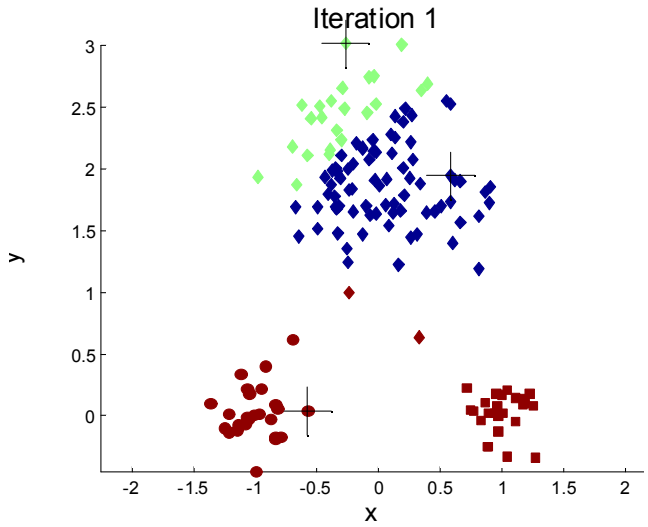

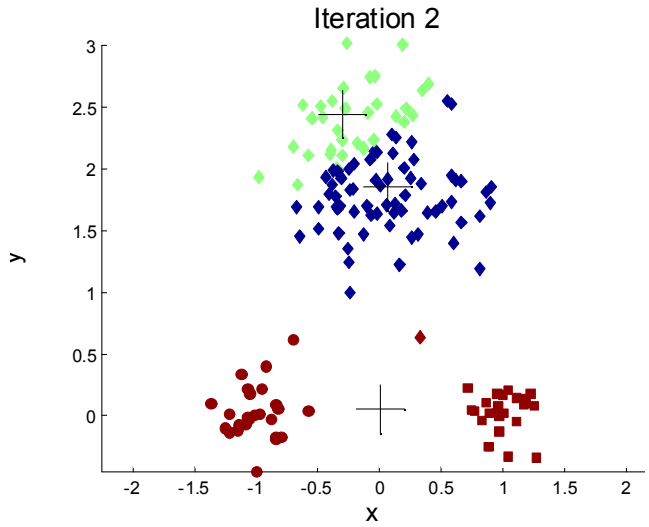

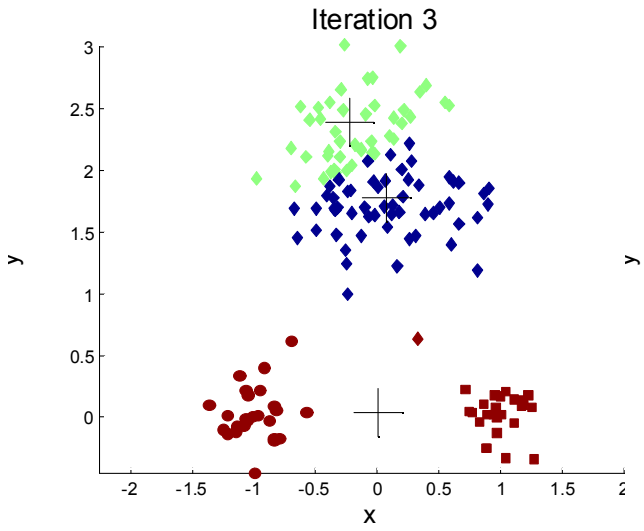

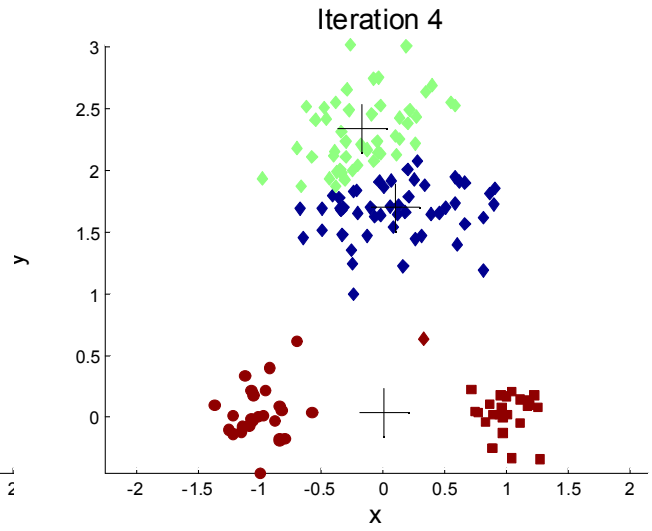

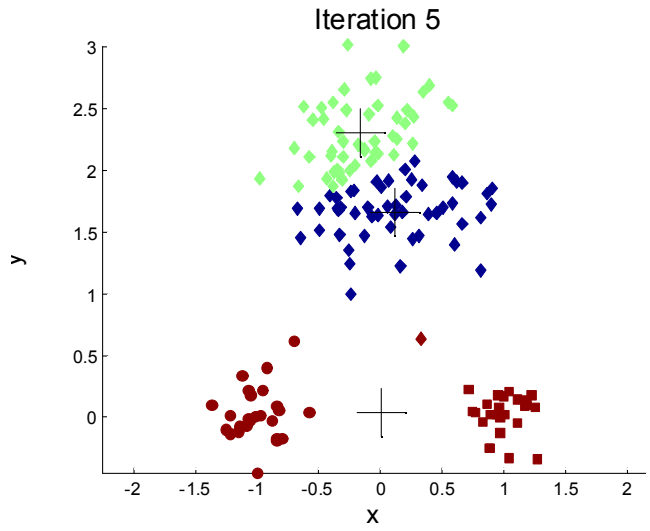

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Evaluating K-means Clusters

- 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 (center) point for cluster C_i

  - Given two clusters, we can choose the one with the smallest error
  - One easy way to reduce SSE is to increase K, the number of clusters

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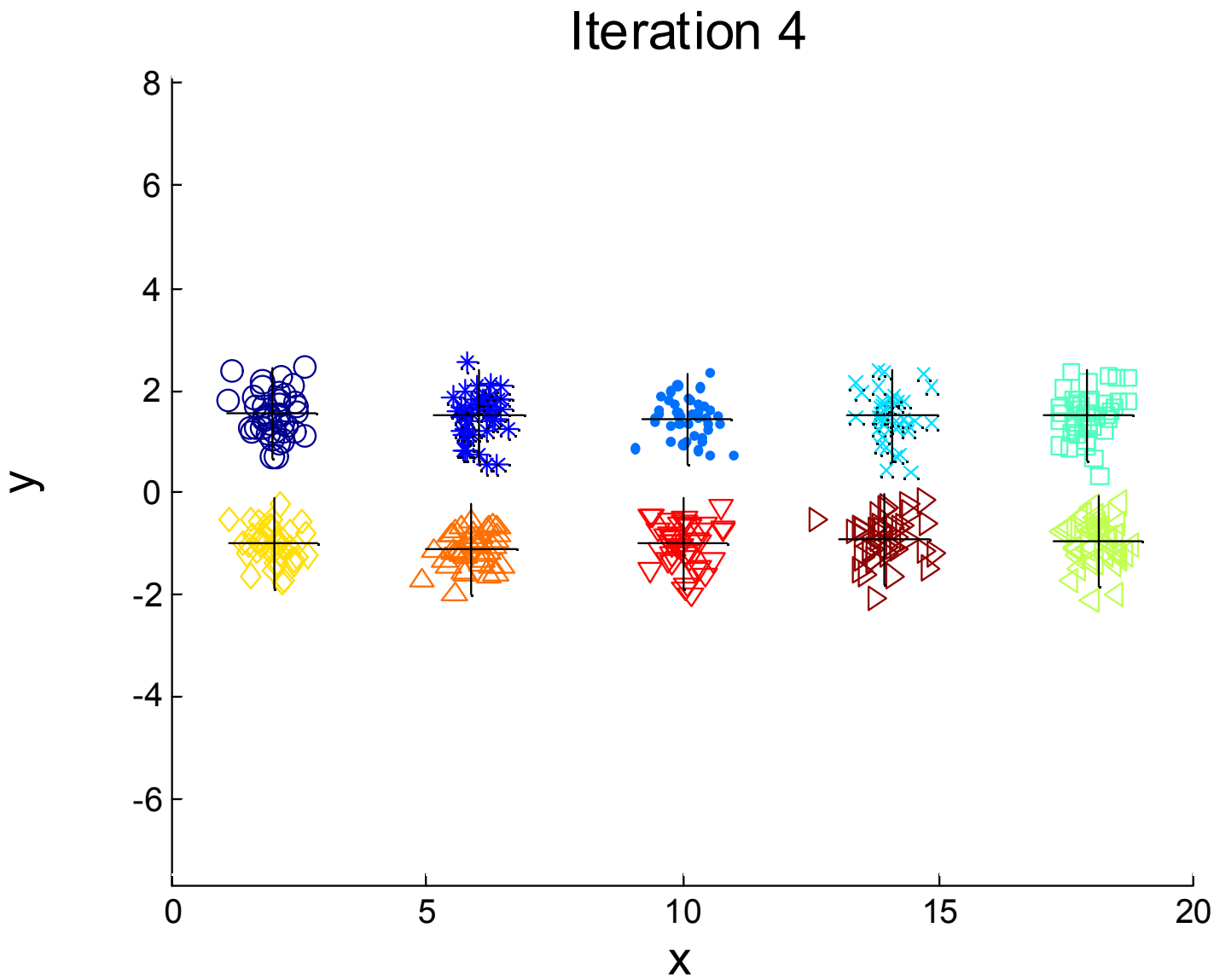
Problems with Selecting Initial Points

- If there are K 'real' clusters then the chance of selecting one centroid from each cluster is small.
  - Especially when K is large
  - Sometimes the initial centroids will readjust themselves in 'right' way, and sometimes they don't
  - Consider an example of five pairs of clusters

10 Clusters Example (A)



Starting with two initial centroids in one cluster of each pair of clusters

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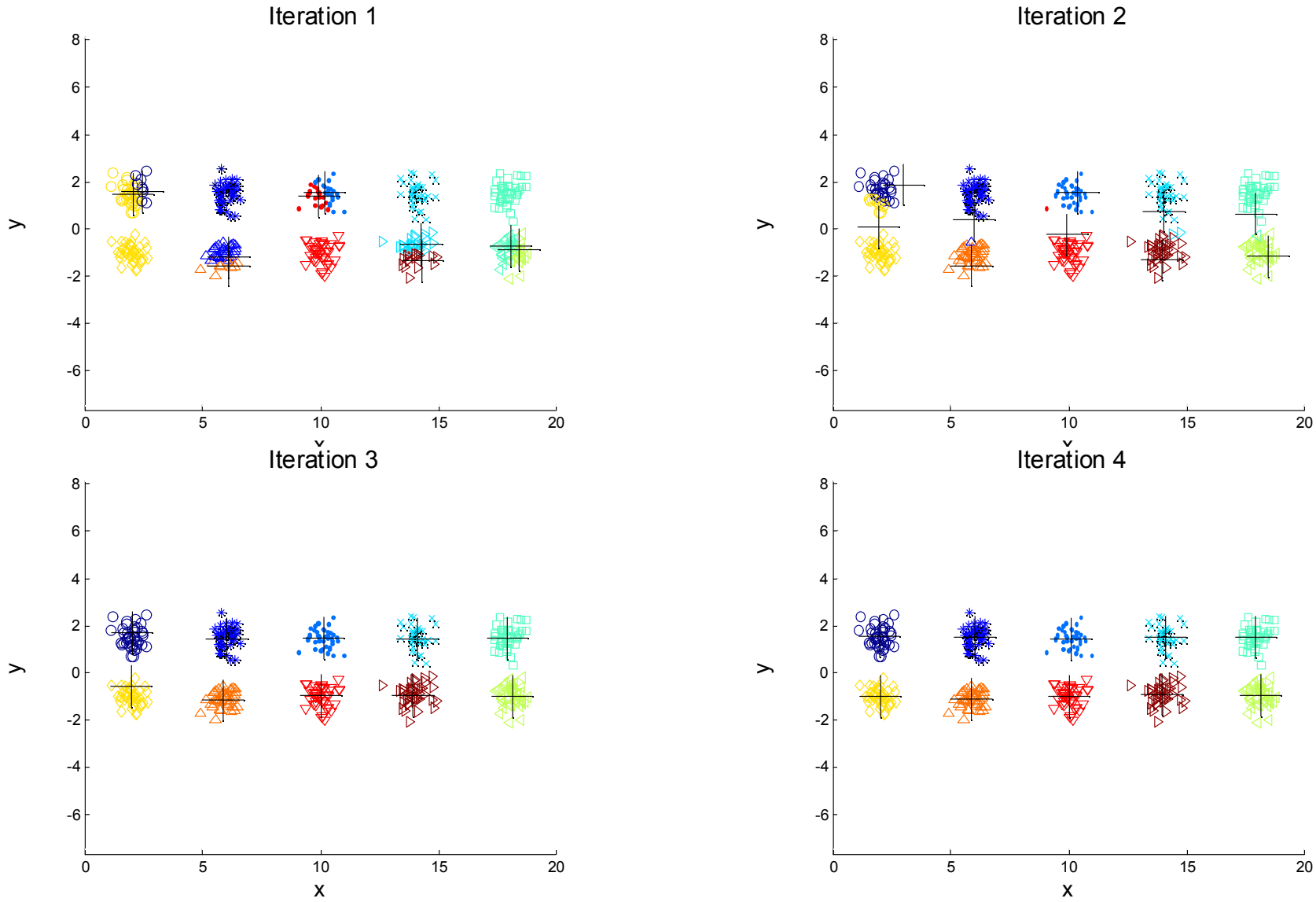
10 Clusters Example (A)



Starting with two initial centroids in one cluster of each pair of clusters

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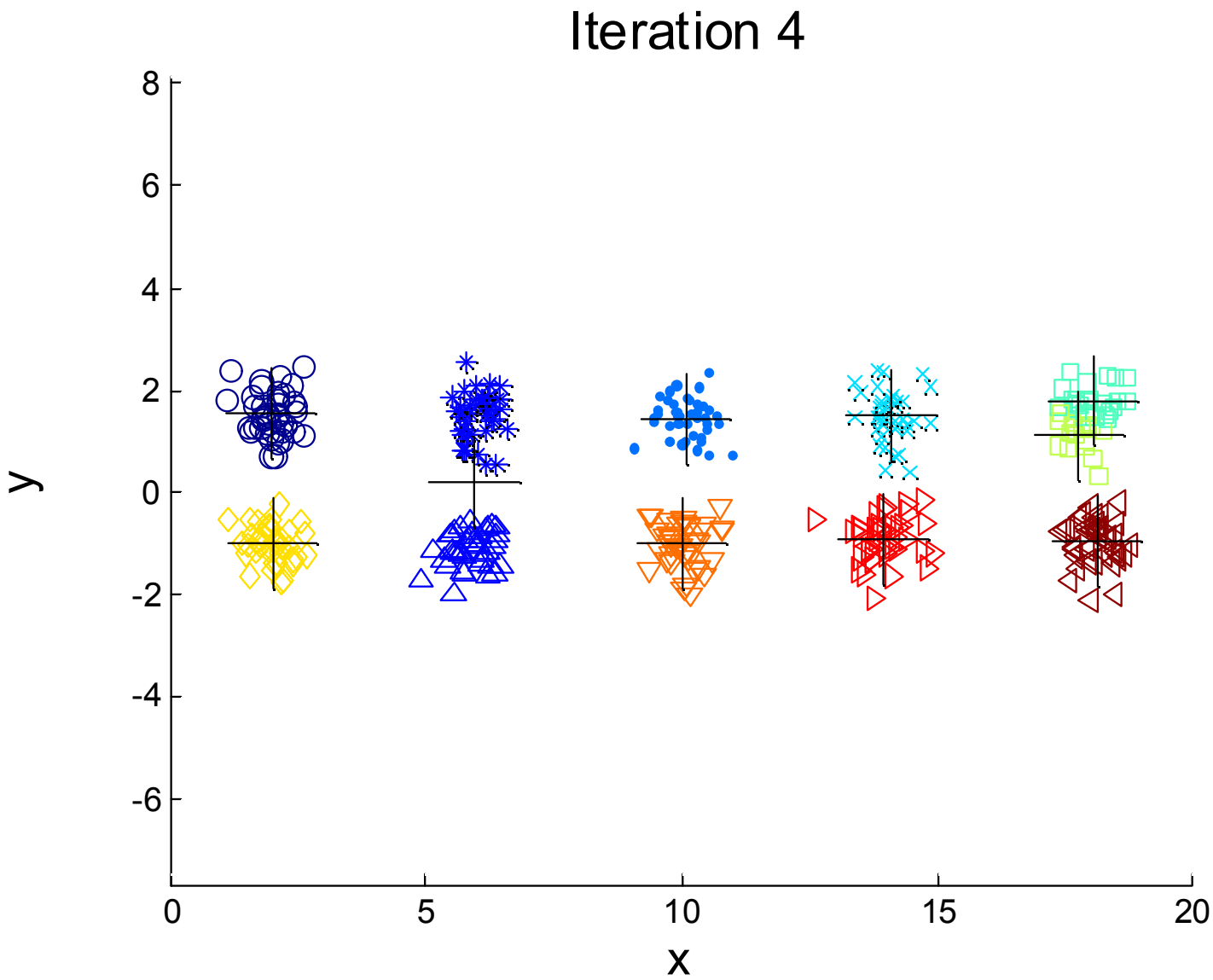
10 Clusters Example (B)



Starting with some pairs of clusters having three initial centroids, while other have only one or two.

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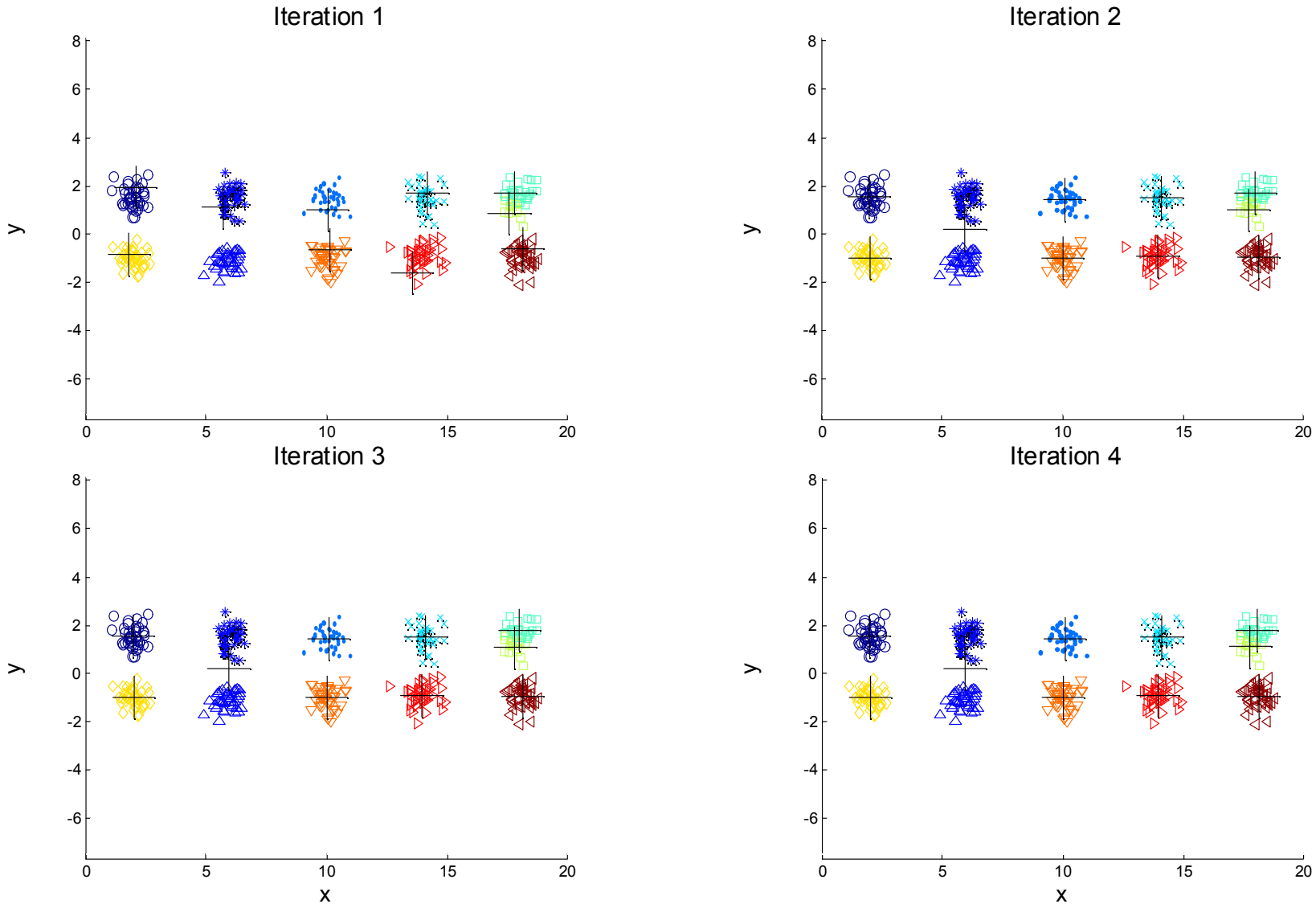

Starting with some pairs of clusters having three initial centroids, while other have only one or two.

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Solutions to Initial Centroids Problem

- Multiple runs
  - Helps, but probability is not on your side
- Sample and use hierarchical clustering to determine initial centroids
- Select more than k initial centroids and then select among these initial centroids
  - Select most widely separated
- Postprocessing
- Bisecting K-means
  - Start with one cluster, and then continuously split
  - Not as susceptible to initialization issues

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Pre-processing and Post-processing

- Pre-processing
  - Normalize the data
  - Eliminate outliers
- Post-processing
  - Eliminate small clusters that may represent outliers
  - Split ‘loose’ clusters, i.e., clusters with relatively high SSE
  - Merge clusters that are ‘close’ and that have relatively low SSE

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Bisecting K-means

- Bisecting K-means algorithm
  - Start with one cluster and split continuously
  - No need to determine the number of clusters
  - Variant of K-means that can produce a partitional or a hierarchical clustering

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1: Initialize the list of clusters to contain the cluster containing all points.
2: **repeat**
3: Select a cluster from the list of clusters
4: **for** $i = 1$ to $number\_of\_iterations$ **do**
5: Bisect the selected cluster using basic K-means
6: **end for**
7: Add the two clusters from the bisection with the lowest SSE to the list of clusters.
8: **until** Until the list of clusters contains K clusters

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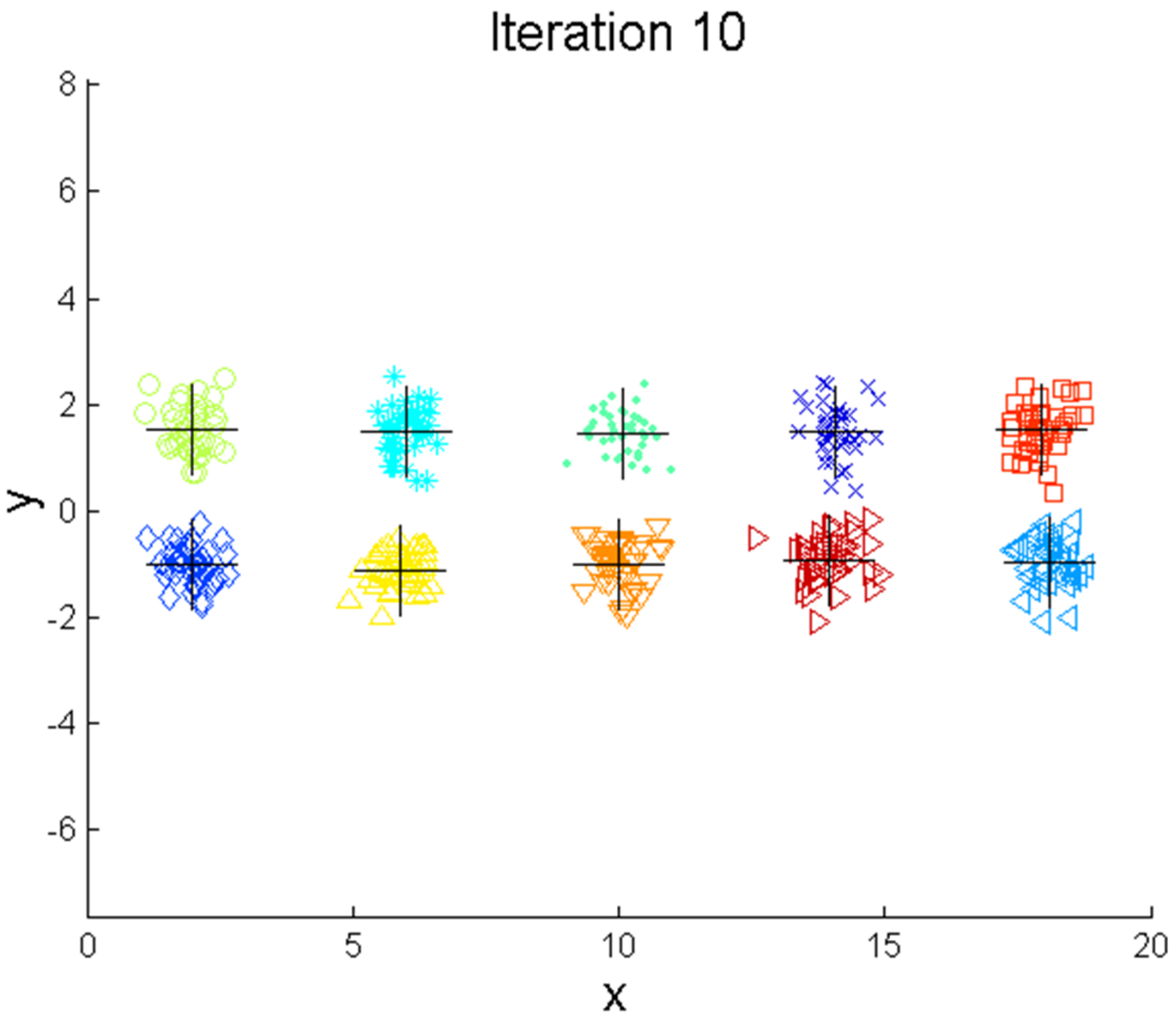
Bisecting K-means Example



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Limitations of K-means

- K-means has problems when clusters are of differing
  - Sizes
  - Densities
  - Non-globular shapes

- K-means has problems when the data contains outliers.

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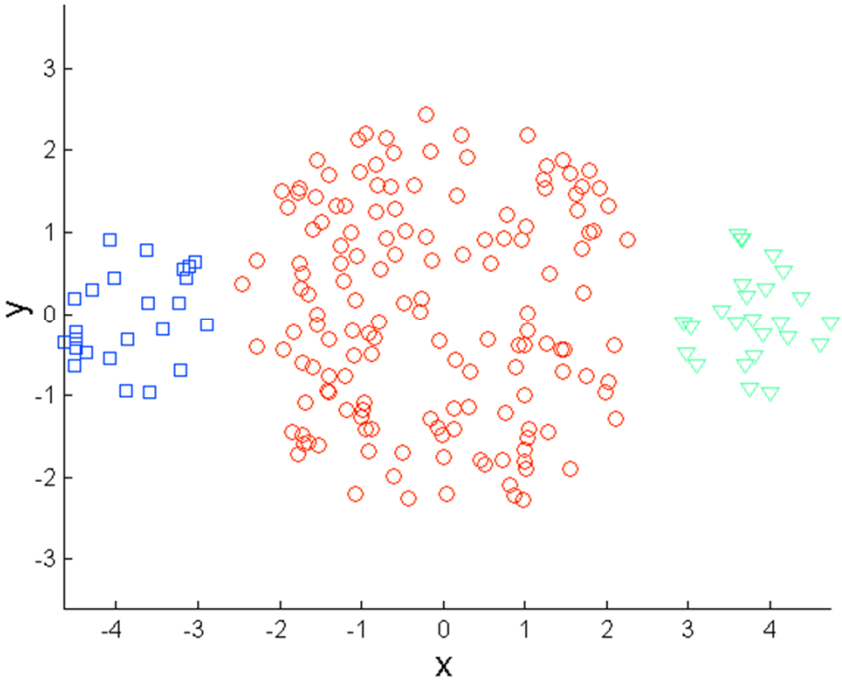
Limitations of K-means: Differing Sizes



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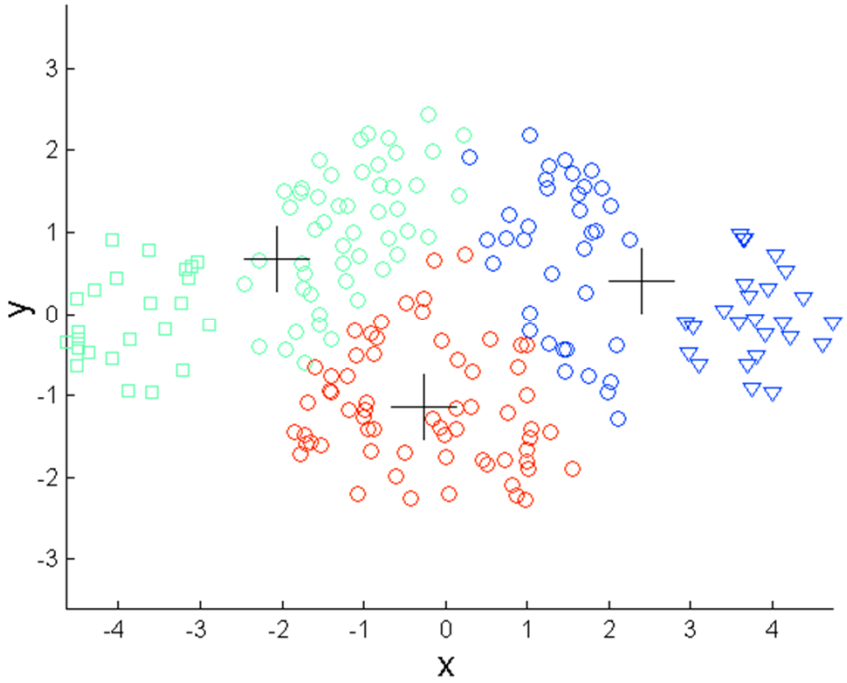

K-means (3 Clusters)

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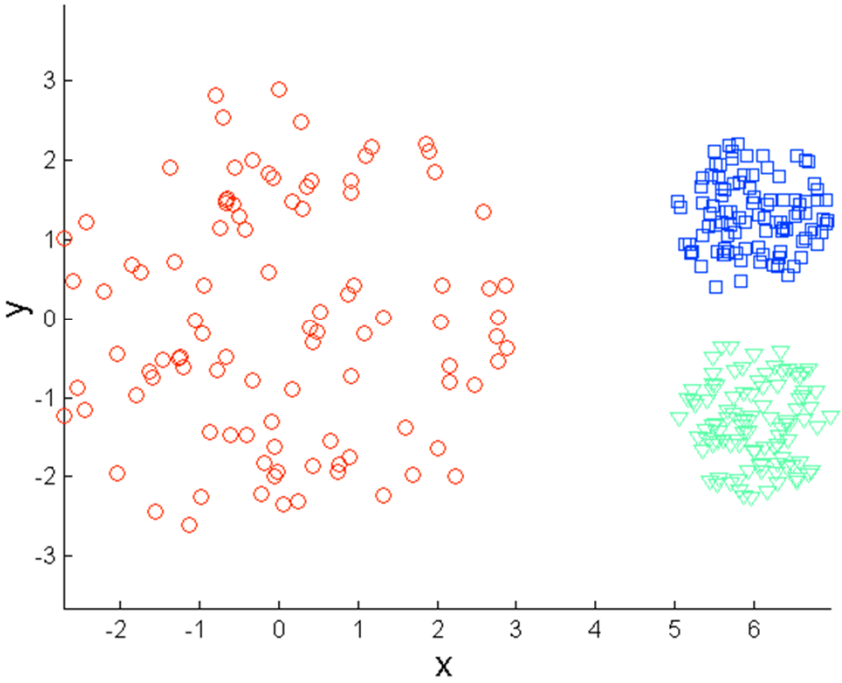
Limitations of K-means: Differing Density



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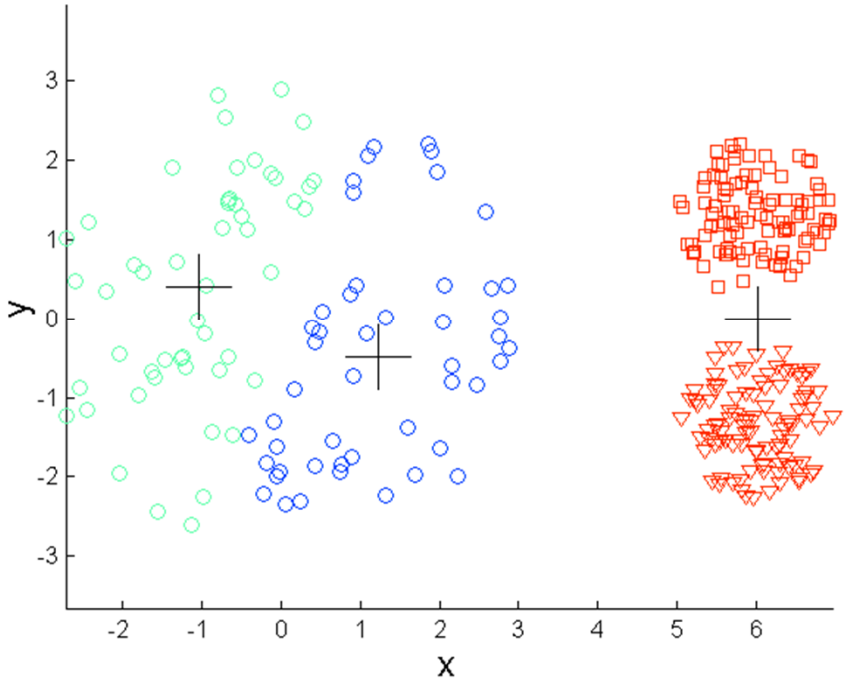

K-means (3 Clusters)

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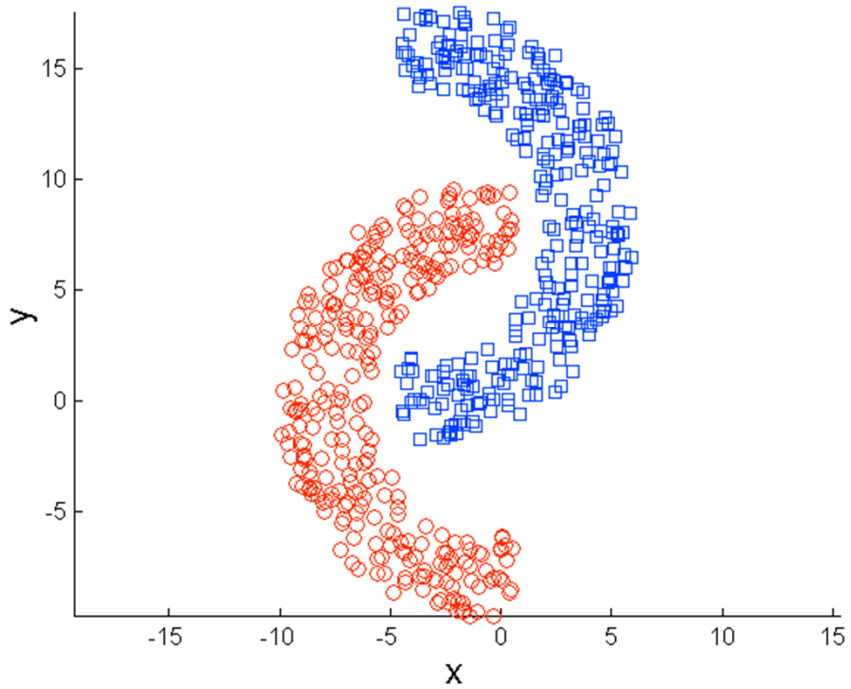
Limitations of K-means: Non-globular Shapes



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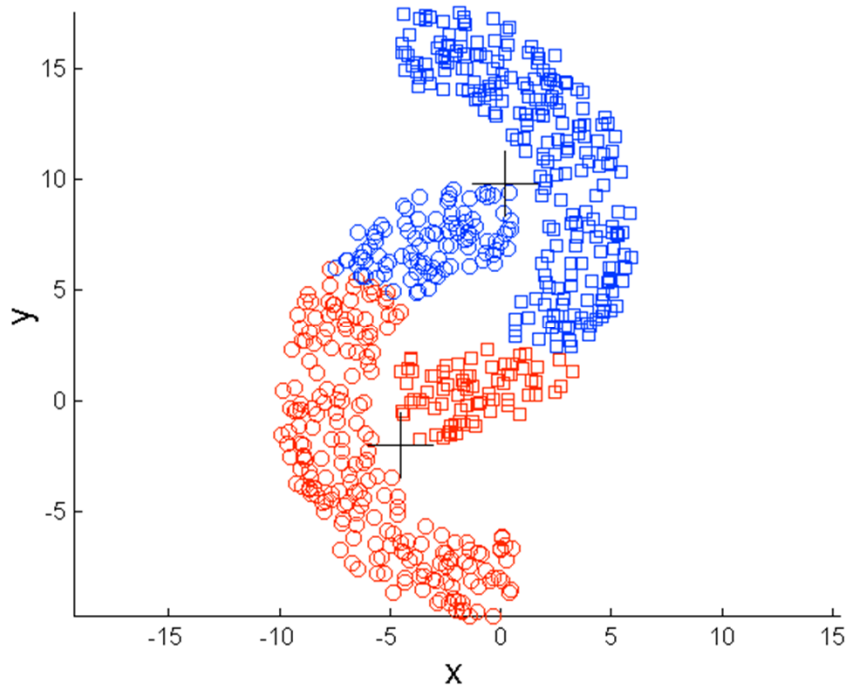

K-means (2 Clusters)

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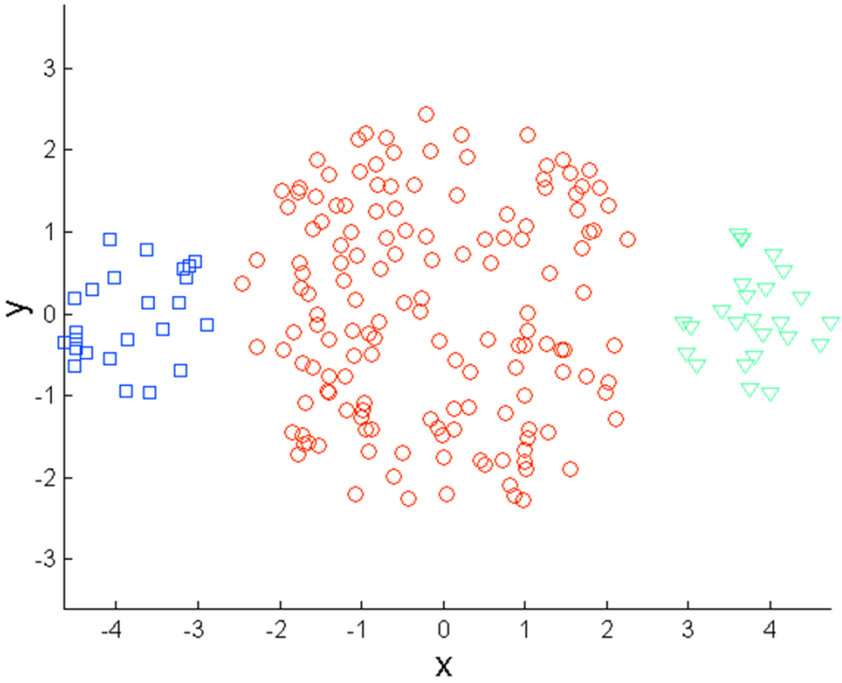
Overcoming K-means Limitations



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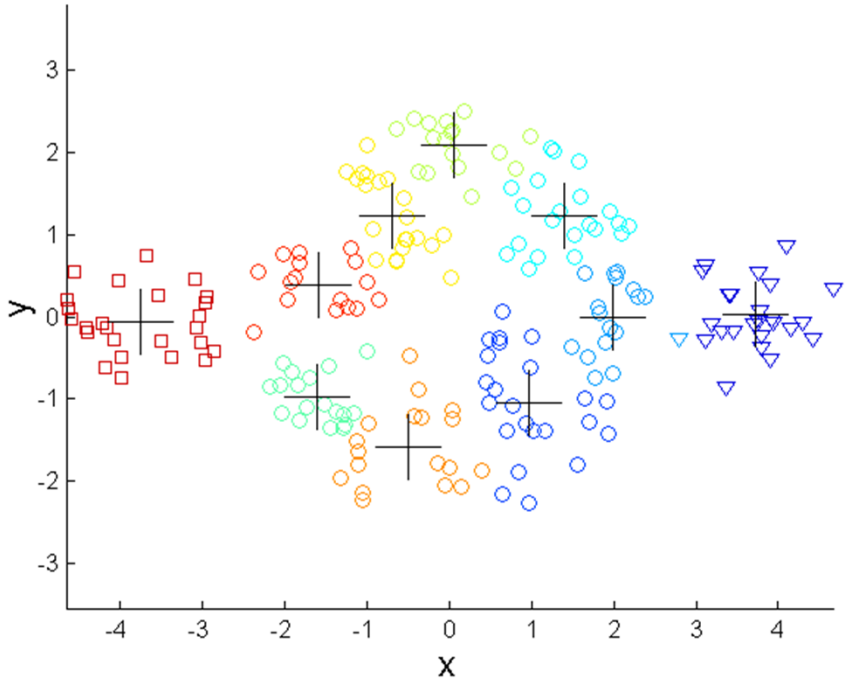

K-means Clusters

One solution is to use many clusters.
Find parts of clusters, but need to put together.

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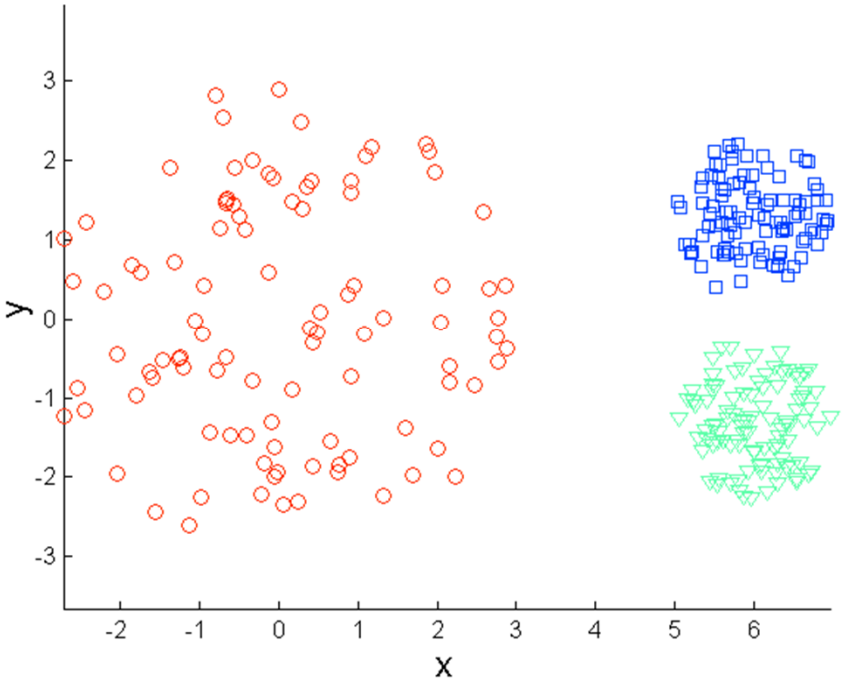
Overcoming K-means Limitations



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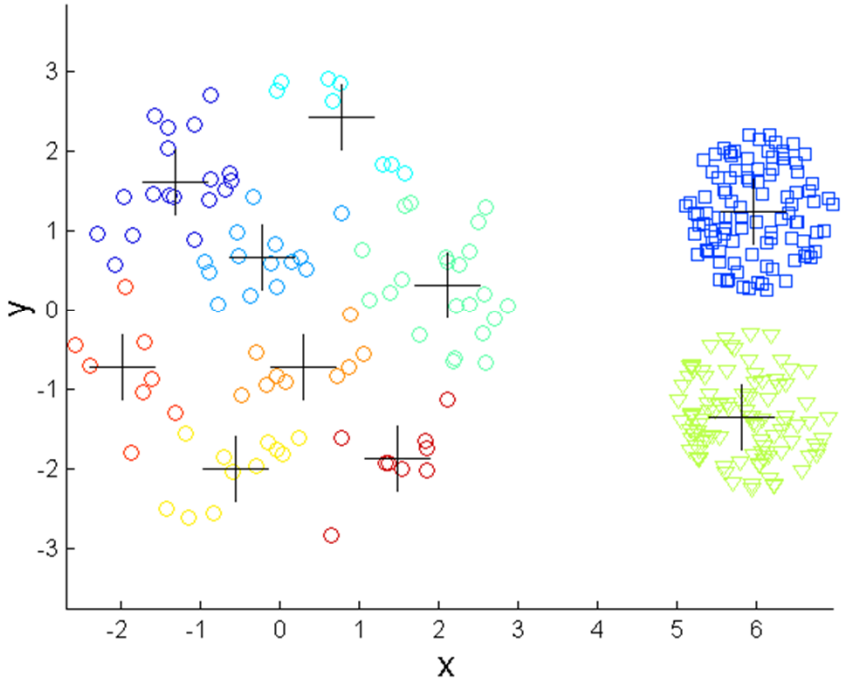

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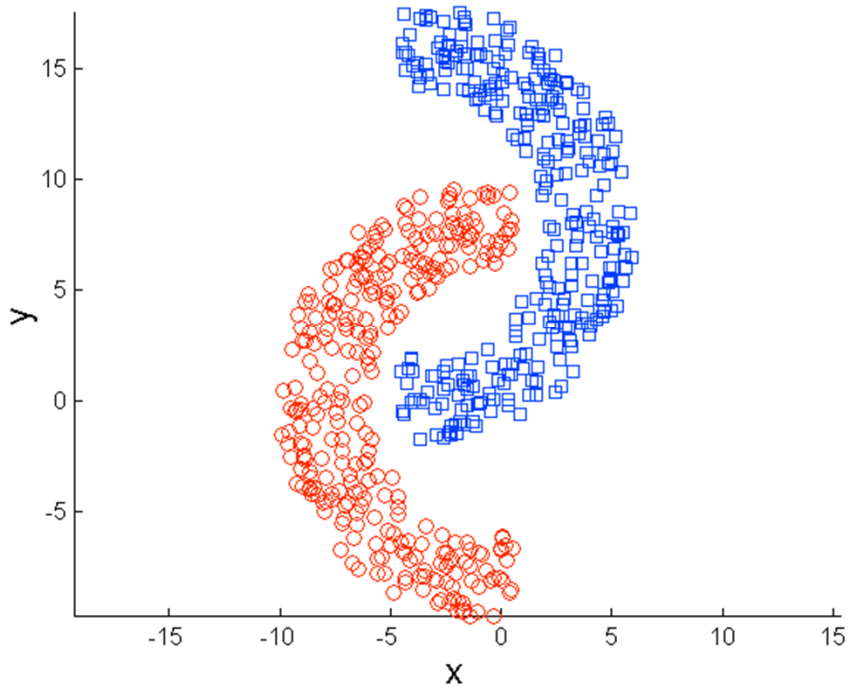
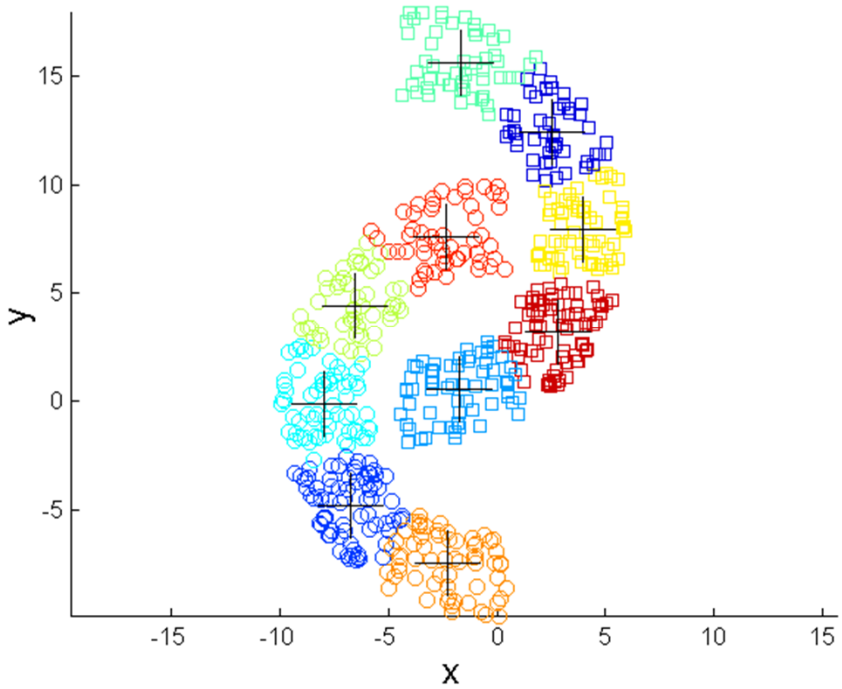


Original Points

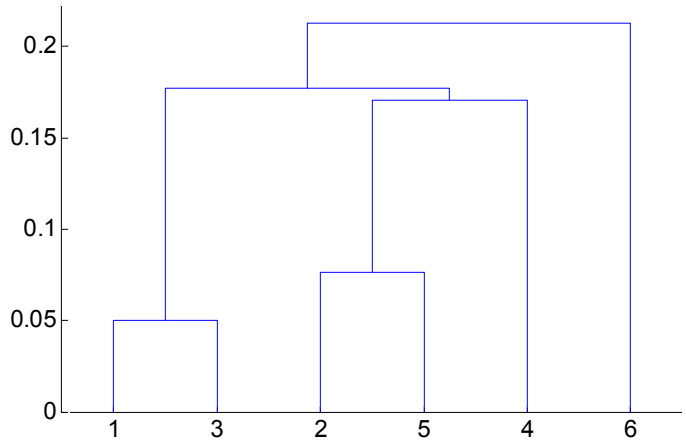


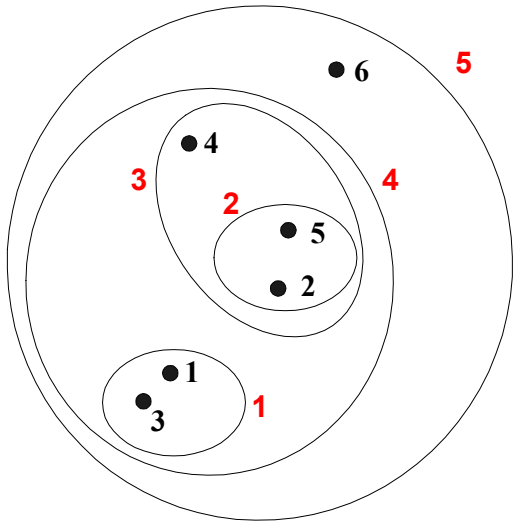
K-means Clusters

Adapted from:
Tan,Steinbach, Kumar - Introduction to Data Mining
Han, Kamber - Data Mining: Concepts and Techniques

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





Adapted from:
Tan,Steinbach, Kumar - Introduction to Data Mining
Han, Kamber - Data Mining: Concepts and Techniques

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

Adapted from:
Tan,Steinbach, Kumar - Introduction to Data Mining
Han, Kamber - Data Mining: Concepts and Techniques

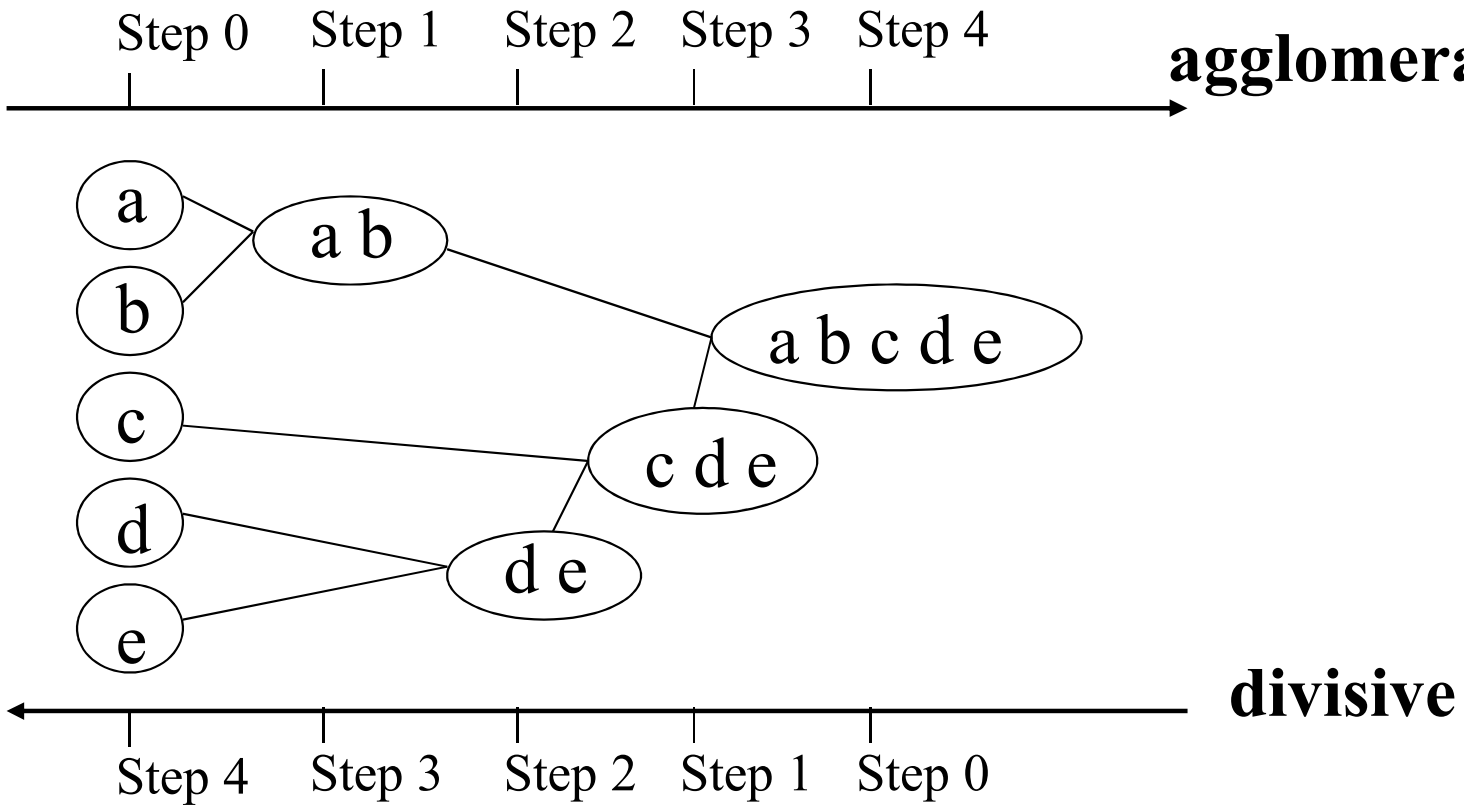
Hierarchical Clustering

- 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

Adapted from:
Tan,Steinbach, Kumar - Introduction to Data Mining
Han, Kamber - Data Mining: Concepts and Techniques

Hierarchical Clustering

- This method does not require the number of clusters ***k*** as an input, but needs a termination condition



Adapted from:
Tan,Steinbach, Kumar - Introduction to Data Mining
Han, Kamber - Data Mining: Concepts and Techniques

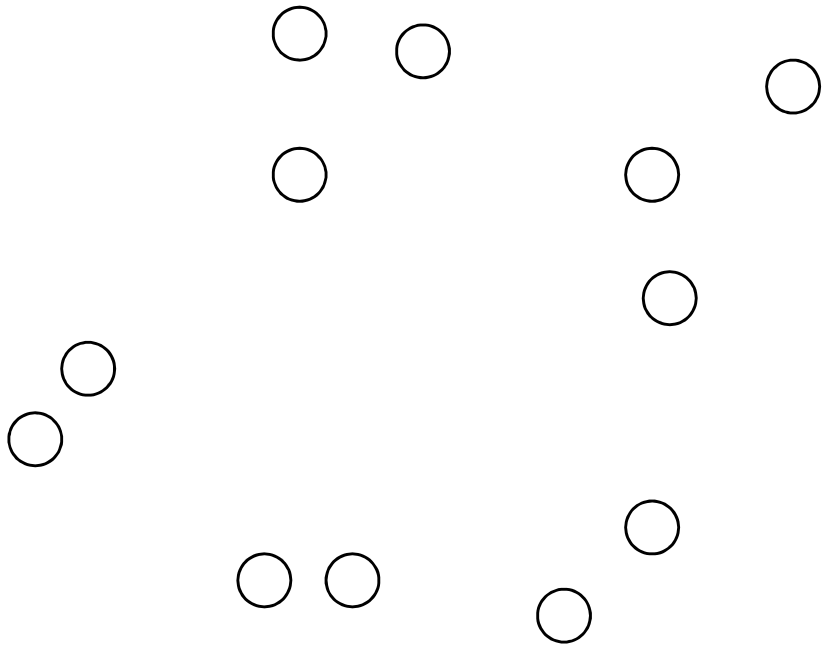
Agglomerative Clustering Algorithm

- 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

Adapted from:
Tan,Steinbach, Kumar - Introduction to Data Mining
Han, Kamber - Data Mining: Concepts and Techniques

Starting Situation

- Start with clusters of individual points and a proximity matrix



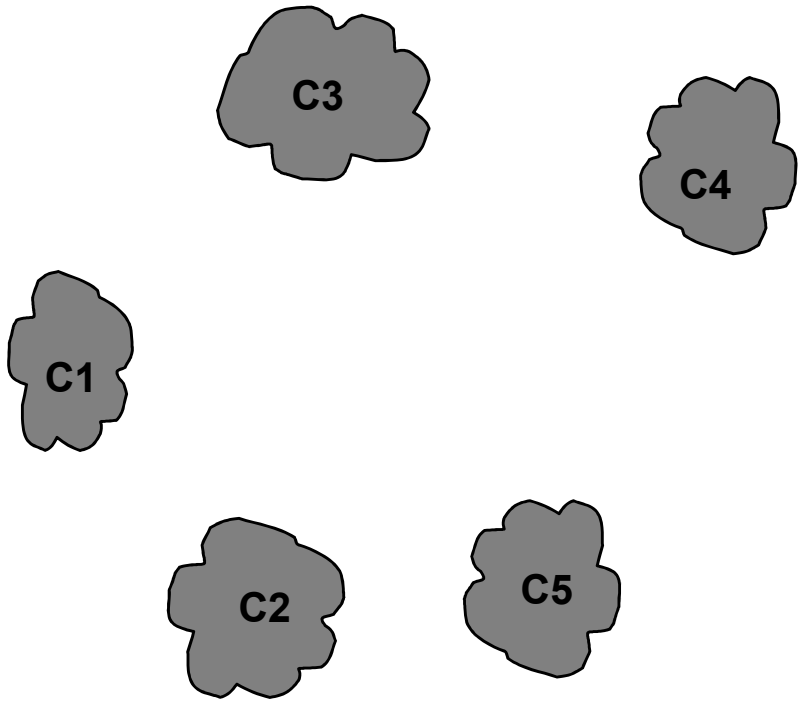
	p1	p2	p3	p4	p5	. . .
p1						
p2						
p3						
p4						
p5						
.						
.						
.						

Proximity Matrix

Adapted from:
Tan,Steinbach, Kumar - Introduction to Data Mining
Han, Kamber - Data Mining: Concepts and Techniques

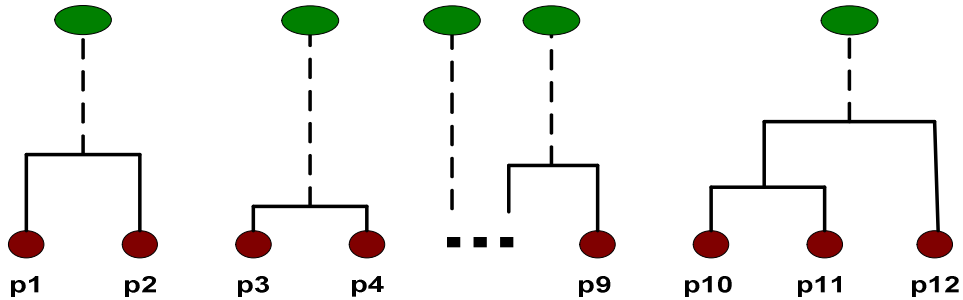
Intermediate Situation

- After some merging steps, we have some clusters



	C1	C2	C3	C4	C5
C1					
C2					
C3					
C4					
C5					

Proximity Matrix



Adapted from:
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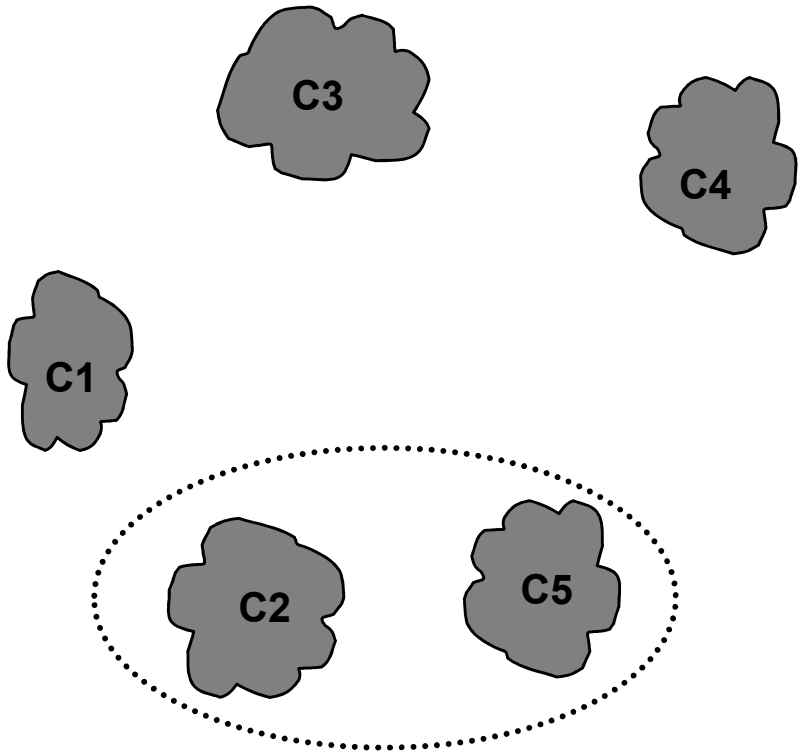
Han, Kamber - Data Mining: Concepts and Techniques

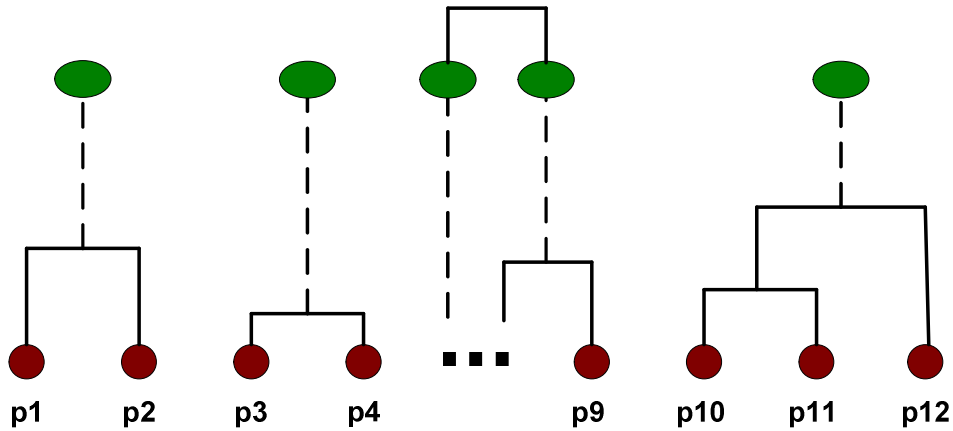
Intermediate Situation

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



	C1	C2	C3	C4	C5
C1					
C2					
C3					
C4					
C5					

Proximity Matrix



Adapted from:
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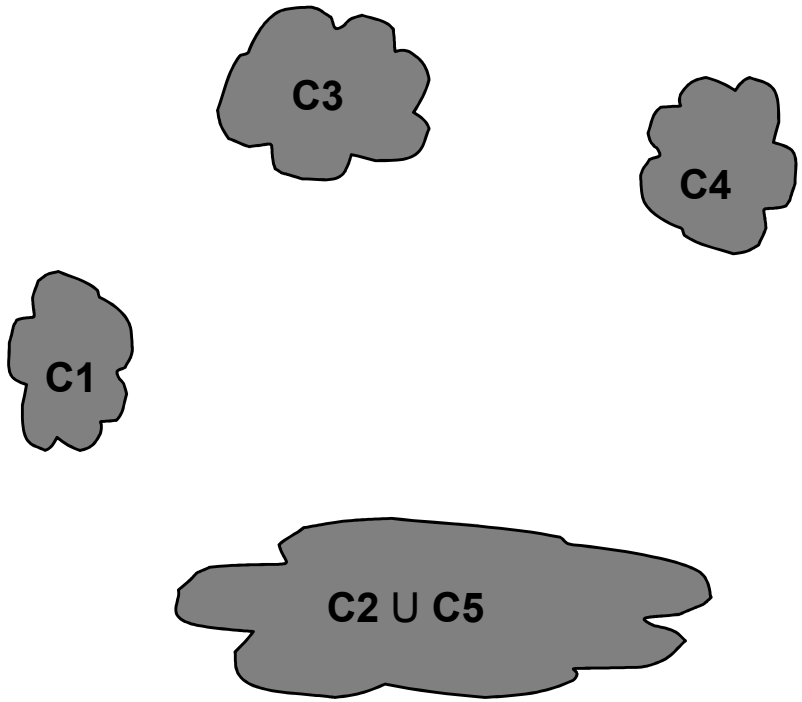
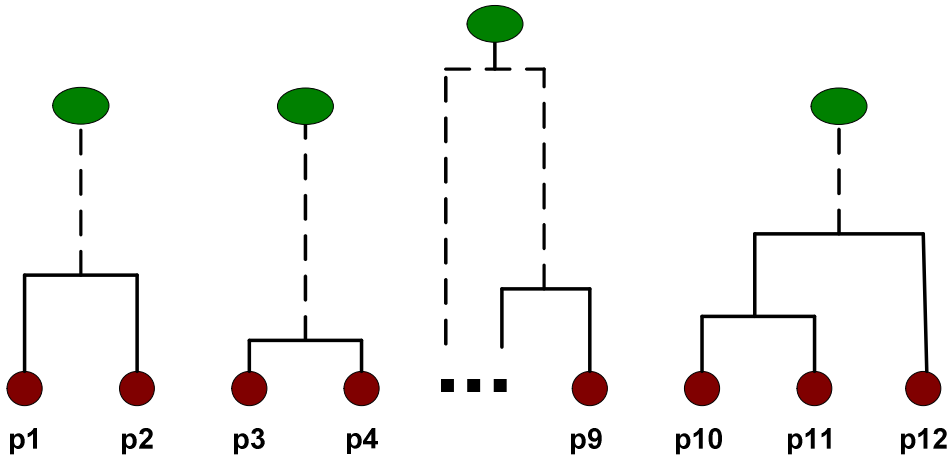
After Merging

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



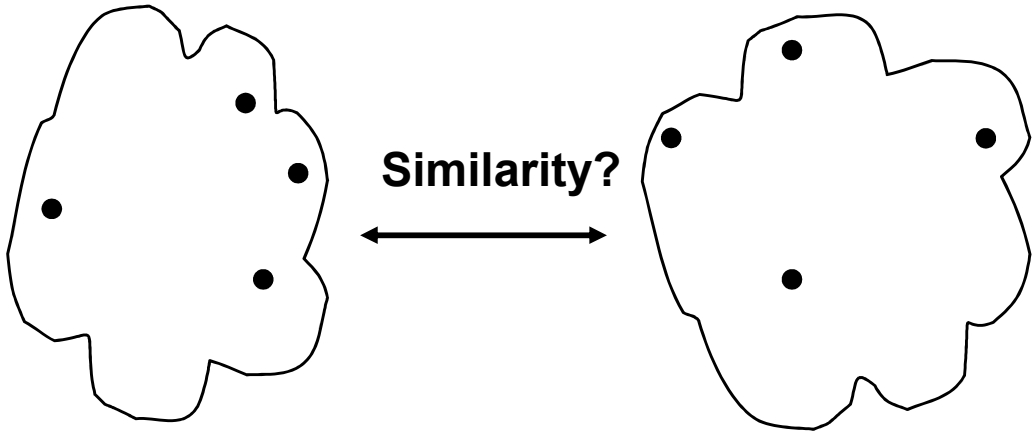
	C1	C2 U C5	C3	C4
C1		?		
C2 U C5	?	?	?	?
C3		?		
C4		?		

Proximity Matrix



Adapted from:
Tan,Steinbach, Kumar - Introduction to Data Mining
Han, Kamber - Data Mining: Concepts and Techniques

How to Define Inter-Cluster Similarity



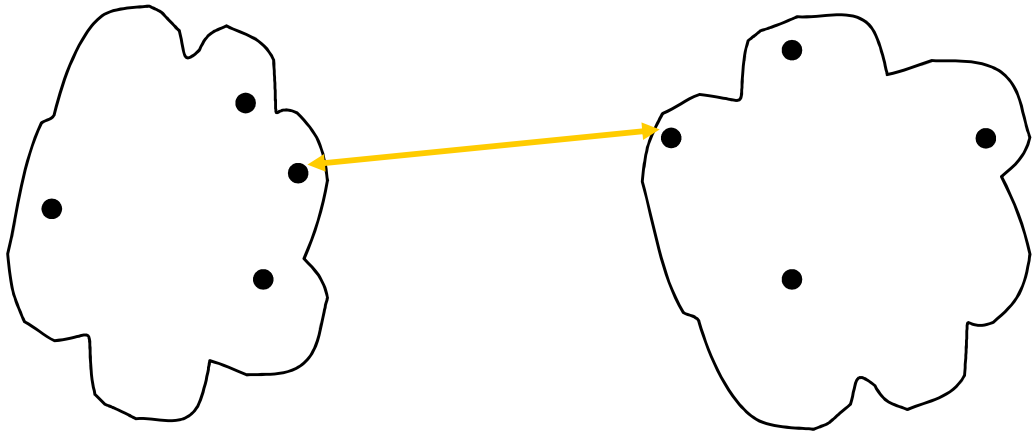
	p1	p2	p3	p4	p5	. . .
p1						
p2						
p3						
p4						
p5						
.						
.						
.						

Proximity Matrix

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

Adapted from:
Tan,Steinbach, Kumar - Introduction to Data Mining
Han, Kamber - Data Mining: Concepts and Techniques

How to Define Inter-Cluster Similarity



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

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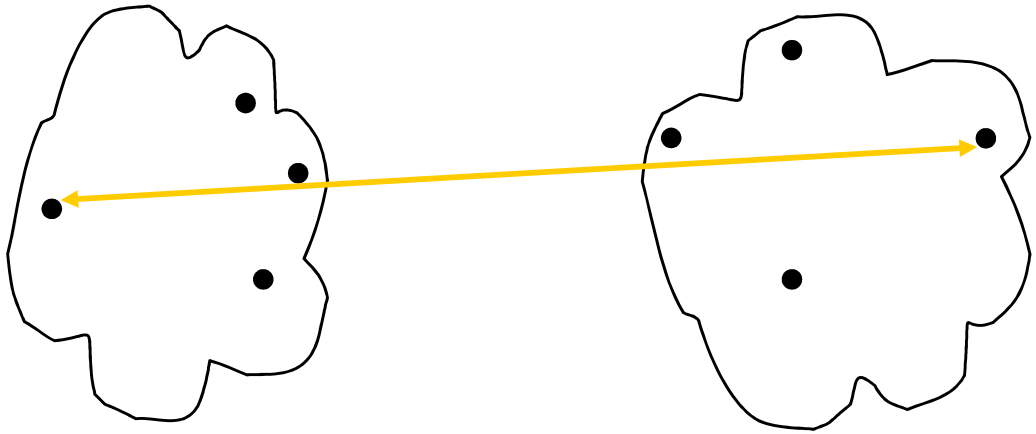
How to Define Inter-Cluster Similarity



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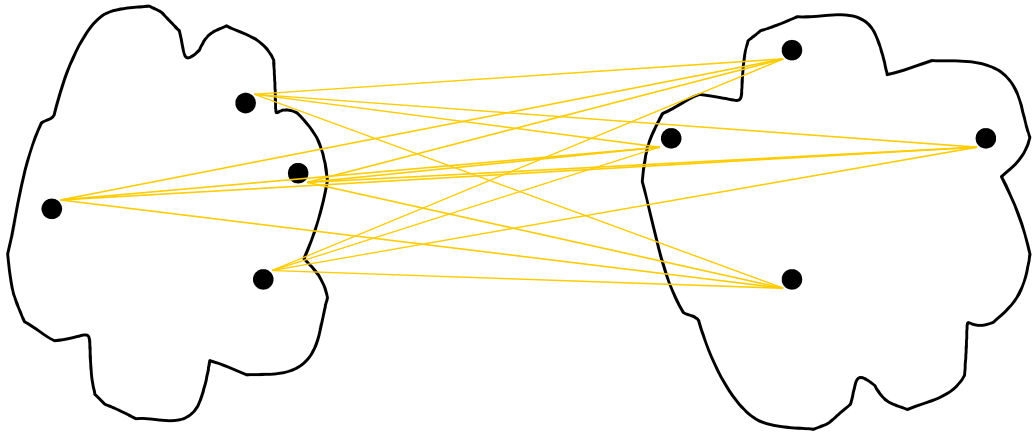
How to Define Inter-Cluster Similarity



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

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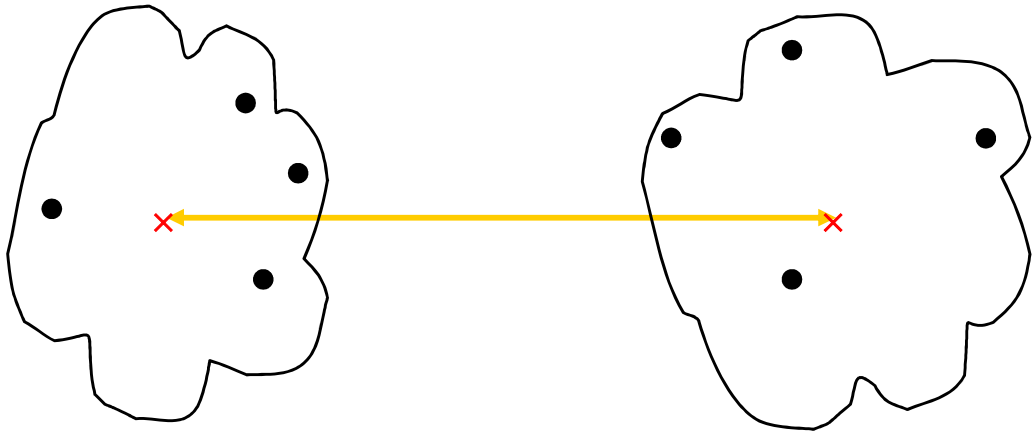
How to Define Inter-Cluster Similarity



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

Proximity Matrix

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

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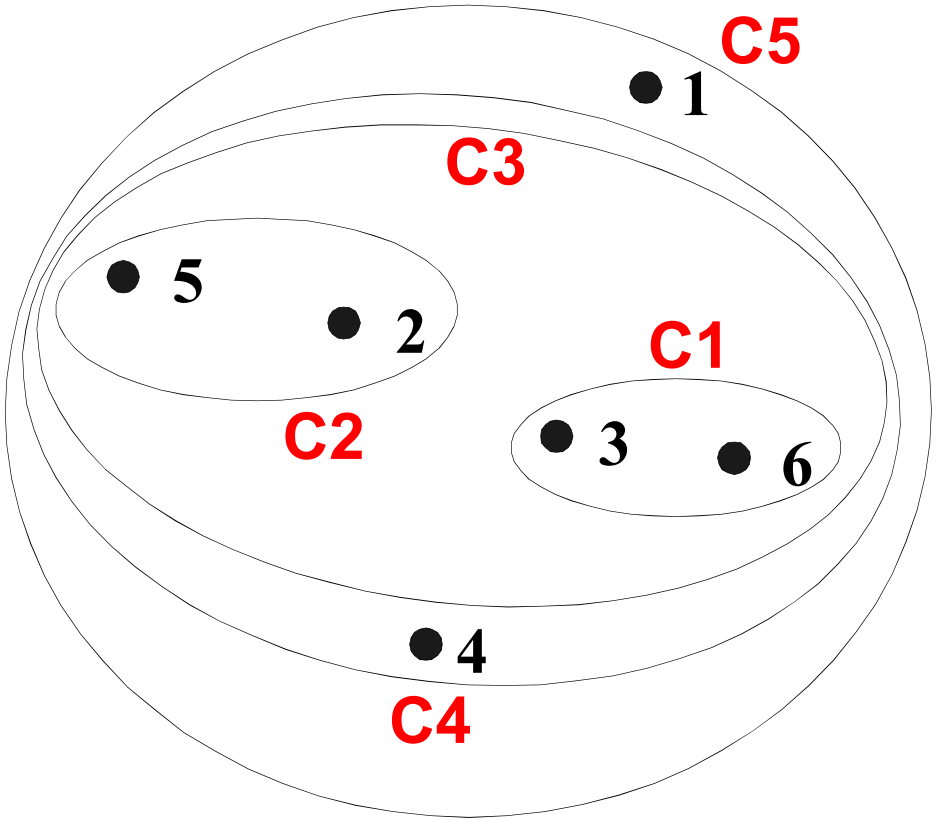
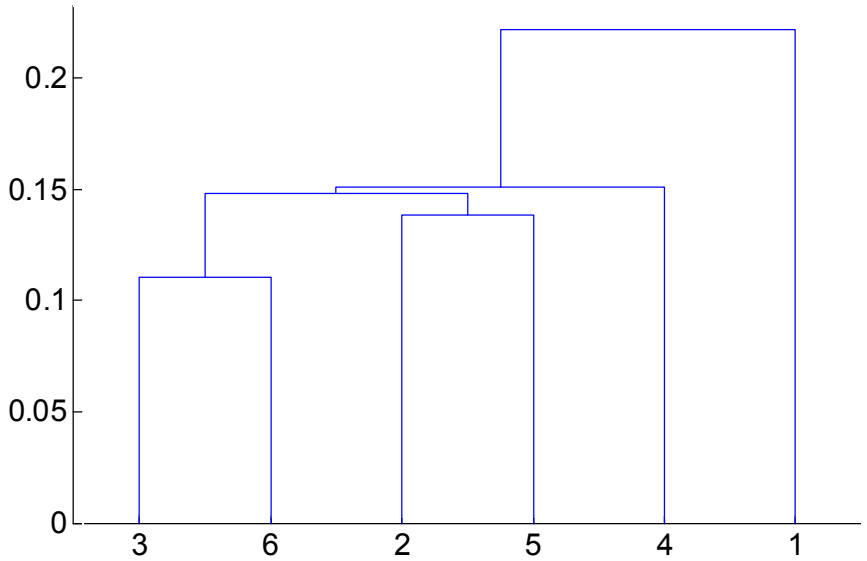
Han, Kamber - Data Mining: Concepts and Techniques

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.

Hierarchical Clustering: MIN



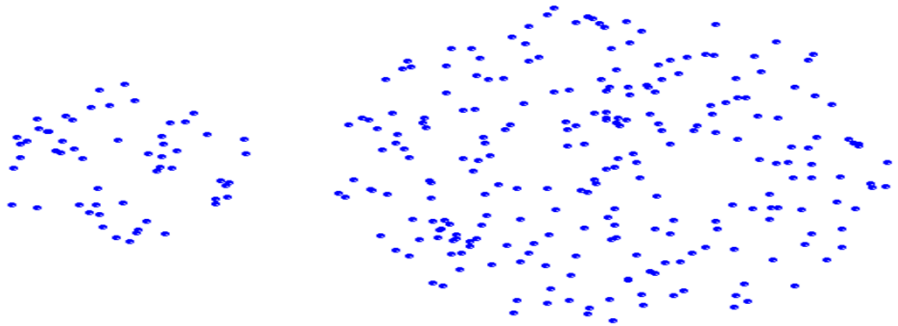


Nested Clusters

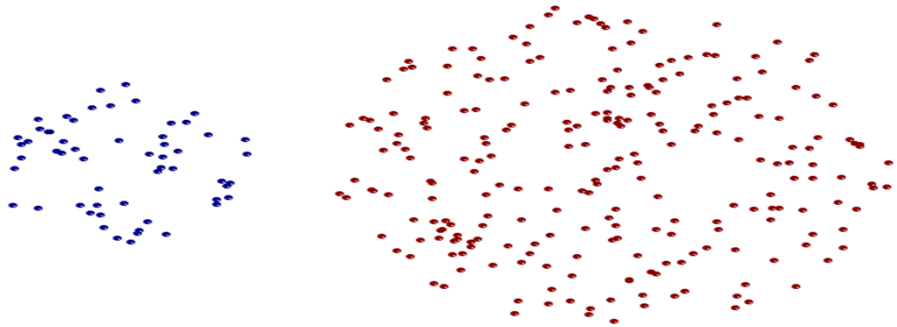
Dendrogram

Adapted from:
Tan,Steinbach, Kumar - Introduction to Data Mining
Han, Kamber - Data Mining: Concepts and Techniques

Strength of MIN



Original Points

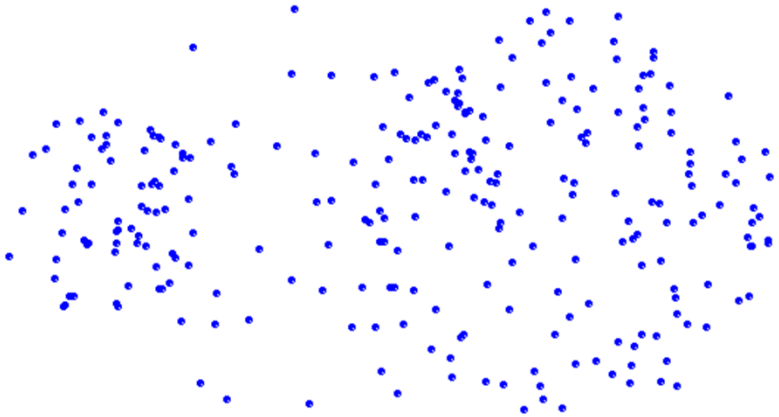


Two Clusters

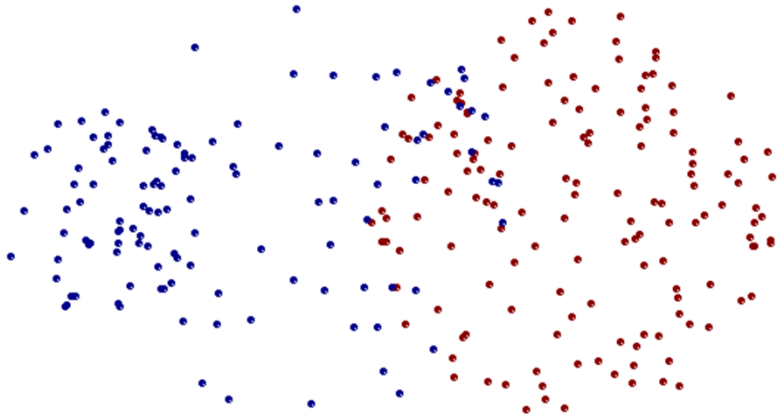
- **Can handle non-elliptical shapes**

Adapted from:
Tan,Steinbach, Kumar - Introduction to Data Mining
Han, Kamber - Data Mining: Concepts and Techniques

Limitations of MIN



Original Points



Two Clusters

- **Sensitive to noise and outliers**

Adapted from:
Tan,Steinbach, Kumar - Introduction to Data Mining
Han, Kamber - Data Mining: Concepts and Techniques

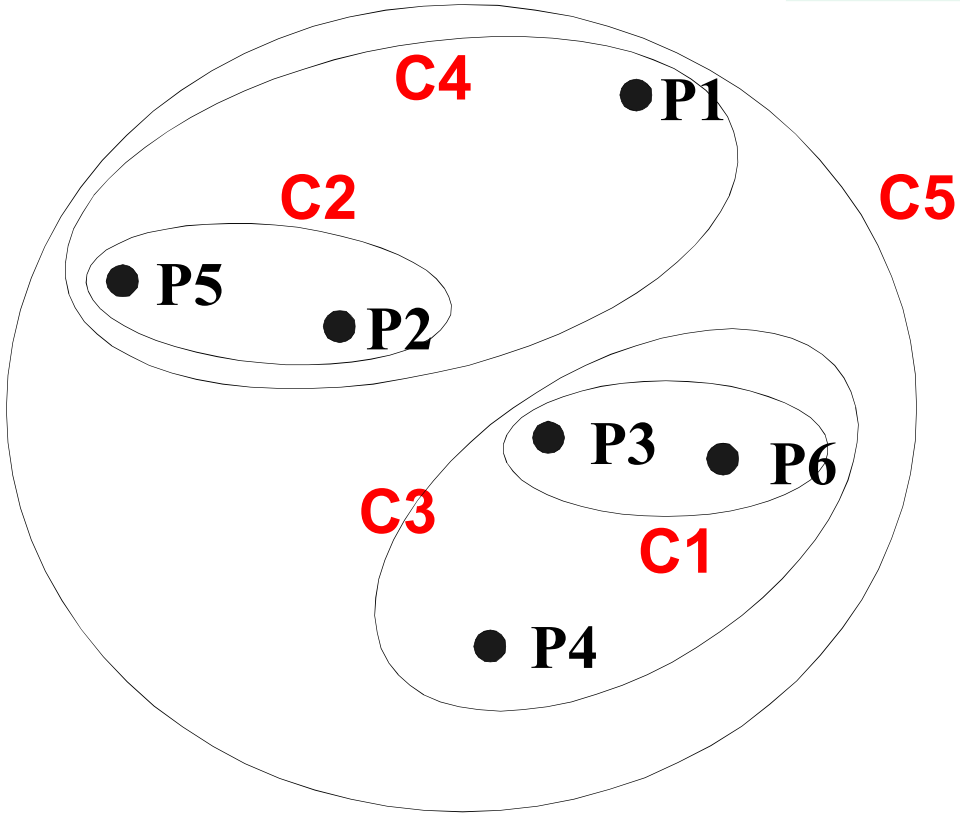
Cluster Similarity: MAX or Complete Linkage

- 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

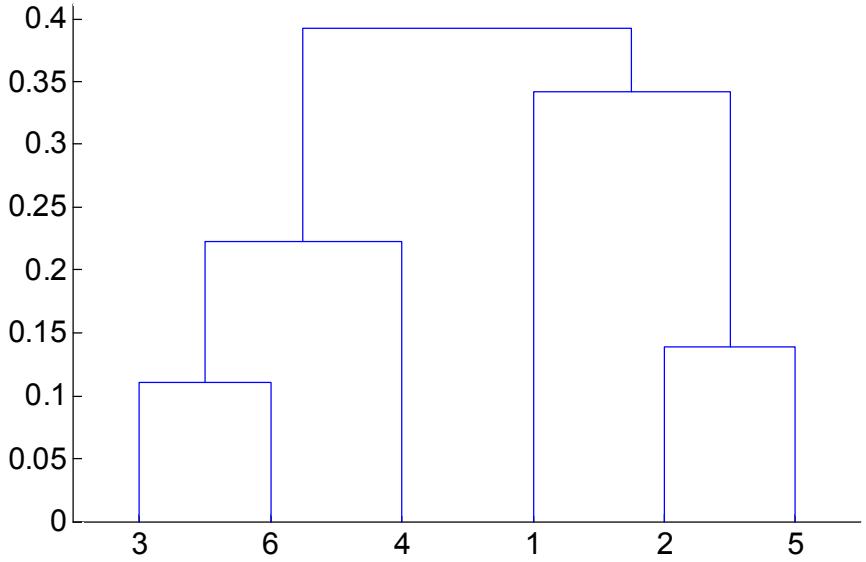
Hierarchical Clustering: MAX

	C1 or C2	P1	P4
C1(P3, P6)	P5 & P6	P1 & P6	P4 & P6
C2(P2, P5)	P5 & P6	P1 & P5	P4 & P5

**MAX → then, FIND MIN among MAX*



Nested Clusters



Dendrogram

Adapted from:
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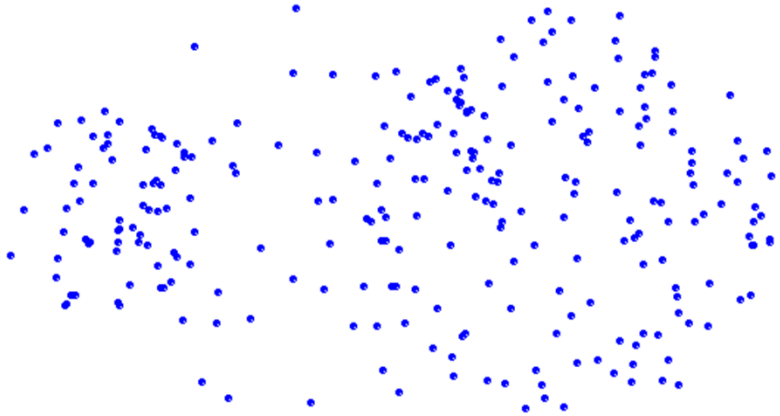
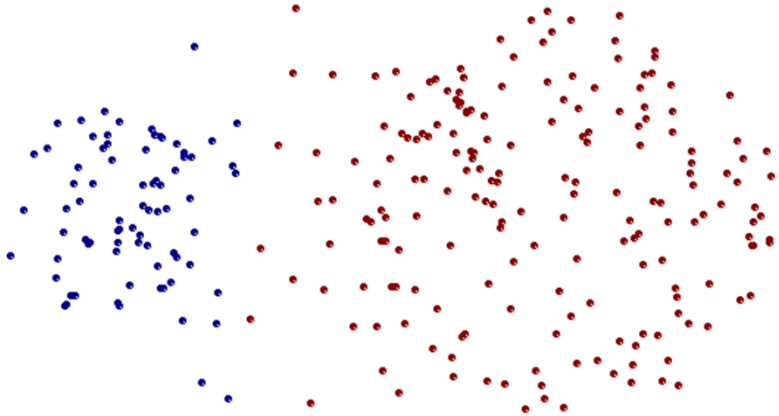
Strength of MAX



Original Points



Two Clusters

- **Less susceptible to noise and outliers**

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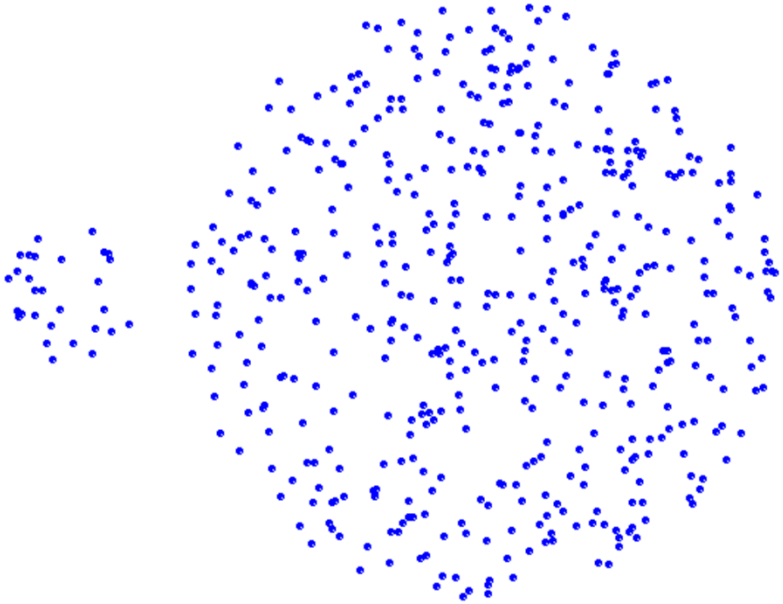
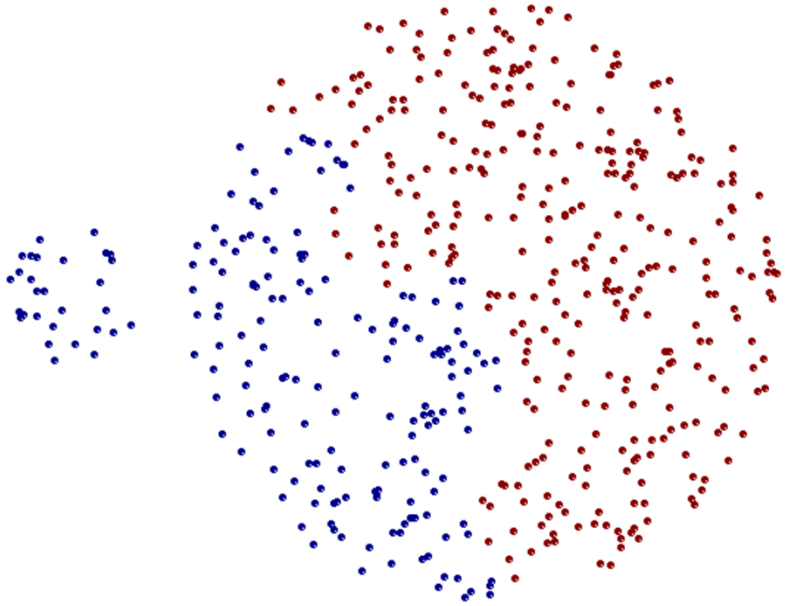
Han, Kamber - Data Mining: Concepts and Techniques

Limitations of MAX



Original Points



Two Clusters

- **Tends to break large clusters**
- **Biased towards globular clusters**

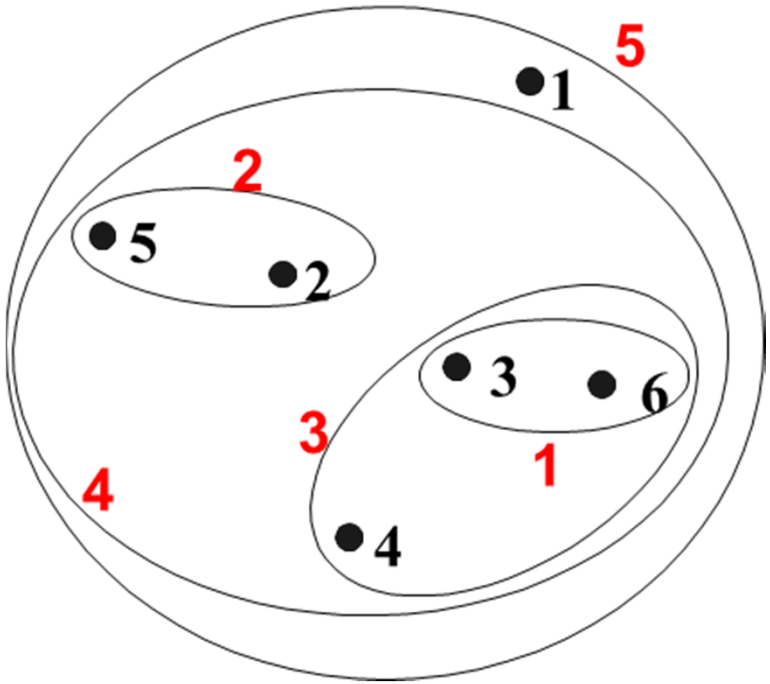
Adapted from:
Tan,Steinbach, Kumar - Introduction to Data Mining
Han, Kamber - Data Mining: Concepts and Techniques

Cluster Similarity: Group Average

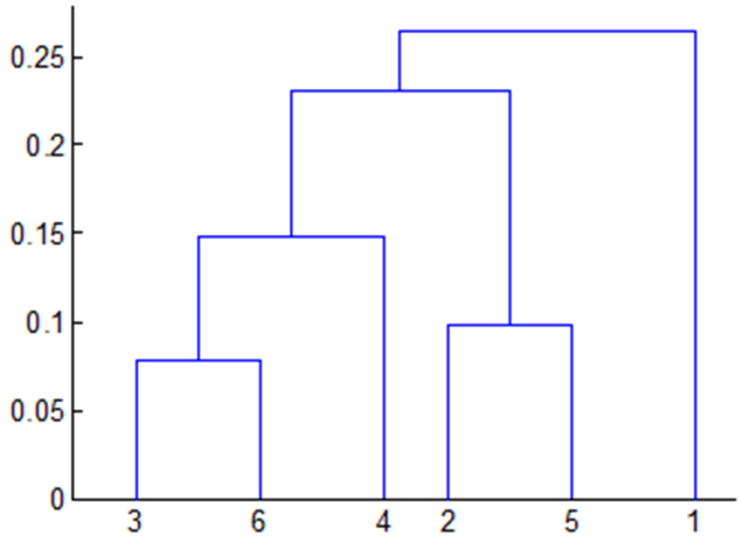
- Proximity of two clusters is the average of pairwise proximity between points in the two clusters.

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

Hierarchical Clustering: Group Average



Nested Clusters



Dendrogram

Adapted from:
Tan,Steinbach, Kumar - Introduction to Data Mining
Han, Kamber - Data Mining: Concepts and Techniques

Hierarchical Clustering: Group Average

- Compromise between Single and Complete Link

- Strengths
  - Less susceptible to noise and outliers

- Limitations
  - Biased towards globular clusters

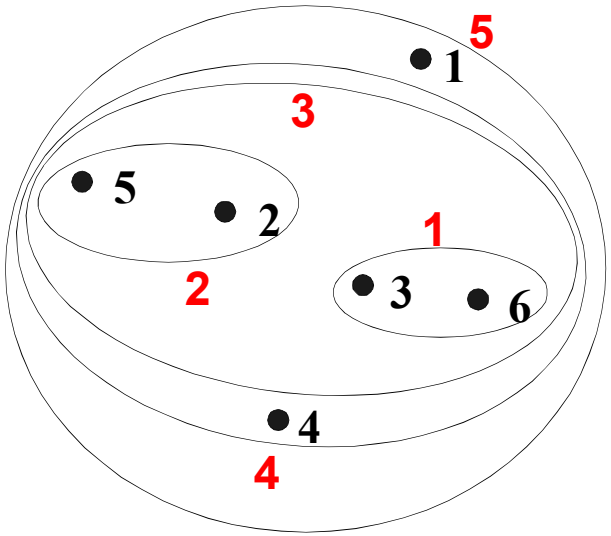
Adapted from:
Tan,Steinbach, Kumar - Introduction to Data Mining
Han, Kamber - Data Mining: Concepts and Techniques

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

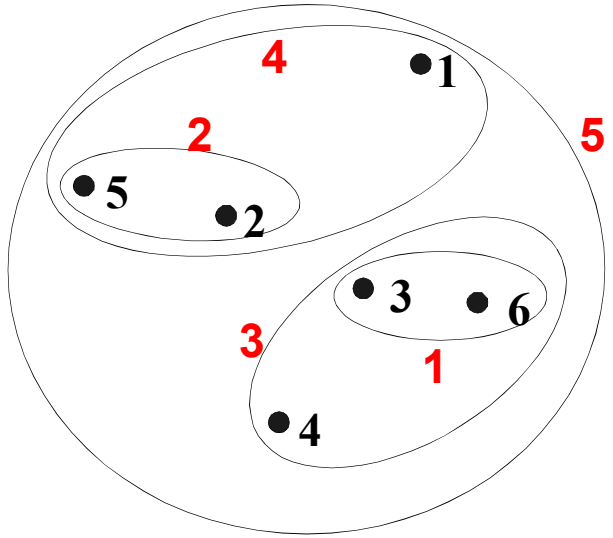
Adapted from:
Tan,Steinbach, Kumar - Introduction to Data Mining
Han, Kamber - Data Mining: Concepts and Techniques

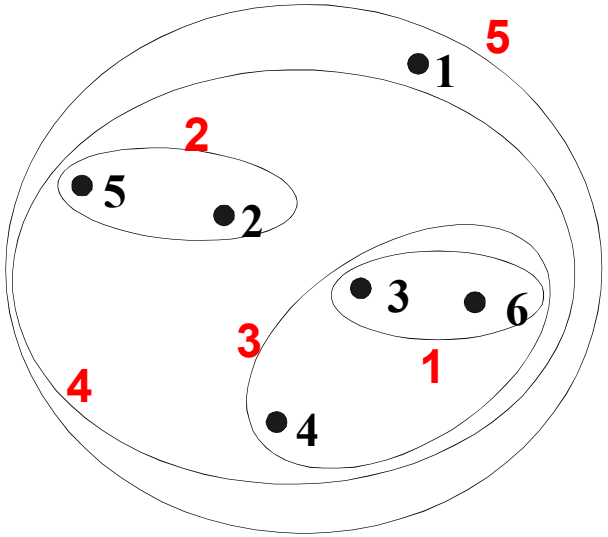
Hierarchical Clustering: Comparison



MIN

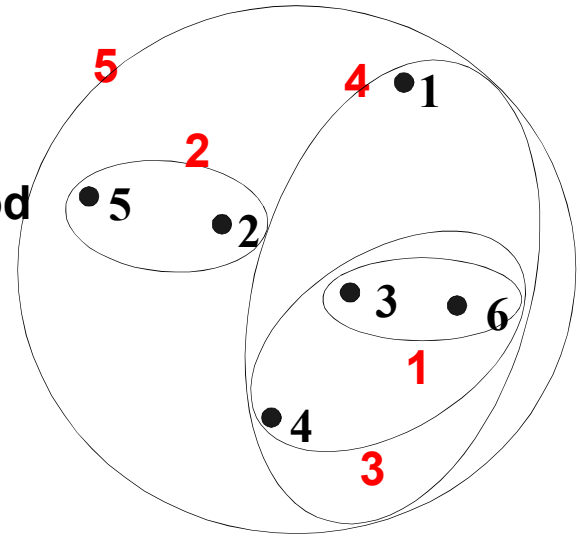
MAX





Group Average

Ward's Method



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Hierarchical Clustering: Limitations

- Once a decision is made to combine two clusters, it cannot be undone
- No objective function (SSE) 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

Adapted from:
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Han, Kamber - Data Mining: Concepts and Techniques

Density-Based Clustering Methods

- Clustering based on density (local cluster criterion), such as density-connected points
- Major features:
  - Discover clusters of arbitrary shape
  - Handle noise
  - One scan
  - Need density parameters as termination condition
- Several interesting studies:
  - DBSCAN: Ester, et al. (KDD'96)
  - OPTICS: Ankerst, et al (SIGMOD'99).
  - DENCLUE: Hinneburg & D. Keim (KDD'98)
  - CLIQUE: Agrawal, et al. (SIGMOD'98)

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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 more than a specified number of points (MinPts) within Eps
    - These are points that are at the interior of a cluster
  - A border point has fewer than MinPts within Eps, 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.

Adapted from:
Tan,Steinbach, Kumar - Introduction to Data Mining
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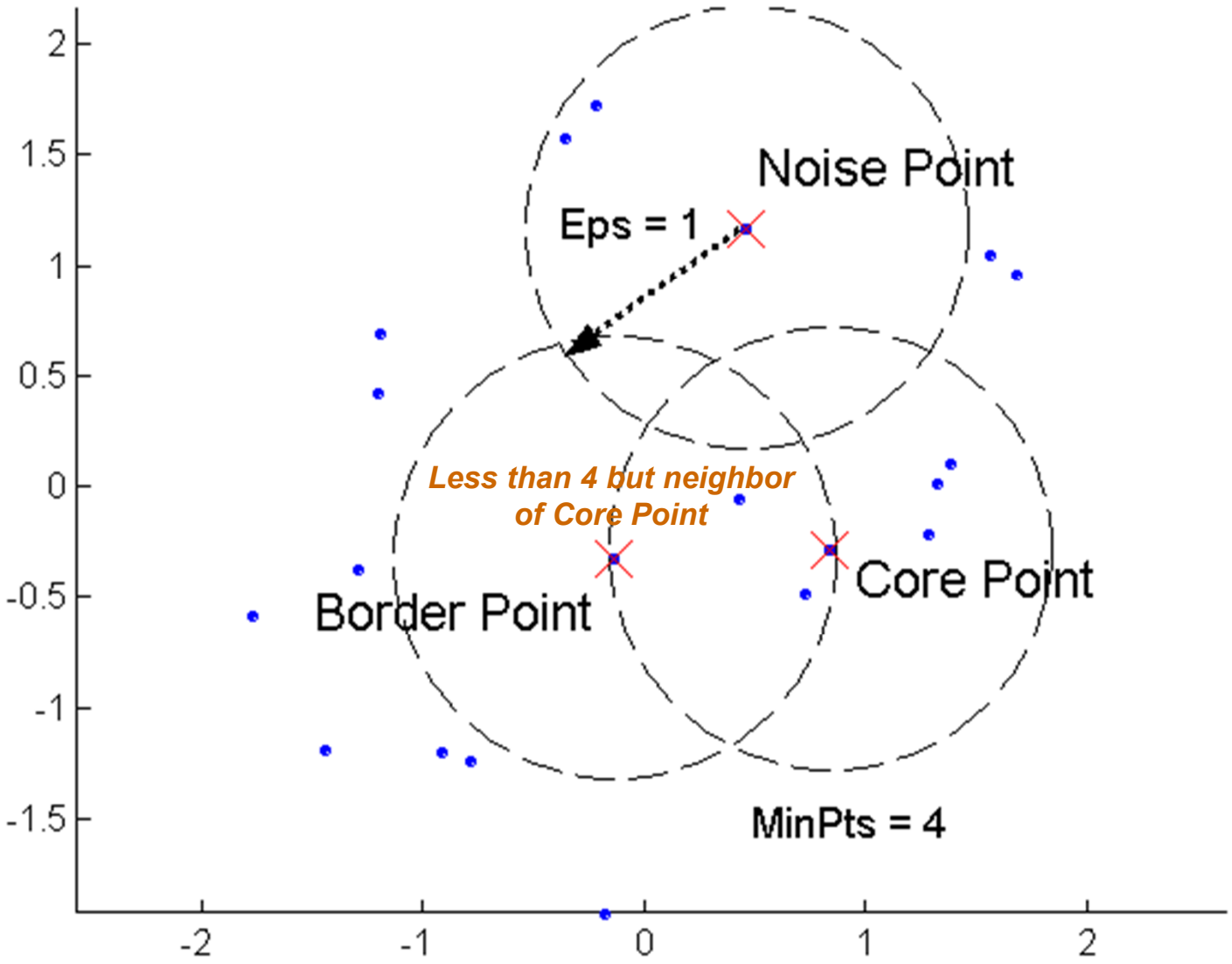
Core, Border, and Noise Points



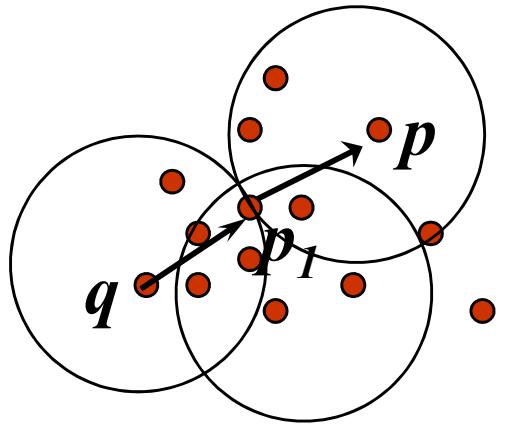
Adapted from:

Tan,Steinbach, Kumar - Introduction to Data Mining

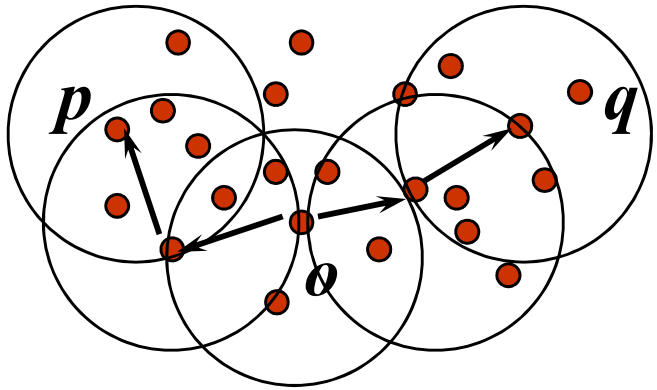
Han, Kamber - Data Mining: Concepts and Techniques

Density-Based Clustering Concepts

- Density-reachable:
  - A point *p* is density-reachable from a point *q* wrt. *Eps*, *MinPts* if there is a chain of points $p_1, \ldots, p_n$, $p_1 = q$, $p_n = p$ such that p_{i+1} is directly density-reachable from p_i



- Density-connected
  - A point *p* is density-connected to a point *q* wrt. *Eps*, *MinPts* if there is a point *o* such that both, *p* and *q* are density-reachable from *o* wrt. *Eps* and *MinPts*.



Adapted from:
Tan,Steinbach, Kumar - Introduction to Data Mining
Han, Kamber - Data Mining: Concepts and Techniques

DBSCAN Algorithm

- Arbitrary select a point ***p***
- Retrieve all points density-reachable from ***p*** wrt ***Eps*** and ***MinPts***.
- If ***p*** is a core point, a cluster is formed.
- If ***p*** is a border point, no points are density-reachable from ***p*** and DBSCAN visits the next point of the database.
- Continue the process until all of the points have been processed.

1. ***Label all points as core, border, or noise***
2. ***Eliminate noise points***
3. ***Put an edge***
4. ***Make each group of connected cores***
5. ***Border points***

Adapted from:
Tan,Steinbach, Kumar - Introduction to Data Mining
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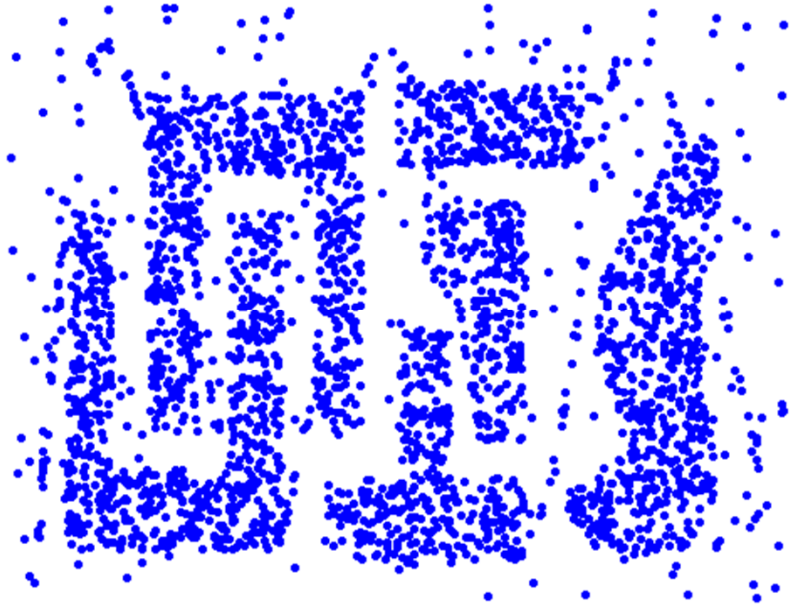
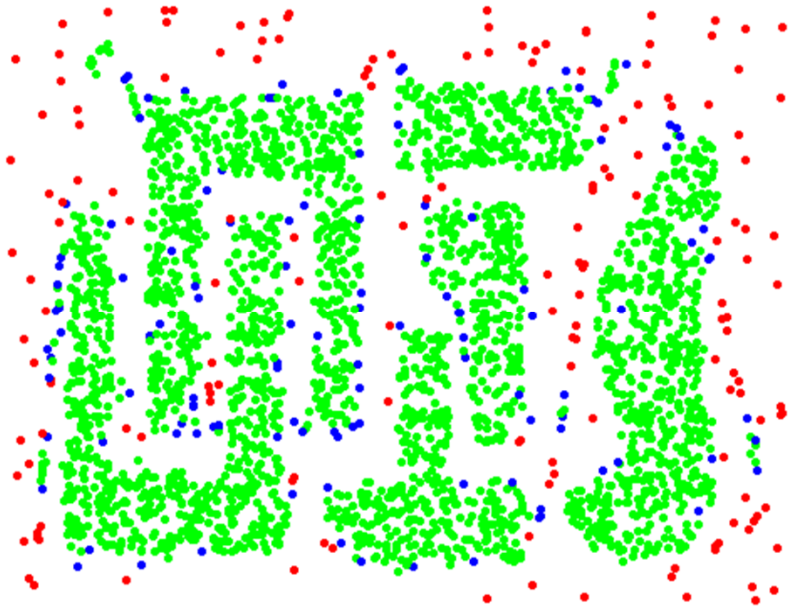
DBSCAN: Core, Border and Noise Points



Original Points



Point types: core, border and noise

Eps = 10, MinPts = 4

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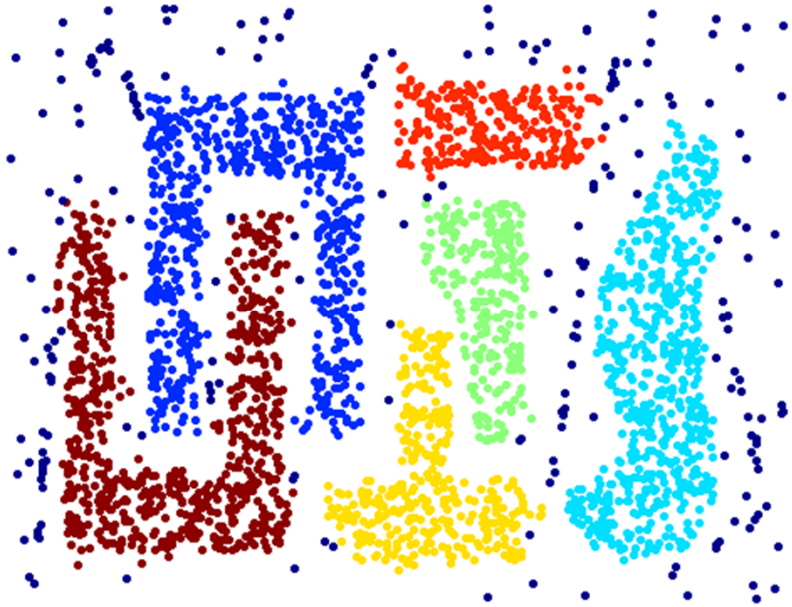
When DBSCAN Works Well

Original Points



Clusters

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

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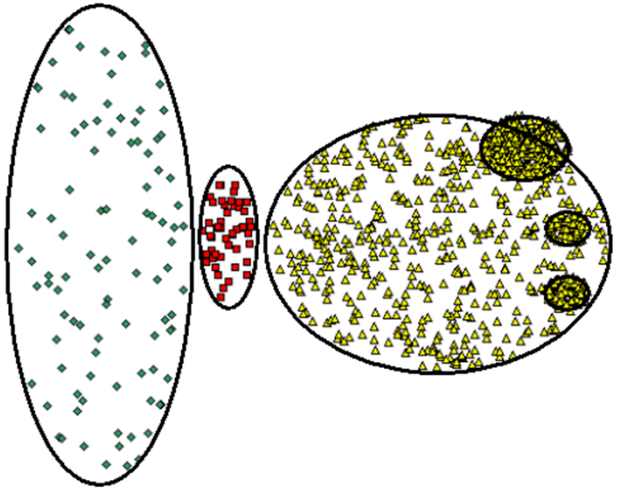
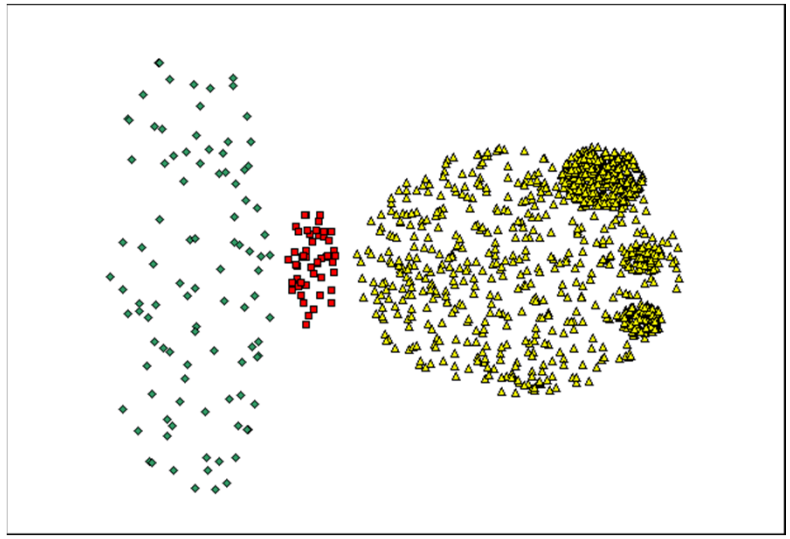
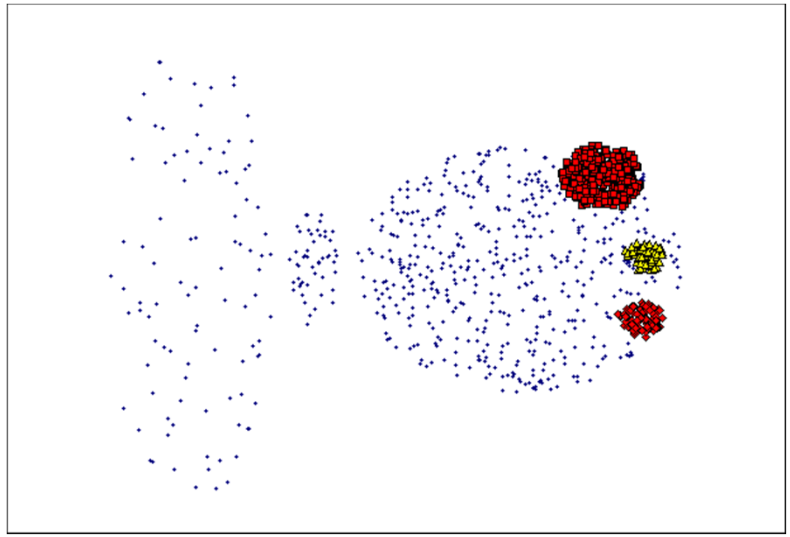
When DBSCAN Does NOT Work Well



Original Points





- **Varying densities**
- **High-dimensional data**
- **Eps = ?, MinPts = ?**

Adapted from:
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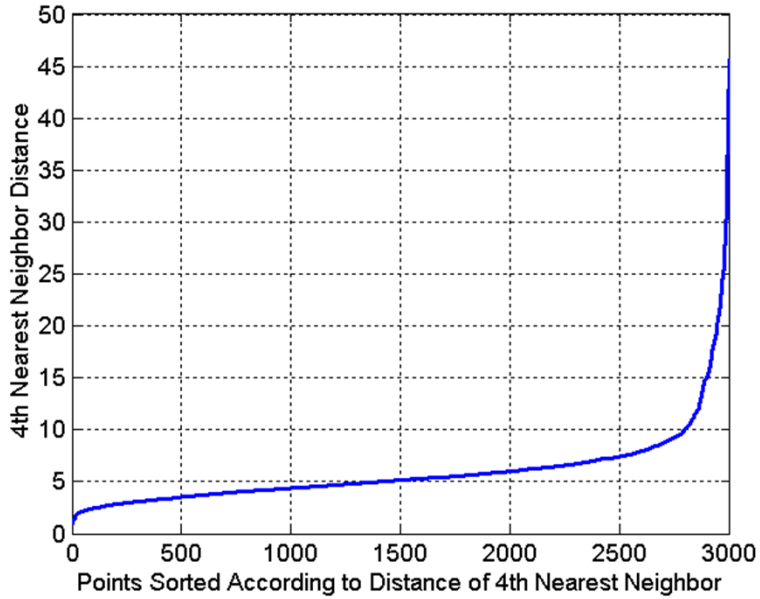
DBSCAN: Determining Eps and MinPts

- Idea: Look at the behavior of the distance from a point to its k^{th} nearest neighbor (k-dist)
- For points that belong to some cluster, the value of k-dist will be small since they have many neighboring points.
- For points that are not in a cluster, such as noise points, the k-dist will be relatively large.
- Thus, compute the k-dist for all the data points → sort them in increasing order → plot the sorted value → find a sharp change for Eps

  → take the value of k as MinPts



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Cluster Validity

- For supervised classification we have a variety of measures to evaluate how good our model is
  - Accuracy, precision, recall
- For cluster analysis, the analogous question is how to evaluate the "goodness" of the resulting clusters?
- But "clusters are in the eye of the beholder"!
- Then why do we want to evaluate them?
  - To avoid finding patterns in noise
  - To compare clustering algorithms
  - To compare two sets of clusters
  - To compare two clusters

Adapted from:
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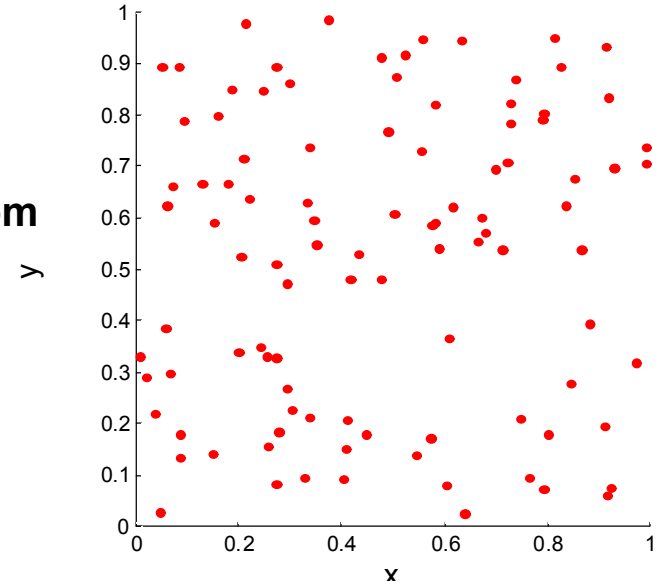
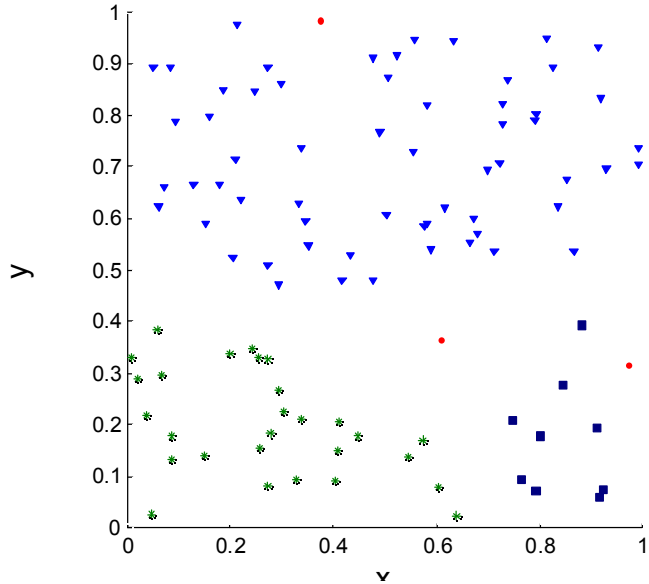
Clusters found in Random Data

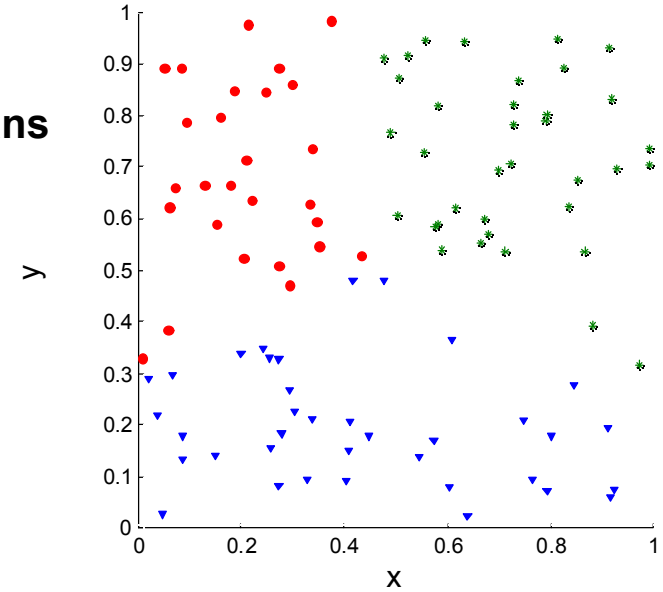
Random Points



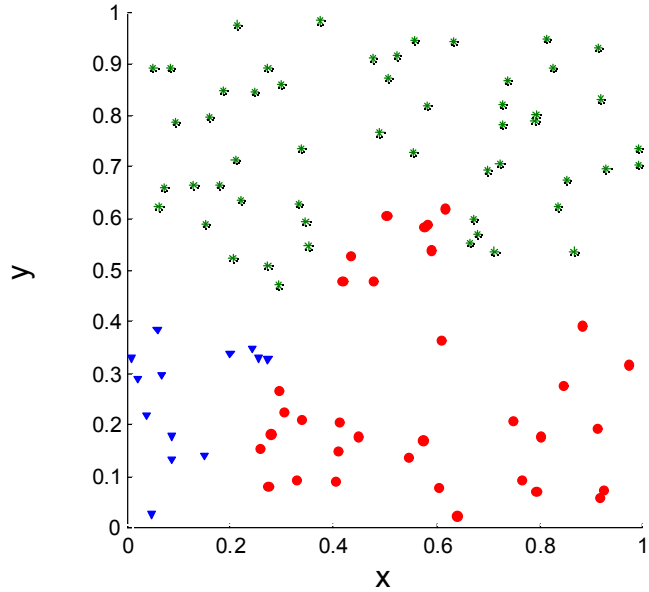
DBSCAN



K-means



Complete Link



Adap

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Different Aspects of Cluster Validation

1. Determining the clustering tendency of a set of data, i.e., distinguishing whether non-random structure actually exists in the data.
2. Comparing the results of a cluster analysis to externally known results, e.g., to externally given class labels.
3. Evaluating how well the results of a cluster analysis fit the data *without* reference to external information.
   - Use only the data
4. Comparing the results of two different sets of cluster analyses to determine which is better.
5. Determining the 'correct' number of clusters.

For 2, 3, and 4, we can further distinguish whether we want to evaluate the entire clustering or just individual clusters.

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Measures of Cluster Validity

- Numerical measures that are applied to judge various aspects of cluster validity, are classified into the following three types.
  - External Index: Used to measure the extent to which cluster labels match externally supplied class labels.
    - e.g.: Entropy
  - Internal Index: Used to measure the goodness of a clustering structure *without* respect to external information.
    - e.g.: Sum of Squared Error (SSE)
  - Relative Index: Used to compare two different clusterings or clusters.
    - Often an external or internal index is used for this function, e.g., SSE or entropy

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Measuring Cluster Validity Via Correlation

- Two matrices:
  - Proximity (similarity) Matrix
  - "Incidence" Matrix
    - One row and one column for each data point
    - An entry is 1 if the associated pair of points belong to the same cluster
    - An entry is 0 if the associated pair of points belongs to different clusters
- Compute the correlation between the two matrices
- High correlation indicates that points that belong to the same cluster are close to each other.
- Not a good measure for some density or contiguity based clusters.

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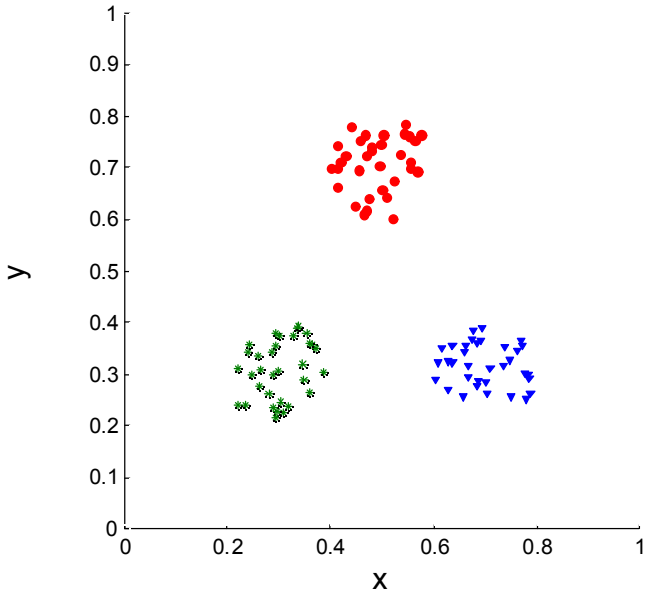
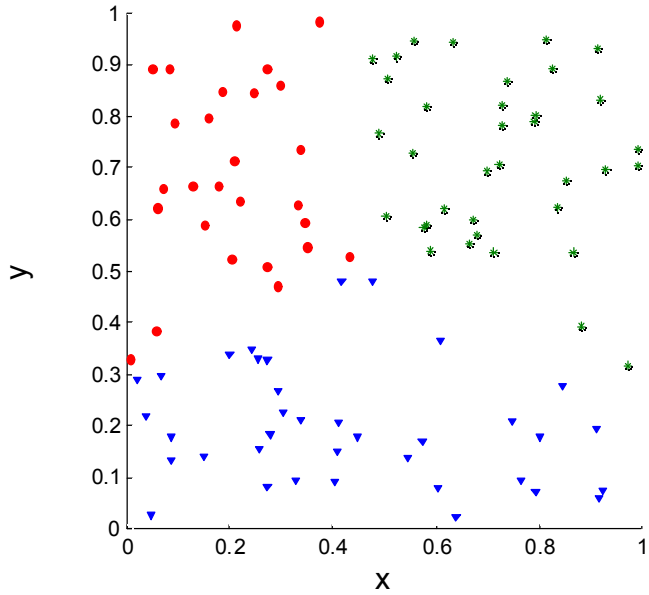
Measuring Cluster Validity Via Correlation

- Correlation of incidence and proximity matrices for the K-means clusterings of the following two data sets.



Corr = -0.9235



Corr = -0.5810

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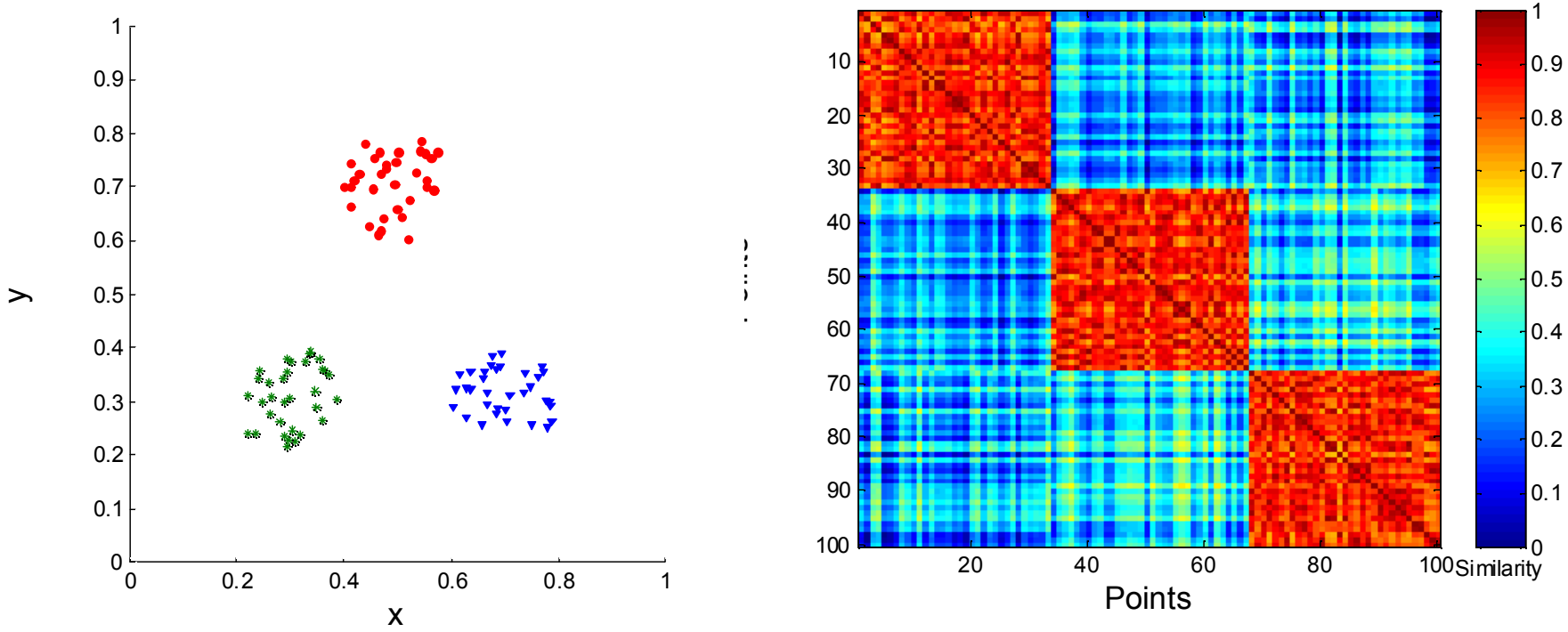
Using Similarity Matrix for Cluster Validation

- Order the similarity matrix with respect to cluster labels and inspect visually.



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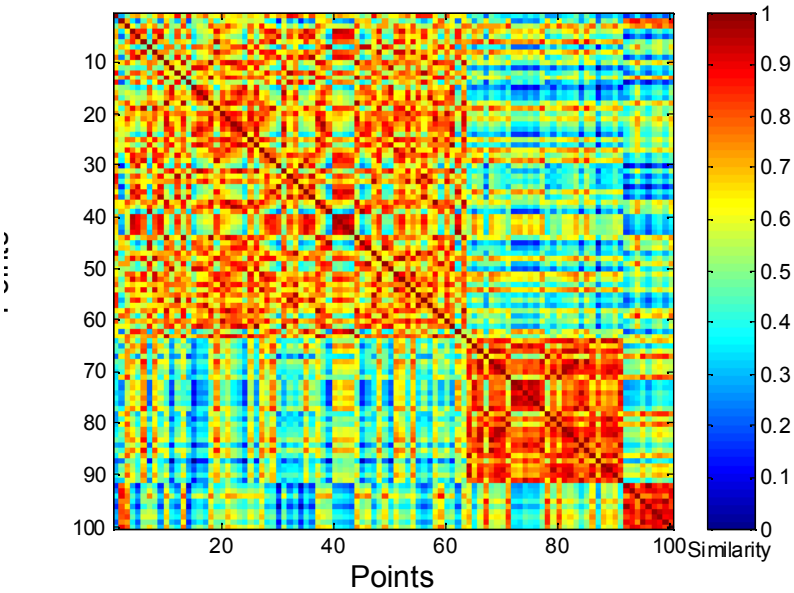
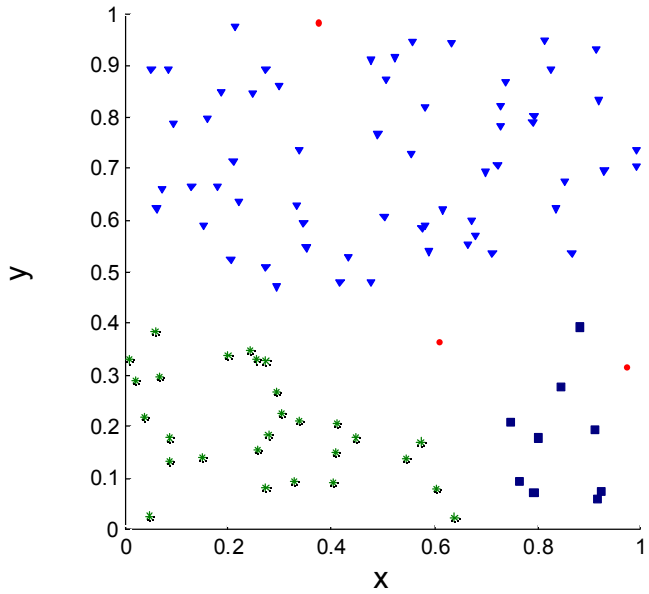
Using Similarity Matrix for Cluster Validation

- Clusters in random data are not so crisp





DBSCAN

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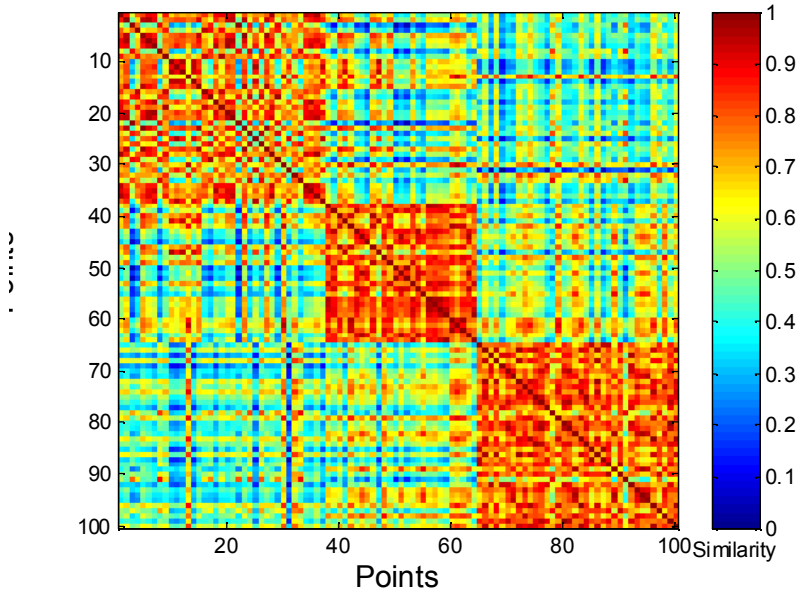
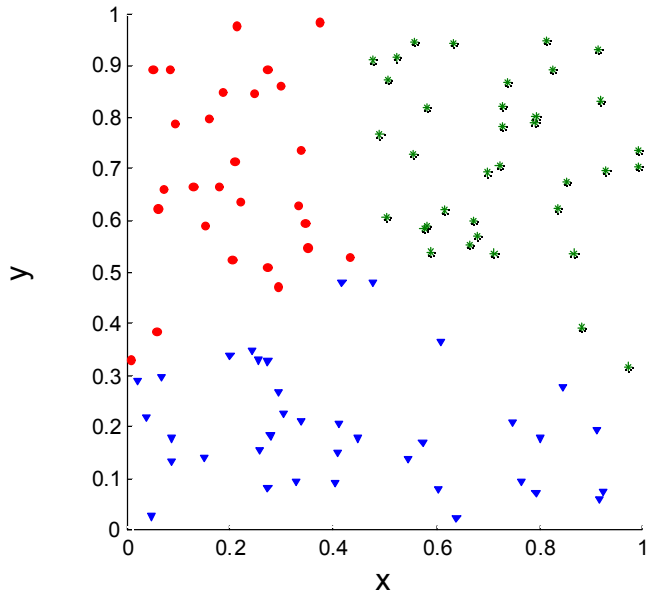
Using Similarity Matrix for Cluster Validation

- Clusters in random data are not so crisp





K-means

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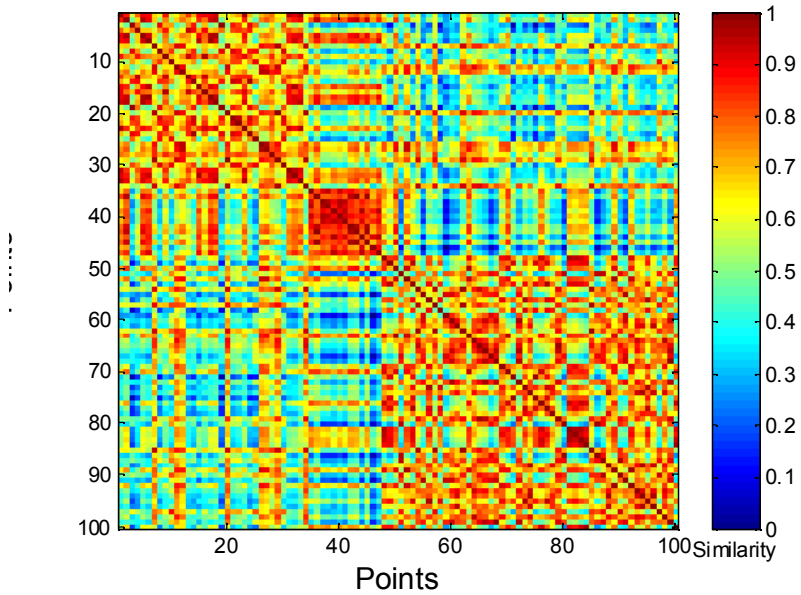
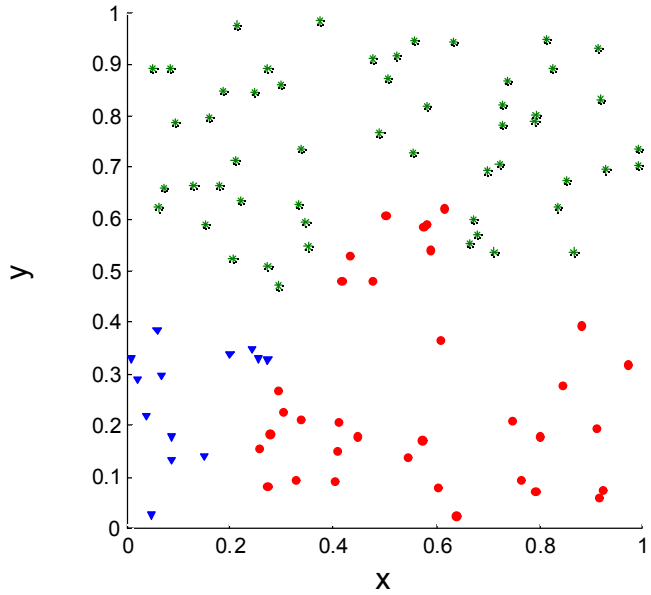
Using Similarity Matrix for Cluster Validation

- Clusters in random data are not so crisp





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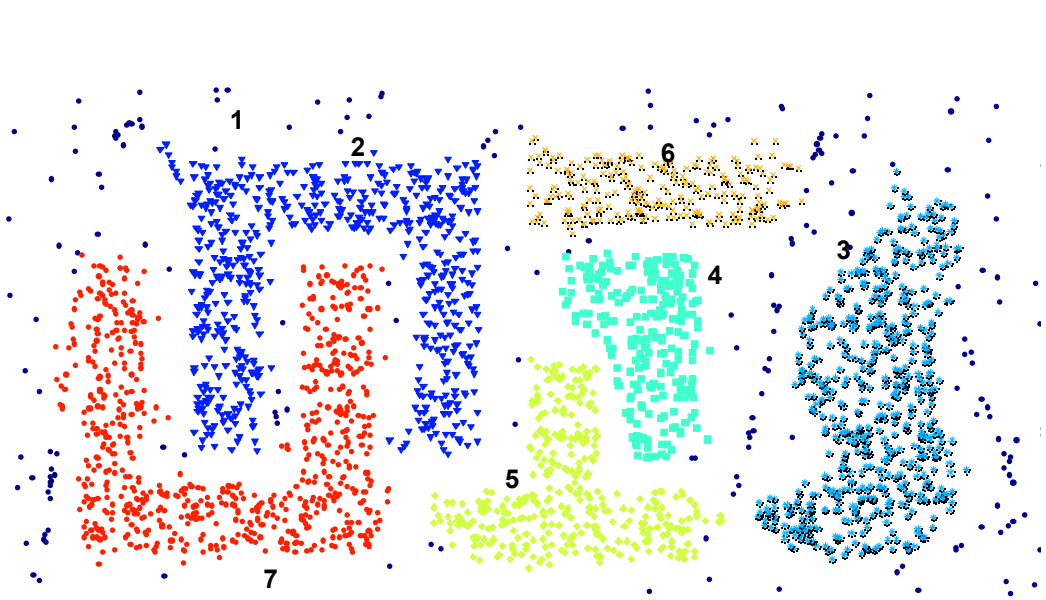
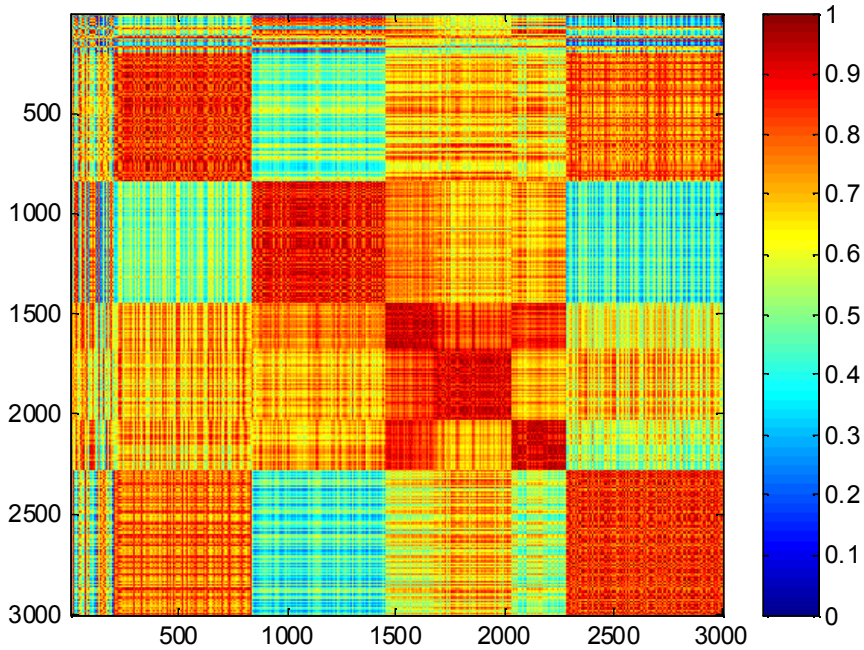
Using Similarity Matrix for Cluster Validation





DBSCAN

Adapted from:
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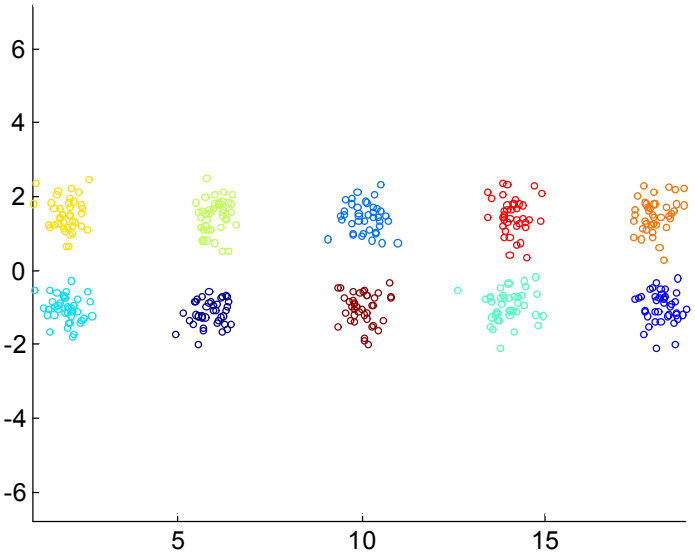
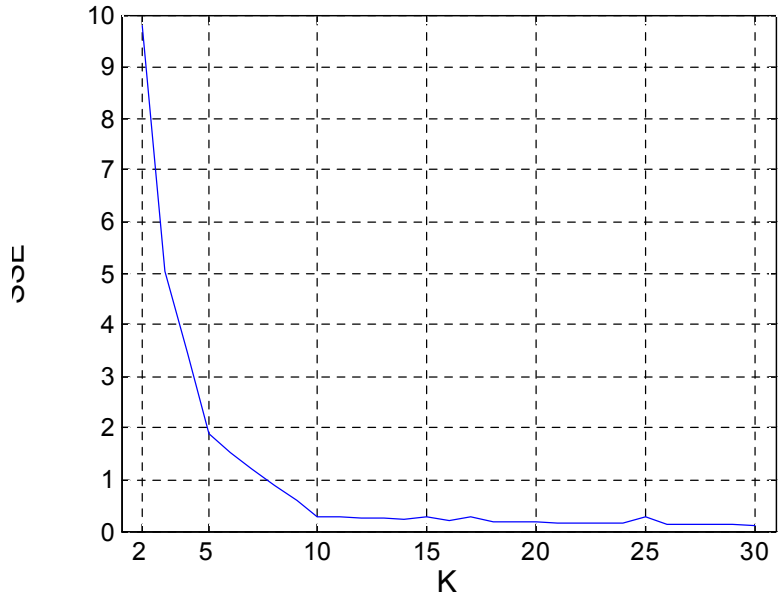
Han, Kamber - Data Mining: Concepts and Techniques

Internal Measures: SSE

- Clusters in more complicated figures aren't well separated
- Internal Index: Used to measure the goodness of a clustering structure without respect to external information
  - SSE
- SSE is good for comparing two clusterings or two clusters (average SSE).
- Can also be used to estimate the number of clusters





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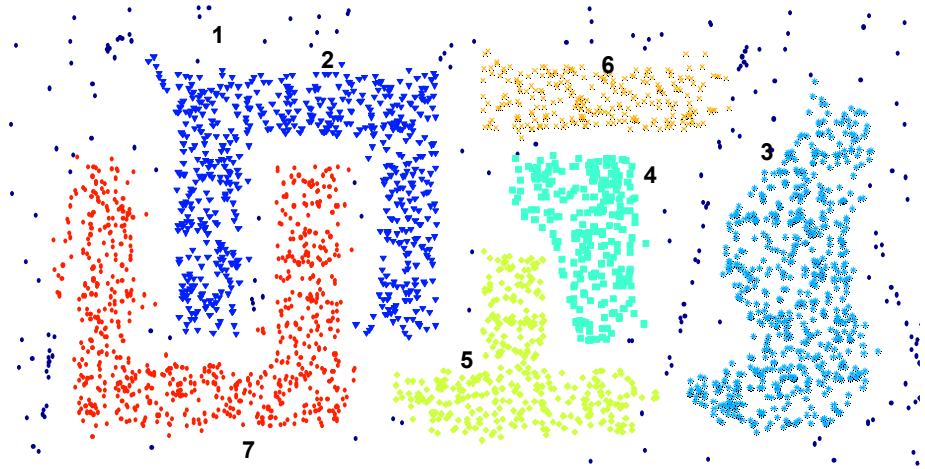
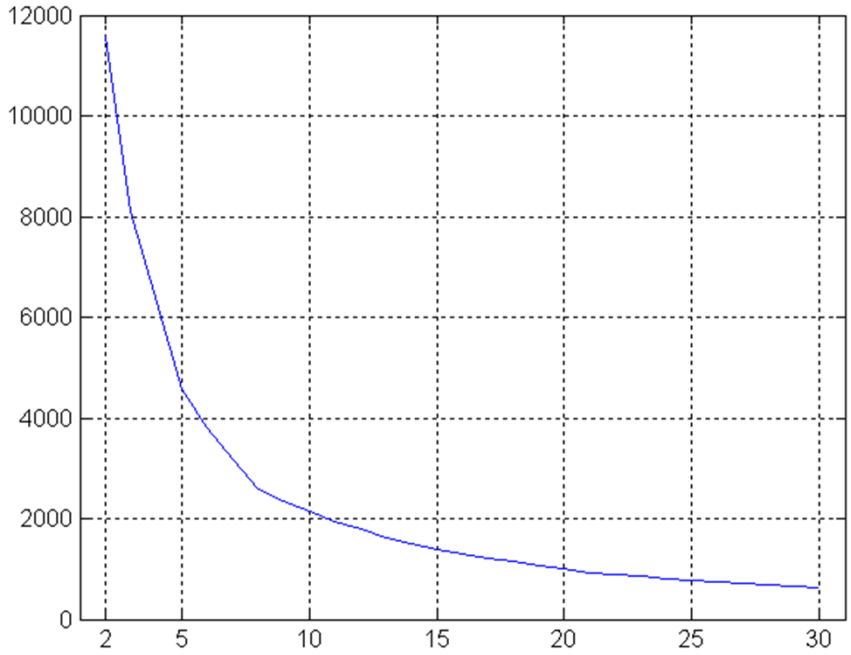
Internal Measures: SSE

- SSE curve for a more complicated data set





SSE of clusters found using K-means

Adapted from:
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Internal Measures: Cohesion and Separation

- Cluster Cohesion: Measures how closely related are objects in a cluster
  - Example: SSE
- Cluster Separation: Measure how distinct or well-separated a cluster is from other clusters
- Example: Squared Error
  - Cohesion is measured by the within cluster sum of squares (SSE)

$$WSS = \sum_{i} \sum_{x \in C_i} (x - m_i)^2$$

  - Separation is measured by the between cluster sum of squares

$$BSS = \sum_{i} |C_i| (m - m_i)^2$$

    - Where $|C_i|$ is the size of cluster i

Adapted from:
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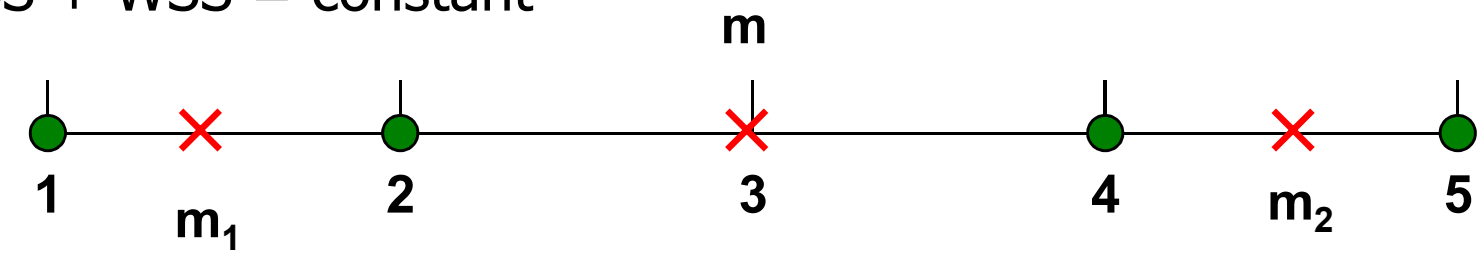
Internal Measures: Cohesion and Separation

- Example: SSE
  - BSS + WSS = constant



K=1 cluster:

$$WSS = (1-3)^2 + (2-3)^2 + (4-3)^2 + (5-3)^2 = 10$$

$$BSS = 4 \times (3-3)^2 = 0$$

$$Total = 10 + 0 = 10$$

K=2 clusters:

$$WSS = (1-1.5)^2 + (2-1.5)^2 + (4-4.5)^2 + (5-4.5)^2 = 1$$

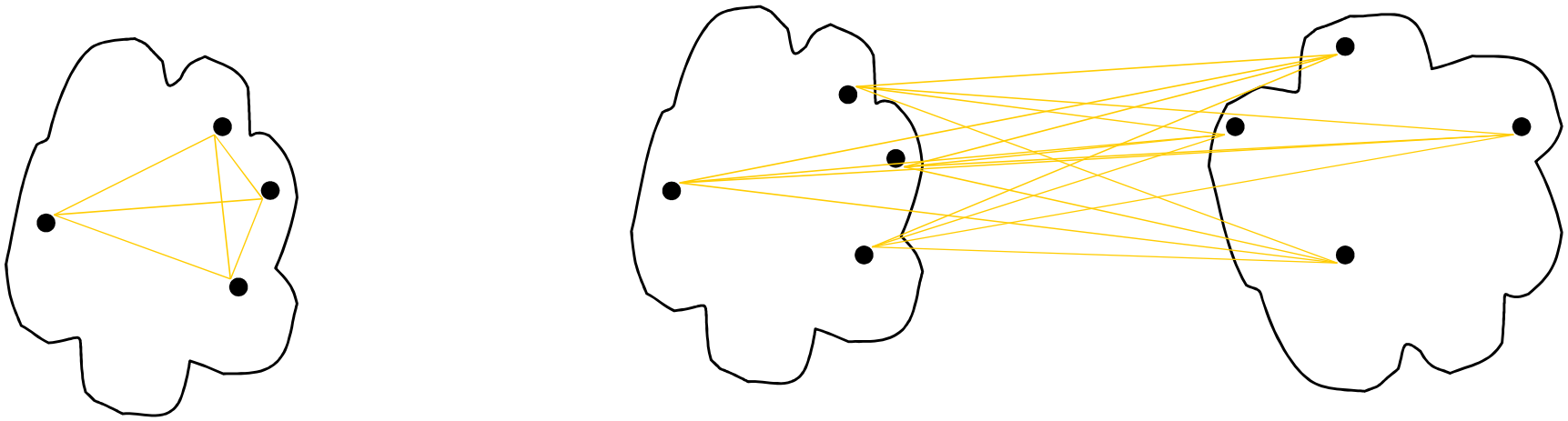
$$BSS = 2 \times (3-1.5)^2 + 2 \times (4.5-3)^2 = 9$$

$$Total = 1 + 9 = 10$$

Adapted from:
Tan,Steinbach, Kumar - Introduction to Data Mining
Han, Kamber - Data Mining: Concepts and Techniques

Internal Measures: Cohesion and Separation

- A proximity graph based approach can also be used for cohesion and separation.
  - Cluster cohesion is the sum of the weight of all links within a cluster.
  - Cluster separation is the sum of the weights between nodes in the cluster and nodes outside the cluster.



cohesion separation

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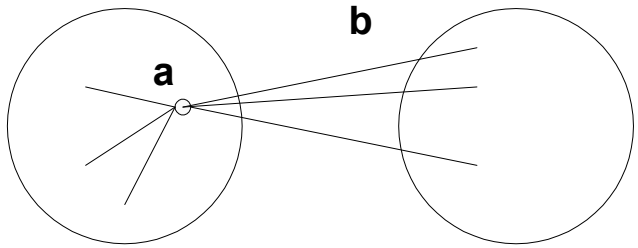
Internal Measures: Silhouette Coefficient

- Silhouette Coefficient combine ideas of both cohesion and separation, but for individual points, as well as clusters and clusterings

- For an individual point, *i*
  - Calculate ***a*** = average distance of *i* to the points in its cluster
  - Calculate ***b*** = min (average distance of *i* to points in another cluster)
  - The silhouette coefficient for a point is then given by

    $s = 1 - a/b$ if $a < b$, (or $s = b/a - 1$ if $a \geq b$, not the usual case)

  - Typically between 0 and 1.
  - The closer to 1 the better.



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External Measures of Cluster Validity: Entropy and Purity

Table 5.9. K-means Clustering Results for LA Document Data Set

Cluster	Entertainment	Financial	Foreign	Metro	National	Sports	Entropy	Purity
1	3	5	40	506	96	27	1.2270	0.7474
2	4	7	280	29	39	2	1.1472	0.7756
3	1	1	1	7	4	671	0.1813	0.9796
4	10	162	3	119	73	2	1.7487	0.4390
5	331	22	5	70	13	23	1.3976	0.7134
6	5	358	12	212	48	13	1.5523	0.5525
Total	354	555	341	943	273	738	1.1450	0.7203

entropy For each cluster, the class distribution of the data is calculated first, i.e., for cluster j we compute p_{ij}, the 'probability' that a member of cluster j belongs to class i as follows: $p_{ij} = m_{ij}/m_j$, where m_j is the number of values in cluster j and m_{ij} is the number of values of class i in cluster j. Then using this class distribution, the entropy of each cluster j is calculated using the standard formula $e_j = \sum_{i=1}^{L} p_{ij} \log_2 p_{ij}$, where the L is the number of classes. The total entropy for a set of clusters is calculated as the sum of the entropies of each cluster weighted by the size of each cluster, i.e., $e = \sum_{i=1}^{K} \frac{m_i}{m} e_j$, where m_j is the size of cluster j, K is the number of clusters, and m is the total number of data points.

purity Using the terminology derived for entropy, the purity of cluster j, is given by $purity_j = \max p_{ij}$ and the overall purity of a clustering by $purity = \sum_{i=1}^{K} \frac{m_i}{m} purity_j$.

Adapted from:
Tan,Steinbach, Kumar - Introduction to Data Mining
Han, Kamber - Data Mining: Concepts and Techniques

Final Comment on Cluster Validity

"The validation of clustering structures is the most difficult and frustrating part of cluster analysis. Without a strong effort in this direction, cluster analysis will remain a black art accessible only to those true believers who have experience and great courage."

Algorithms for Clustering Data, Jain and Dubes