# Clustering fundamentals

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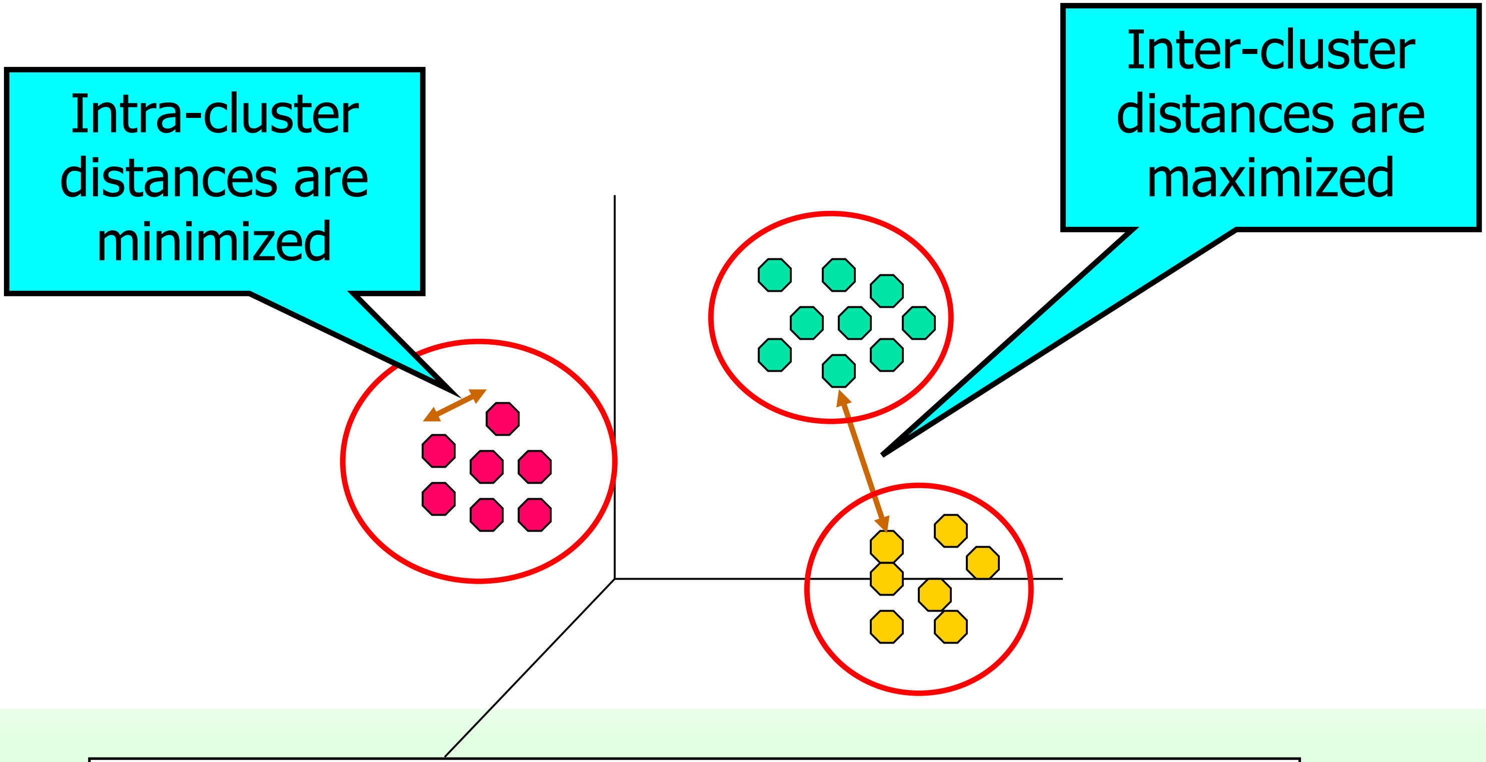
# What is Cluster Analysis?

- 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



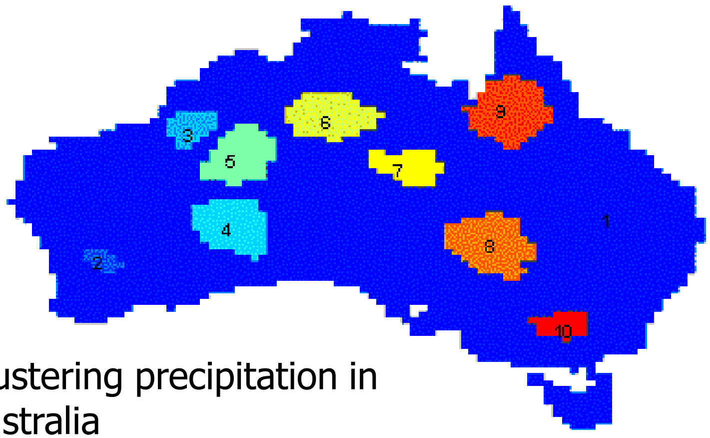

From: Tan,Steinbach, Kumar, Introduction to Data Mining, McGraw Hill 2006

# 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

| | *Discovered Clusters* | *Industry Group* |
|---|---|---|
| **1** | Applied-Matl-DOWN,Bay-Network-Down,3-COM-DOWN, Cabletron-Sys-DOWN,CISCO-DOWN,HP-DOWN, DSC-Comm-DOWN,INTEL-DOWN,LSI-Logic-DOWN, Micron-Tech-DOWN,Texas-Inst-Down,Tellabs-Inc-Down, Natl-Semiconduct-DOWN,Oracl-DOWN,SGI-DOWN, Sun-DOWN | Technology1-DOWN |
| **2** | Apple-Comp-DOWN,Autodesk-DOWN,DEC-DOWN, ADV-Micro-Device-DOWN,Andrew-Corp-DOWN, Computer-Assoc-DOWN,Circuit-City-DOWN, Compaq-DOWN, EMC-Corp-DOWN, Gen-Inst-DOWN, Motorola-DOWN,Microsoft-DOWN,Scientific-Atl-DOWN | Technology2-DOWN |
| **3** | Fannie-Mae-DOWN,Fed-Home-Loan-DOWN, MBNA-Corp-DOWN,Morgan-Stanley-DOWN | Financial-DOWN |
| **4** | Baker-Hughes-UP,Dresser-Inds-UP,Halliburton-HLD-UP, Louisiana-Land-UP,Phillips-Petro-UP,Unocal-UP, Schlumberger-UP | Oil-UP |

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




Clustering precipitation in Australia

From: Tan,Steinbach, Kumar, Introduction to Data Mining, McGraw Hill 2006

# Notion of a Cluster can be Ambiguous

How many clusters?

Six Clusters

Two Clusters

Four Clusters

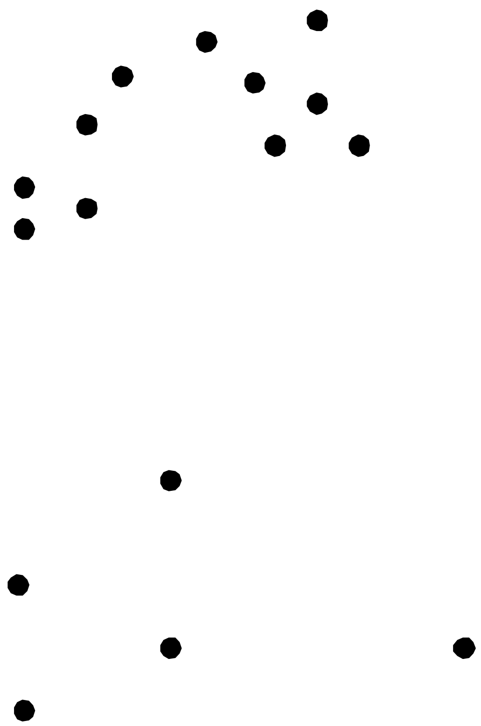
# Types of Clusterings

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

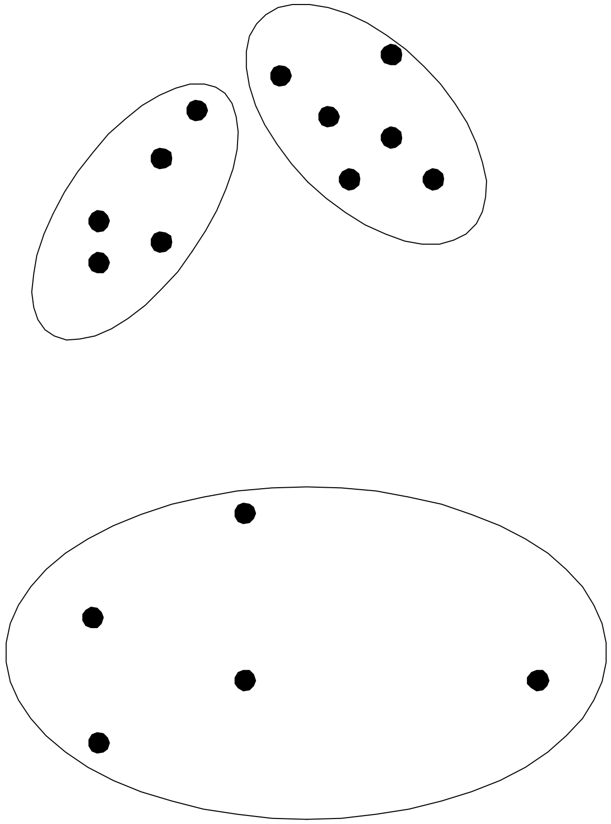


From: Tan,Steinbach, Kumar, Introduction to Data Mining, McGraw Hill 2006

# Partitional Clustering



Original Points

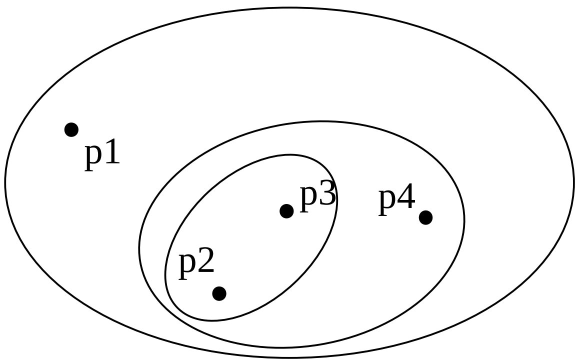


A Partitional Clustering

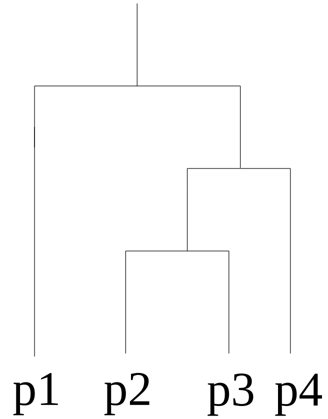


From: Tan,Steinbach, Kumar, Introduction to Data Mining, McGraw Hill 2006

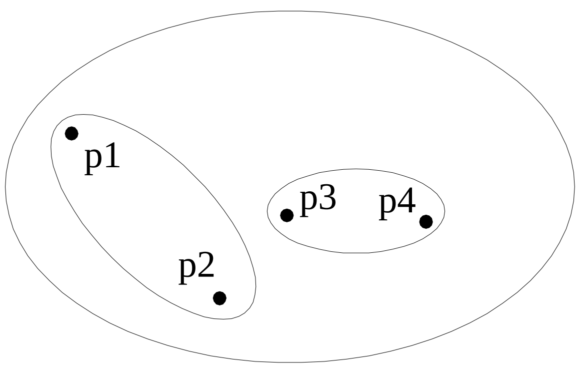
# Hierarchical Clustering



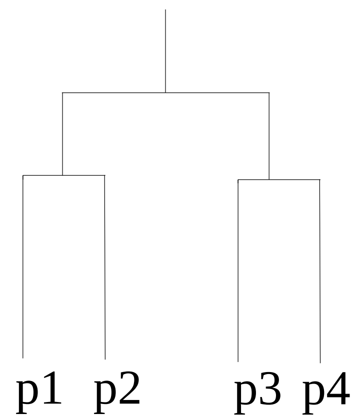

Traditional Hierarchical Clustering




Traditional Dendrogram




Non-traditional Hierarchical Clustering




Non-traditional Dendrogram

From: Tan,Steinbach, Kumar, Introduction to Data Mining, McGraw Hill 2006

# Other Distinctions Between Sets of Clusters

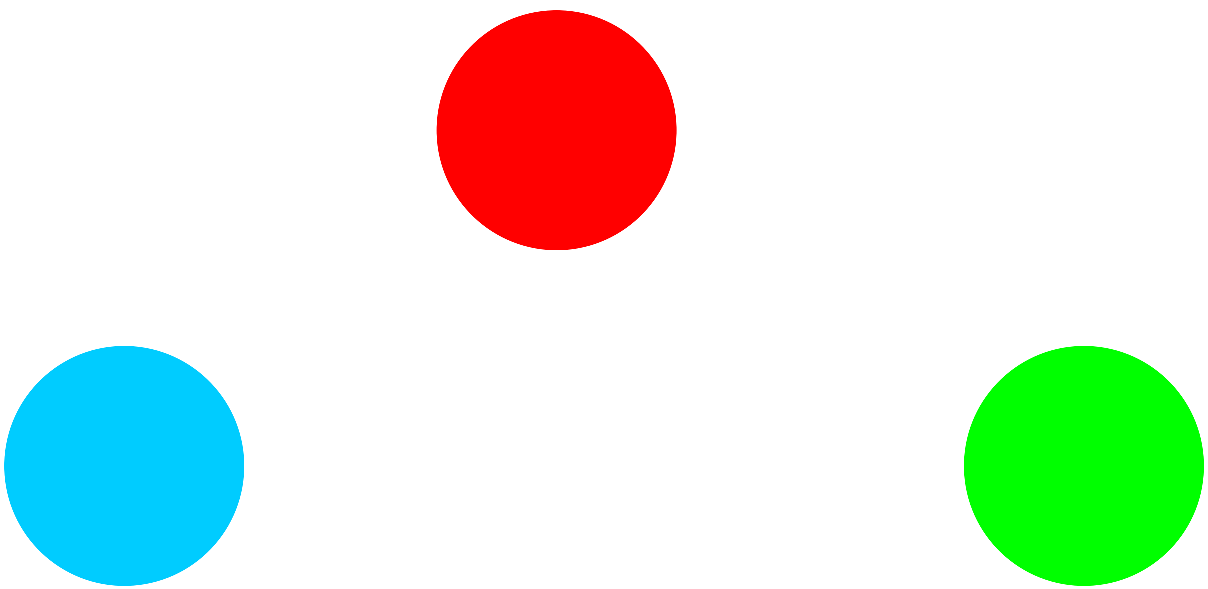
- Exclusive versus non-exclusive
  - In non-exclusive clustering, points may belong to multiple clusters.
- Fuzzy versus non-fuzzy
  - In fuzzy clustering, a point belongs to every cluster with some weight between 0 and 1
  - Weights must sum to 1
  - Probabilistic clustering has similar characteristics
- 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

# Types of Clusters

- Well-separated clusters
- Center-based clusters
- Contiguous clusters
- Density-based clusters
- Property or Conceptual
- Described by an Objective Function

# Types of Clusters: Well Separated

- Well-Separated Clusters:
  - A cluster is a set of points such that any point in a cluster is closer (or more similar) to every other point in the cluster than to any point not in the cluster.

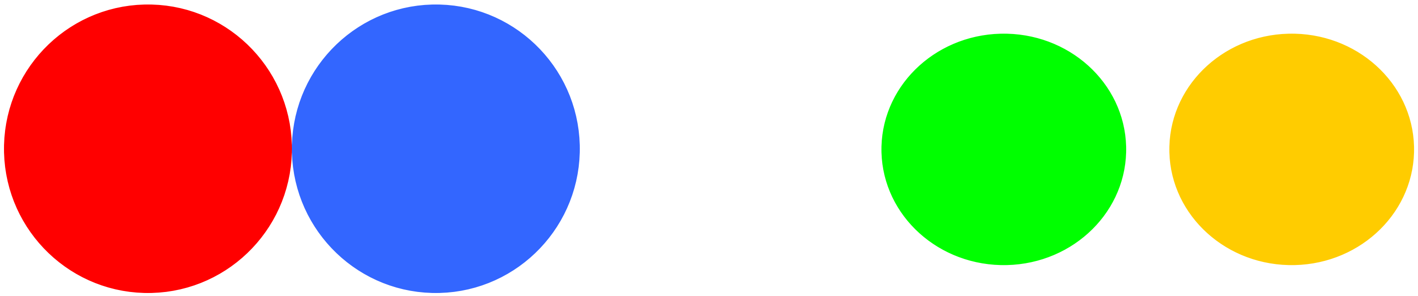


3 well-separated clusters

From: Tan,Steinbach, Kumar, Introduction to Data Mining, McGraw Hill 2006

# Types of Clusters: Center-Based

- Center-based
  - A cluster is a set of objects such that an object in a cluster is closer (more similar) to the "center" of a cluster, than to the center of any other cluster
  - The center of a cluster is often a centroid, the average of all the points in the cluster, or a medoid, the most "representative" point of a cluster

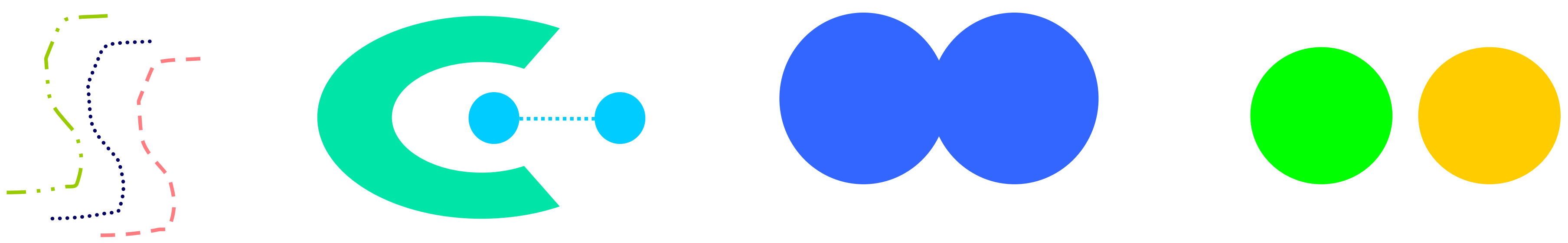


4 center-based clusters

From: Tan,Steinbach, Kumar, Introduction to Data Mining, McGraw Hill 2006

# Types of Clusters: Contiguity-Based

- Contiguous Cluster (Nearest neighbor or Transitive)
  - A cluster is a set of points such that a point in a cluster is closer (or more similar) to one or more other points in the cluster than to any point not in the cluster.

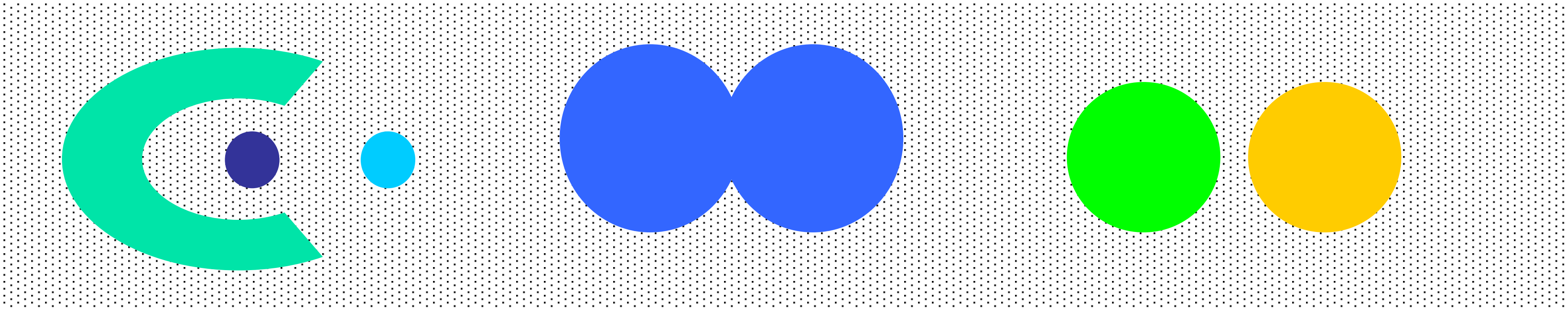


8 contiguous clusters

From: Tan,Steinbach, Kumar, Introduction to Data Mining, McGraw Hill 2006

# Types of Clusters: Density-Based

- Density-based
  - A cluster is a dense region of points, which is separated by low-density regions, from other regions of high density.
  - Used when the clusters are irregular or intertwined, and when noise and outliers are present.



6 density-based clusters

From: Tan,Steinbach, Kumar, Introduction to Data Mining, McGraw Hill 2006

# Types of Clusters: Conceptual Clusters

- Shared Property or Conceptual Clusters
  - Finds clusters that share some common property or represent a particular concept.

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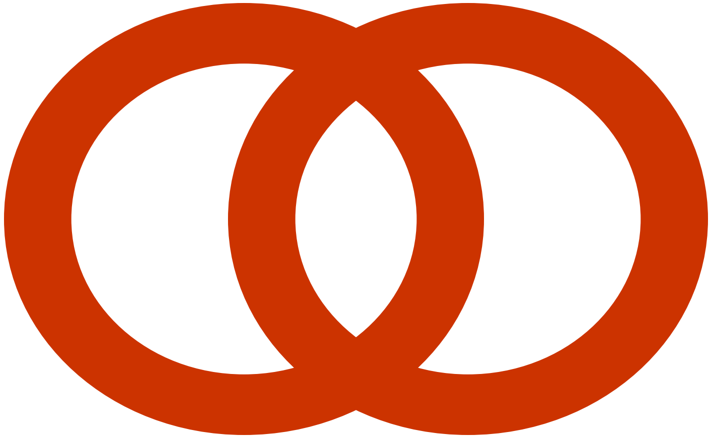


2 Overlapping Circles

From: Tan,Steinbach, Kumar, Introduction to Data Mining, McGraw Hill 2006

# Clustering Algorithms

- K-means and its variants
- Hierarchical clustering
- Density-based clustering



From: Tan,Steinbach, Kumar, Introduction to Data Mining, McGraw Hill 2006

# 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

```
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
```

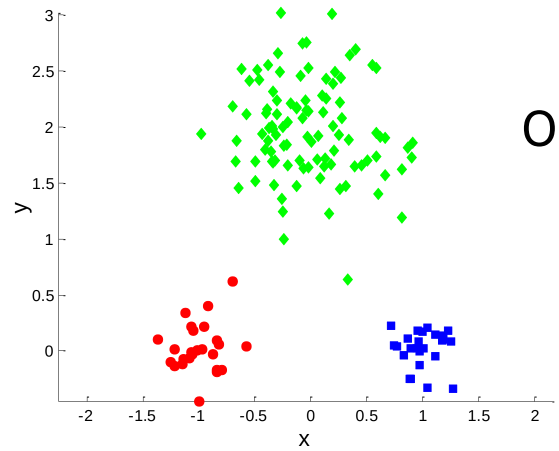
From: Tan,Steinbach, Kumar, Introduction to Data Mining, McGraw Hill 2006

# K-means Clustering – Details

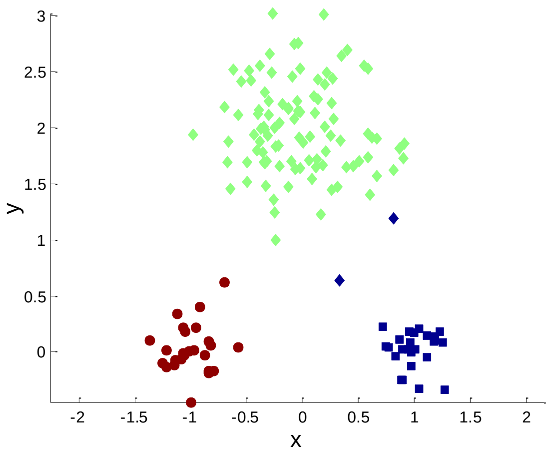
- Initial centroids are often chosen randomly.
  - Clusters produced vary from one run to another.
- The centroid is (typically) the mean of the points in the cluster.
- ‘Closeness’ is measured by Euclidean distance, cosine similarity, correlation, etc.
- K-means will converge for common similarity measures 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’
- Complexity is O( n * K * I * d )
  - n = number of points, K = number of clusters,
    I = number of iterations, d = number of attributes

From: Tan,Steinbach, Kumar, Introduction to Data Mining, McGraw Hill 2006

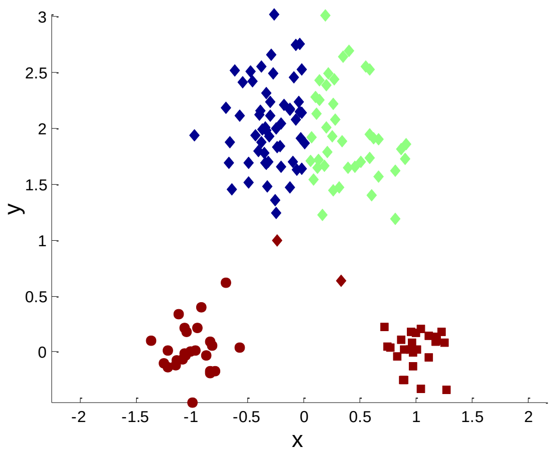
# Two different K-means Clusterings




Original Points



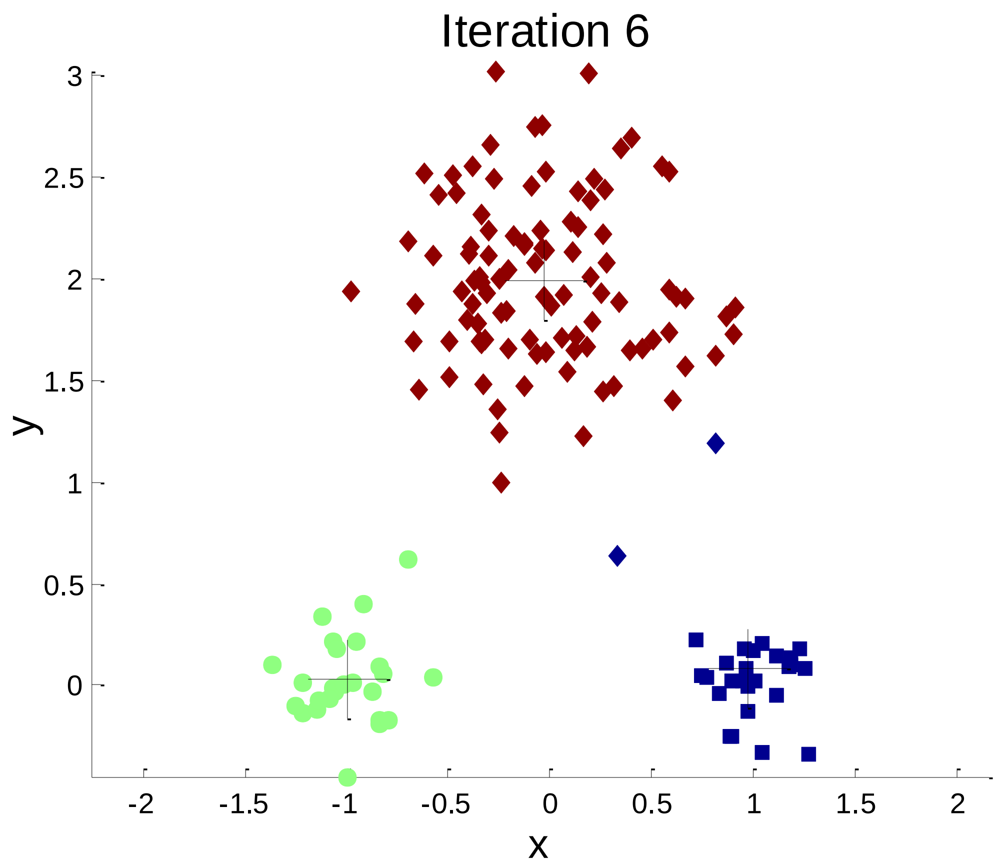

Optimal Clustering




Sub-optimal Clustering

From: Tan,Steinbach, Kumar, Introduction to Data Mining, McGraw Hill 2006

# Importance of Choosing Initial Centroids

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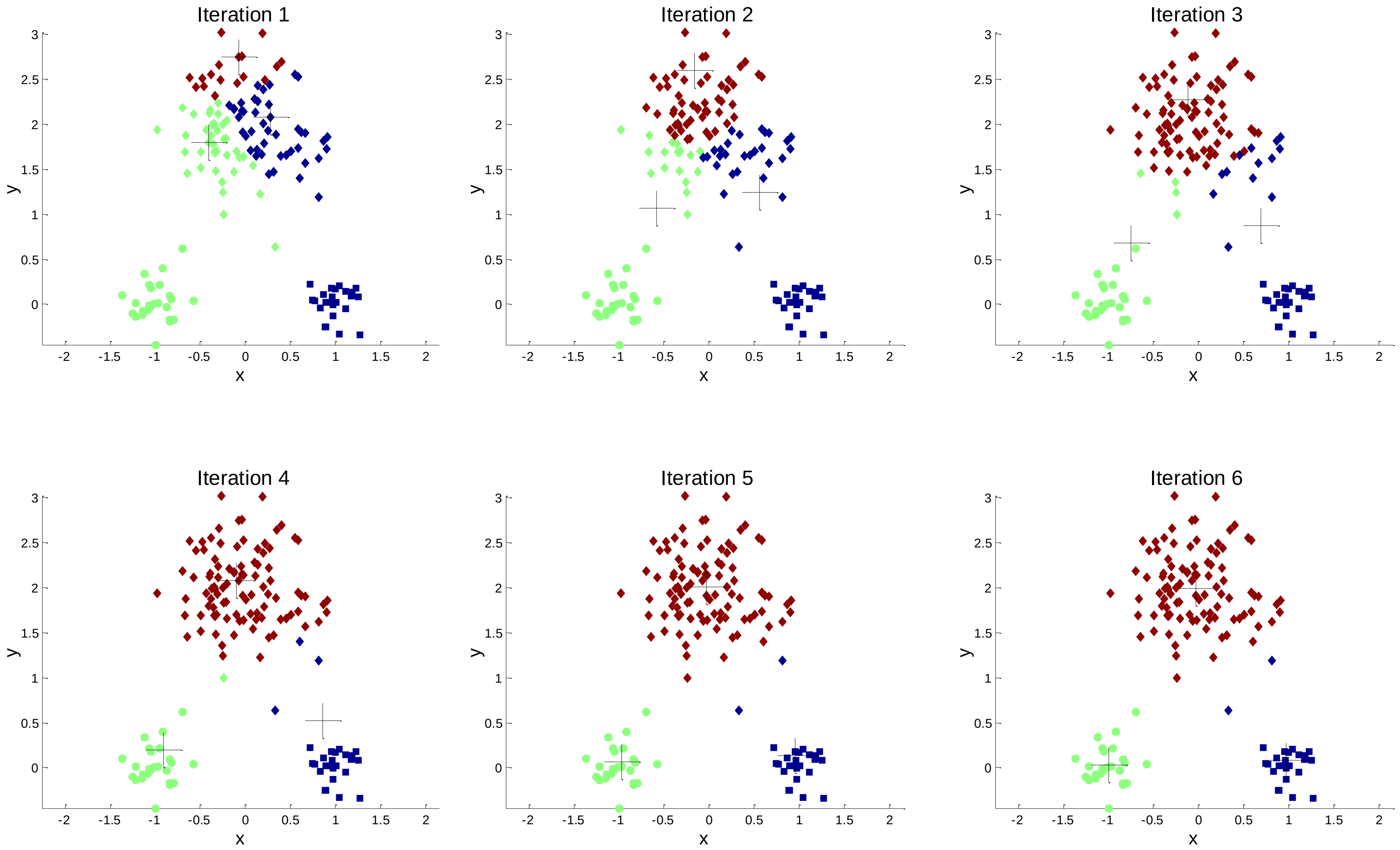


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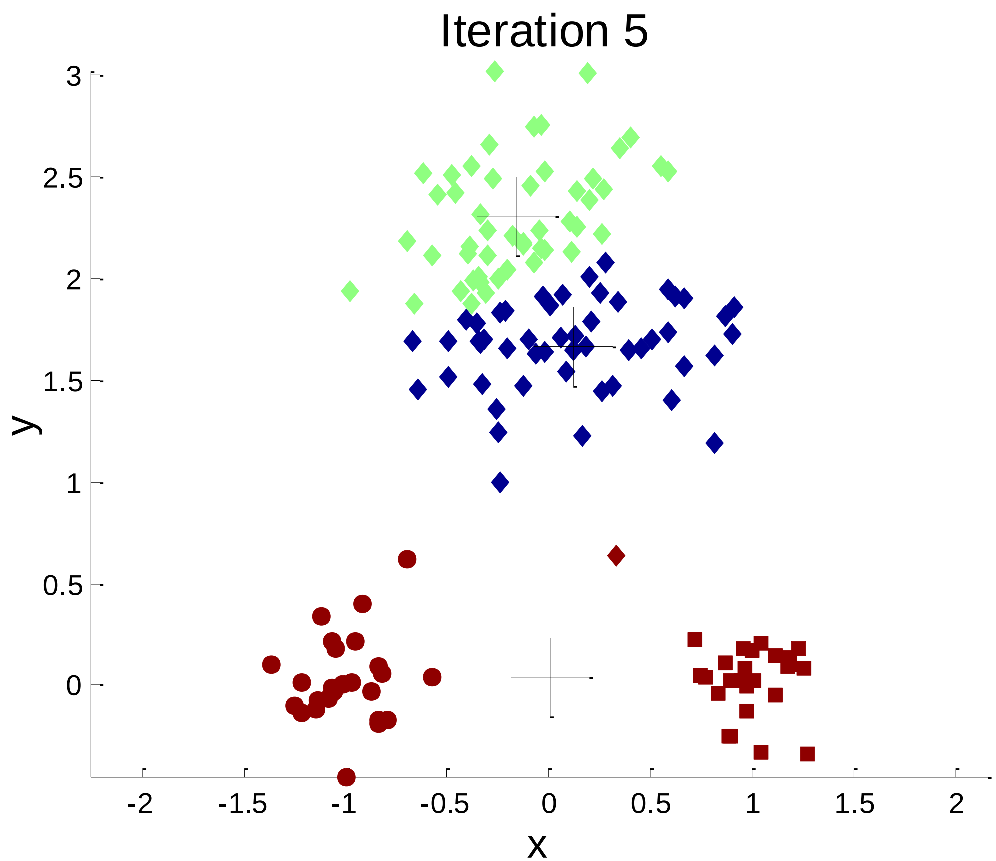

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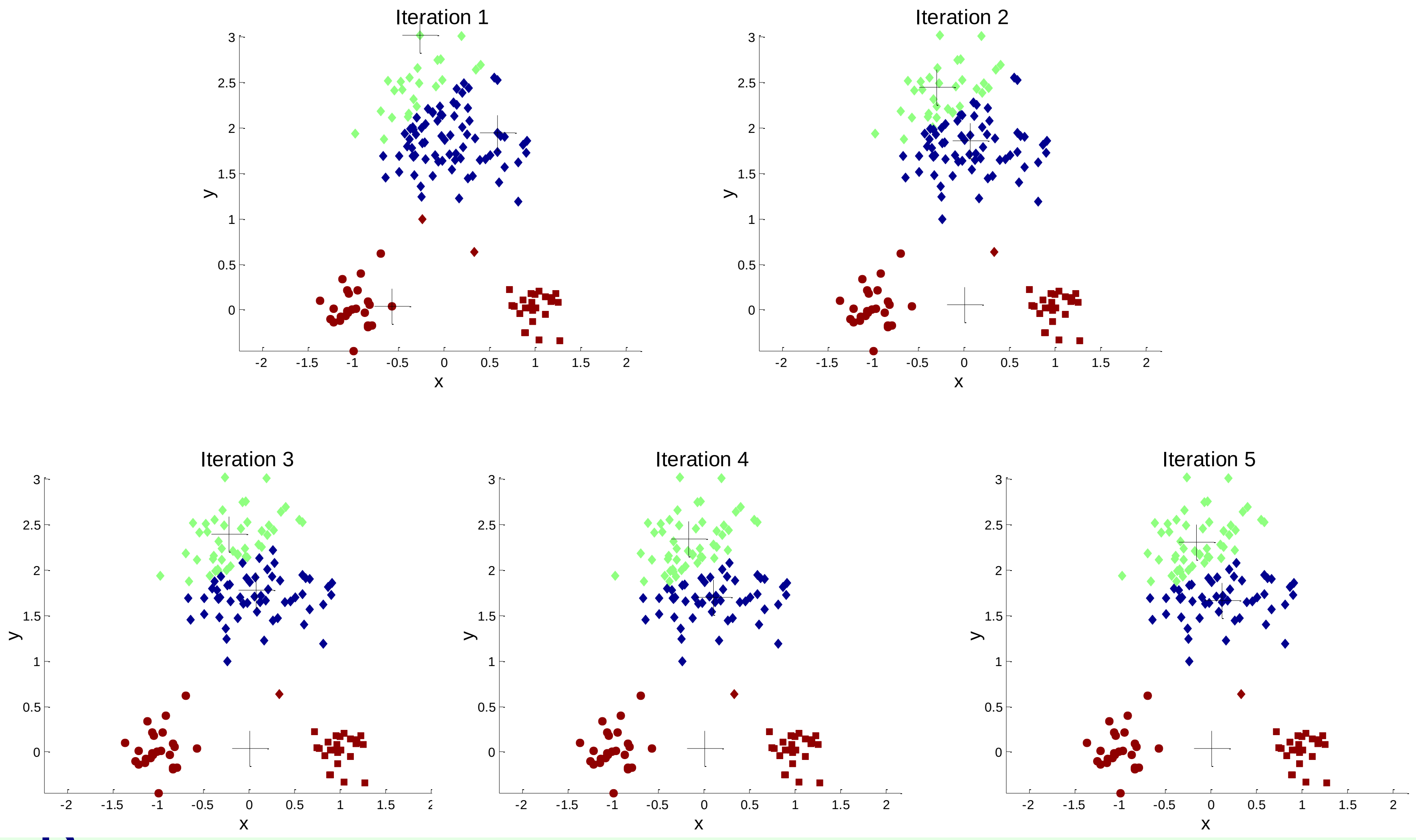



From: Tan,Steinbach, Kumar, Introduction to Data Mining, McGraw Hill 2006

# 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.

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

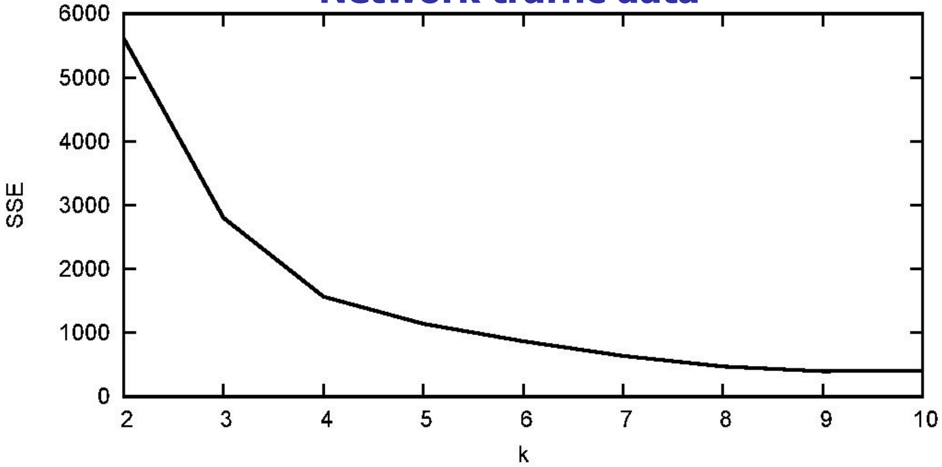
  - $x$ is a data point in cluster $C_i$ and $m_i$ is the representative point for cluster $C_i$
    - can show that $m_i$ corresponds to the center (mean) of the cluster
  - Given two clusters, we can choose the one with the smallest error
  - One easy way to reduce SSE is to increase K, the number of clusters
    - A good clustering with smaller K can have a lower SSE than a poor clustering with higher K

From: Tan,Steinbach, Kumar, Introduction to Data Mining, McGraw Hill 2006

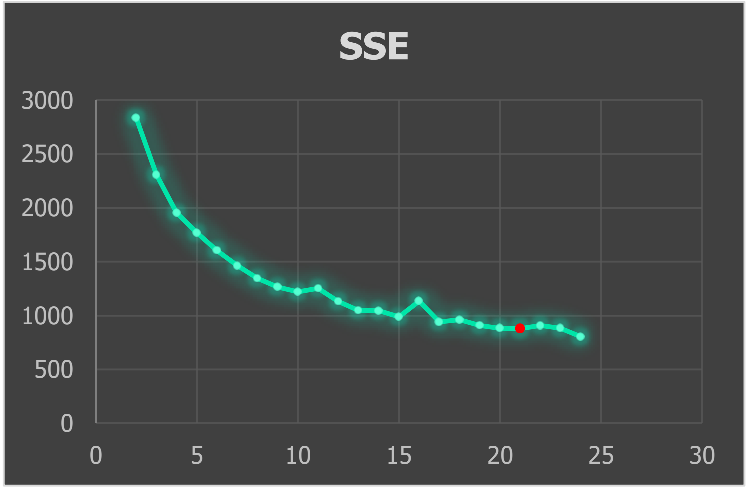
# K-means parameter setting

- Elbow graph (Knee approach)
  - Plotting the quality measure trend (e.g., SSE) against K
  - Choosing the value of K
    - the gain from adding a centroid is negligible
    - The reduction of the quality measure is not interesting anymore

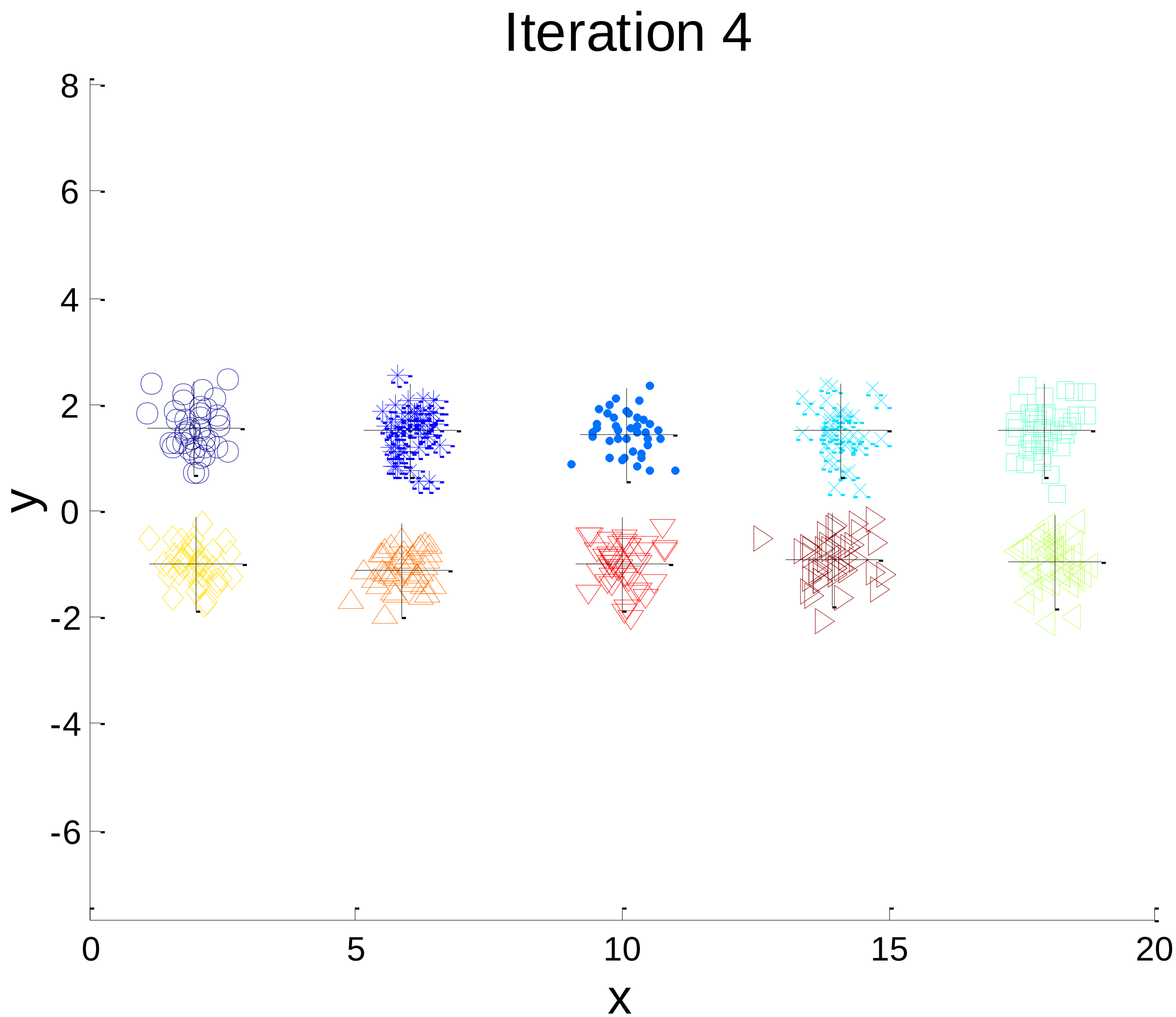
Network traffic data




Medical records



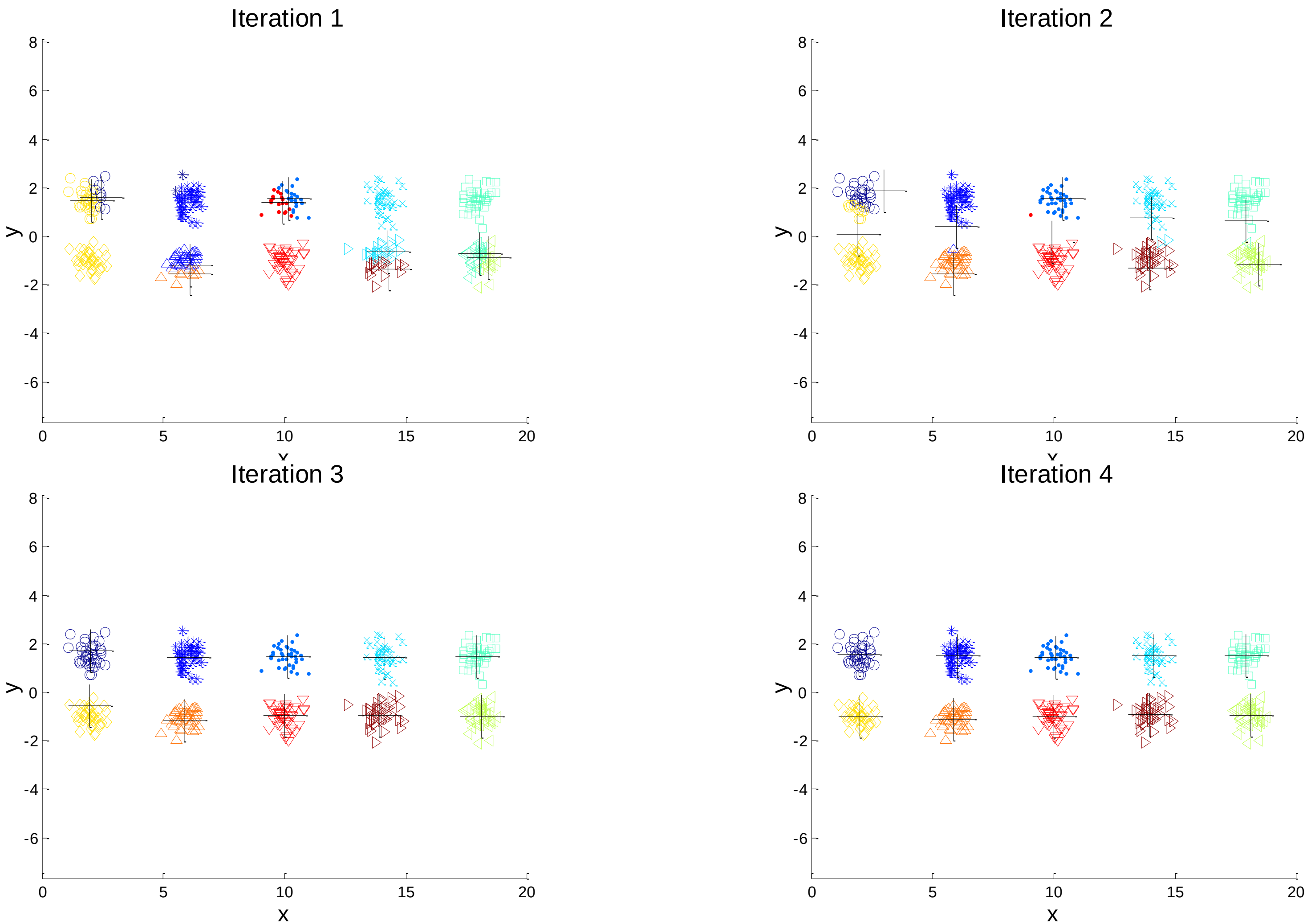
# 10 Clusters Example




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

From: Tan,Steinbach, Kumar, Introduction to Data Mining, McGraw Hill 2006

# 10 Clusters Example

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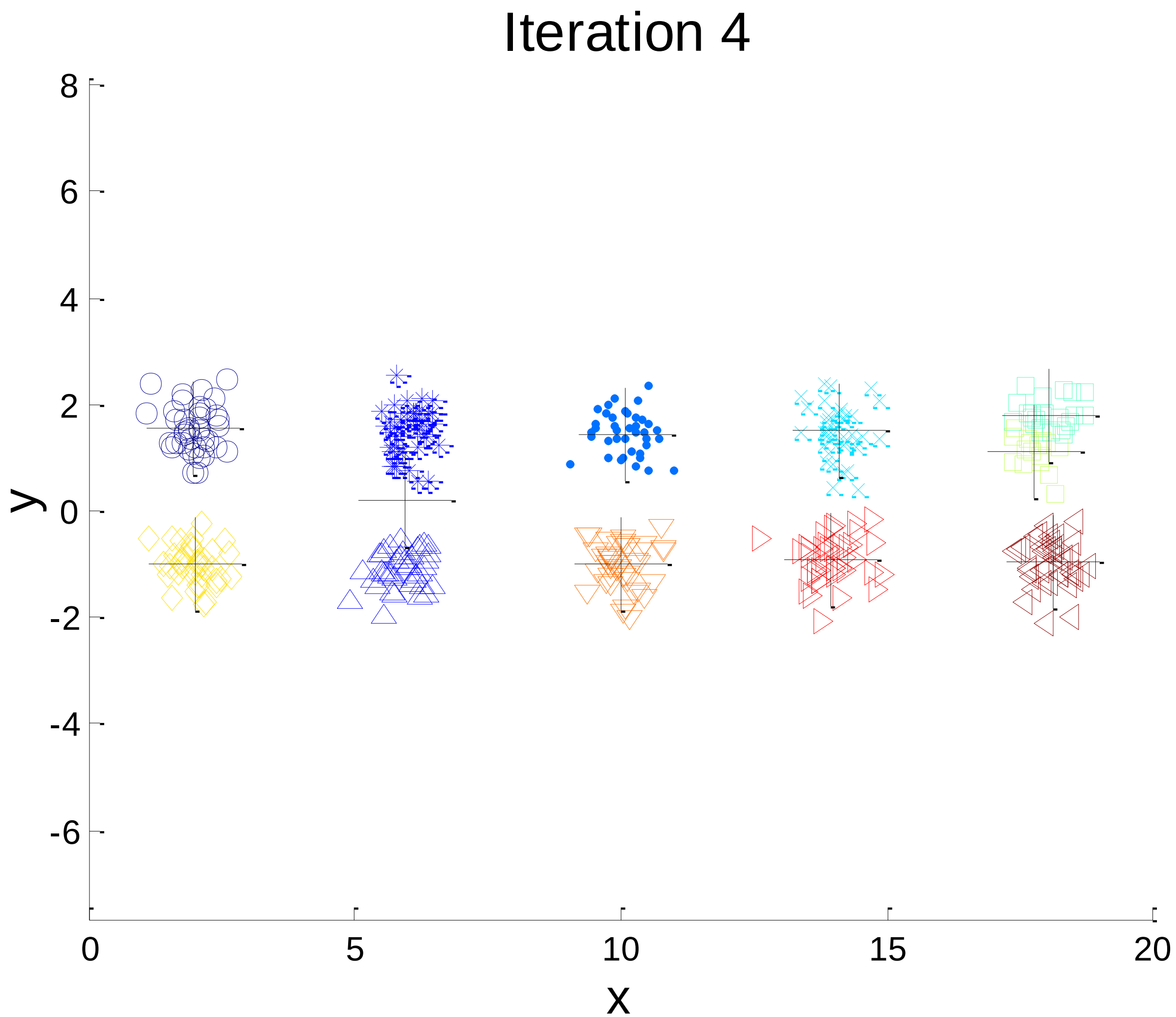
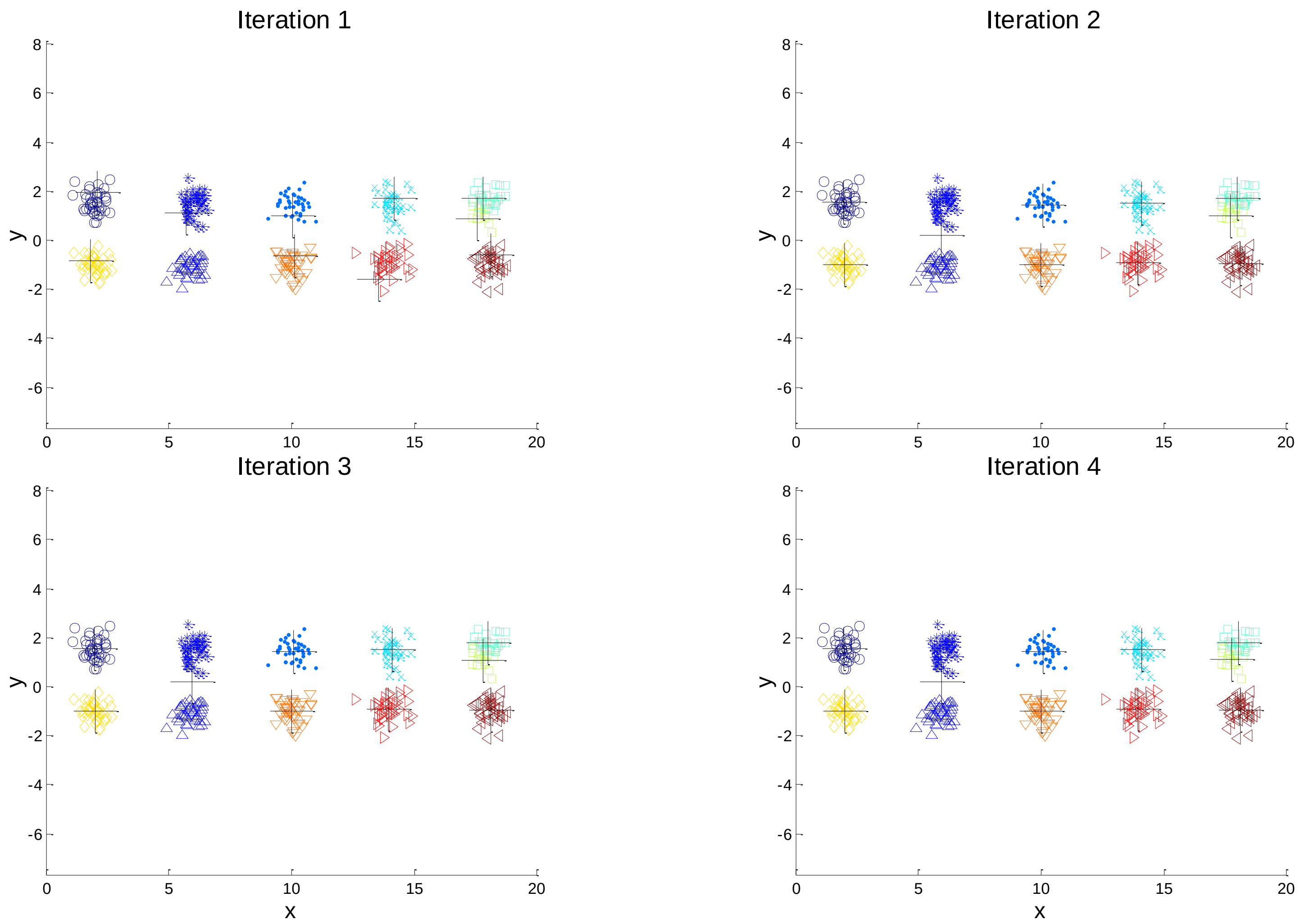



Starting with some pairs of clusters having three initial centroids, while other have only one.

From: Tan,Steinbach, Kumar, Introduction to Data Mining, McGraw Hill 2006

# 10 Clusters Example




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

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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
  - Not as susceptible to initialization issues



From: Tan,Steinbach, Kumar, Introduction to Data Mining, McGraw Hill 2006

# Handling Empty Clusters

- Basic K-means algorithm can yield empty clusters
- Several strategies
  - Choose the point that contributes most to SSE
  - Choose a point from the cluster with the highest SSE
  - If there are several empty clusters, the above can be repeated several times.



From: Tan,Steinbach, Kumar, Introduction to Data Mining, McGraw Hill 2006

# 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
  - Can use these steps during the clustering process



From: Tan,Steinbach, Kumar, Introduction to Data Mining, McGraw Hill 2006

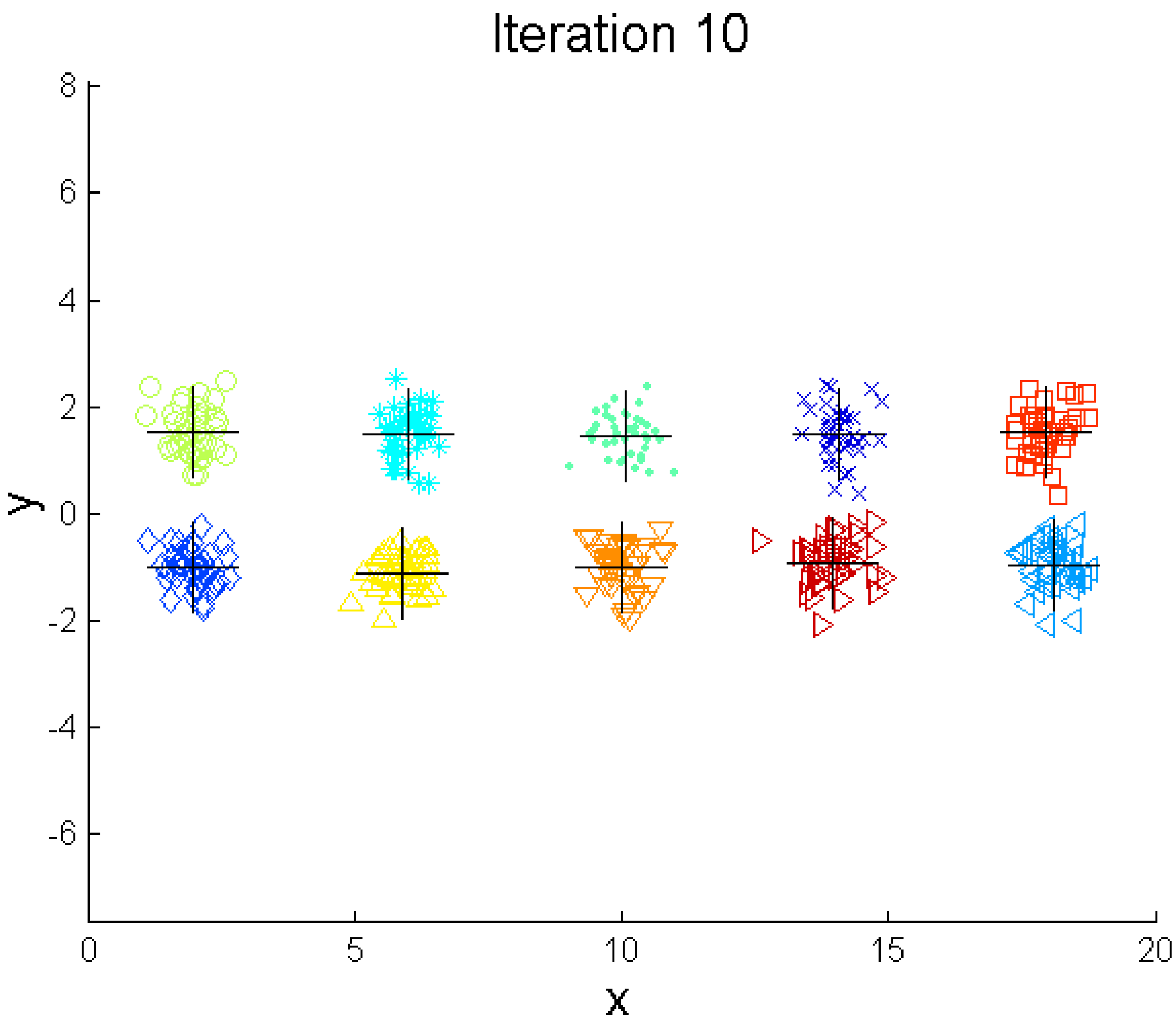
# Bisecting K-means

- **Bisecting K-means algorithm**
  - Variant of K-means that can produce a partitional or a hierarchical clustering

```
Initialize the list of clusters to contain the cluster containing all points.
repeat
   Select a cluster from the list of clusters
   for i = 1 to number_of_iterations do
      Bisect the selected cluster using basic K-means
   end for
   Add the two clusters from the bisection with the lowest SSE to the list of clusters.
until Until the list of clusters contains K clusters
```

From: Tan,Steinbach, Kumar, Introduction to Data Mining, McGraw Hill 2006

# Bisecting K-means Example



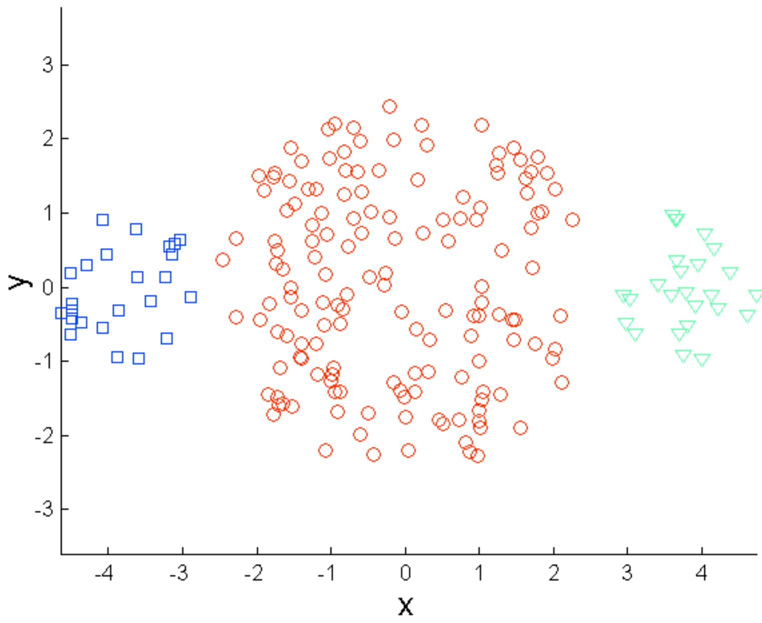

From: Tan,Steinbach, Kumar, Introduction to Data Mining, McGraw Hill 2006

# Limitations of K-means

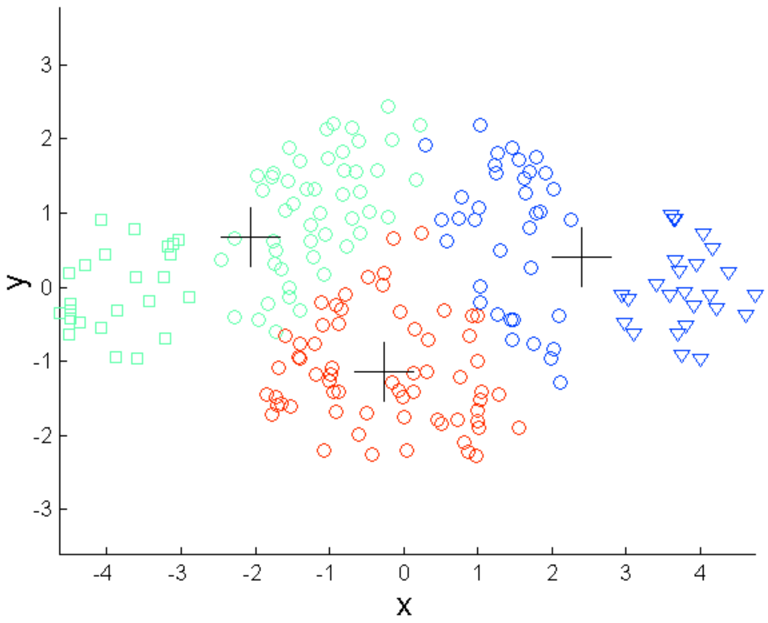
- K-means has problems when clusters are of differing
  - Sizes
  - Densities
  - Non-globular shapes

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

# Limitations of K-means: Differing Sizes

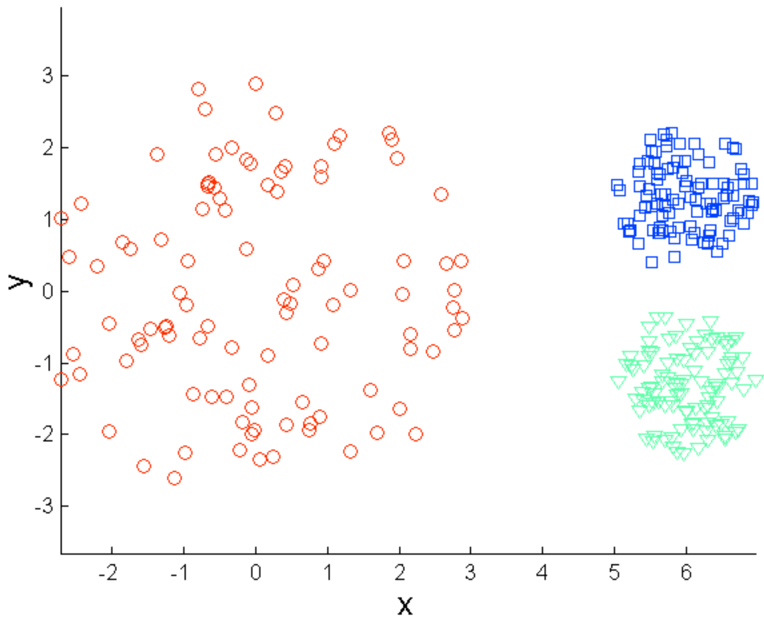



Original Points

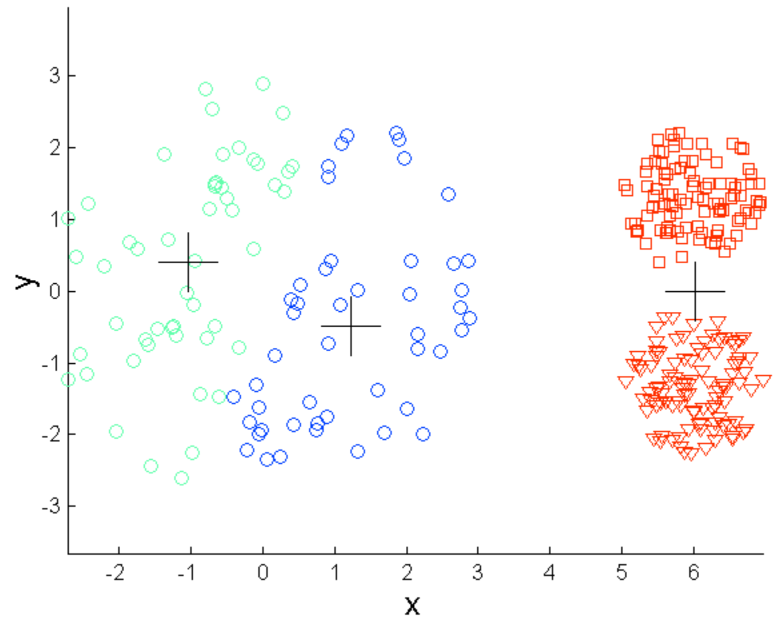



K-means (3 Clusters)

# Limitations of K-means: Differing Density




Original Points




K-means (3 Clusters)

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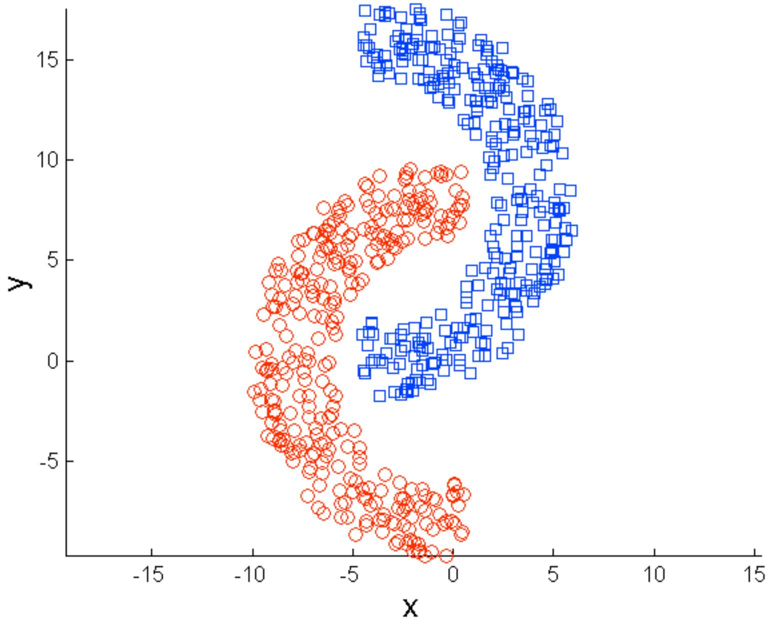
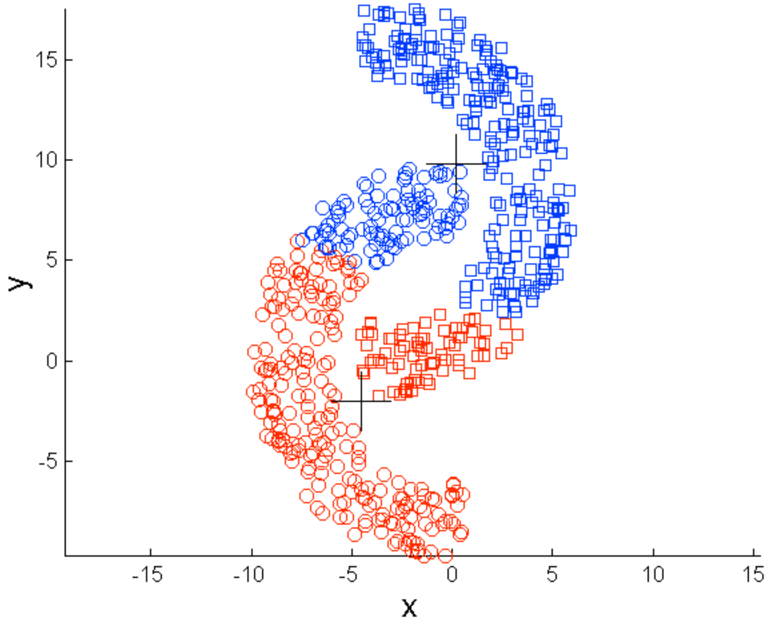
# Limitations of K-means: Non-globular Shapes



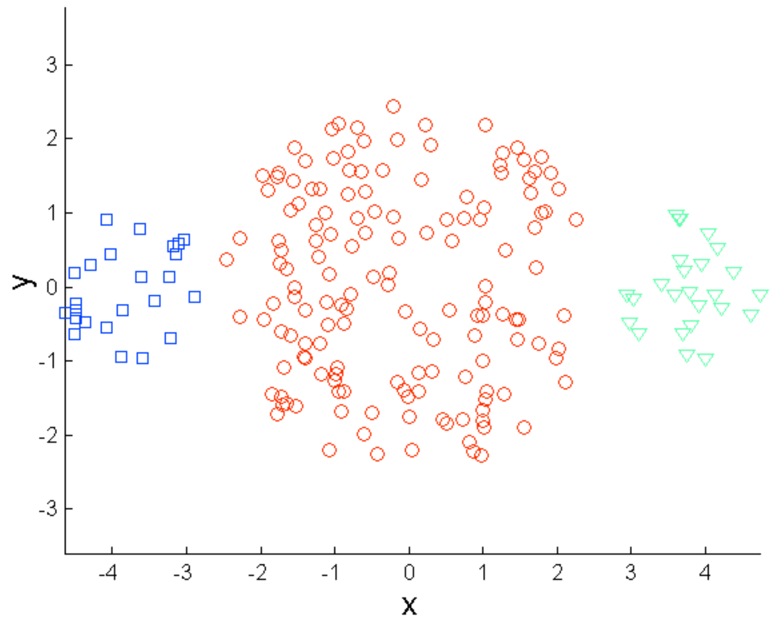

Original Points



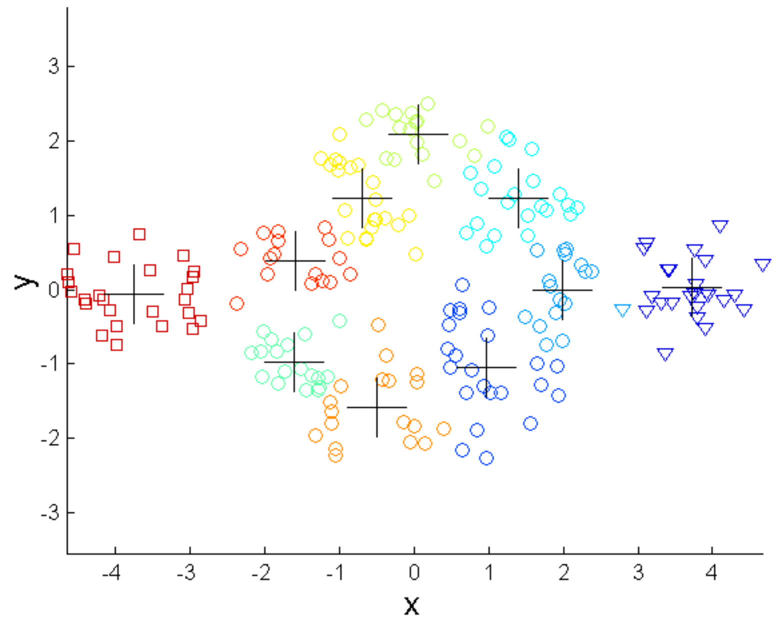

K-means (2 Clusters)

From: Tan,Steinbach, Kumar, Introduction to Data Mining, McGraw Hill 2006

# Overcoming K-means Limitations




Original Points



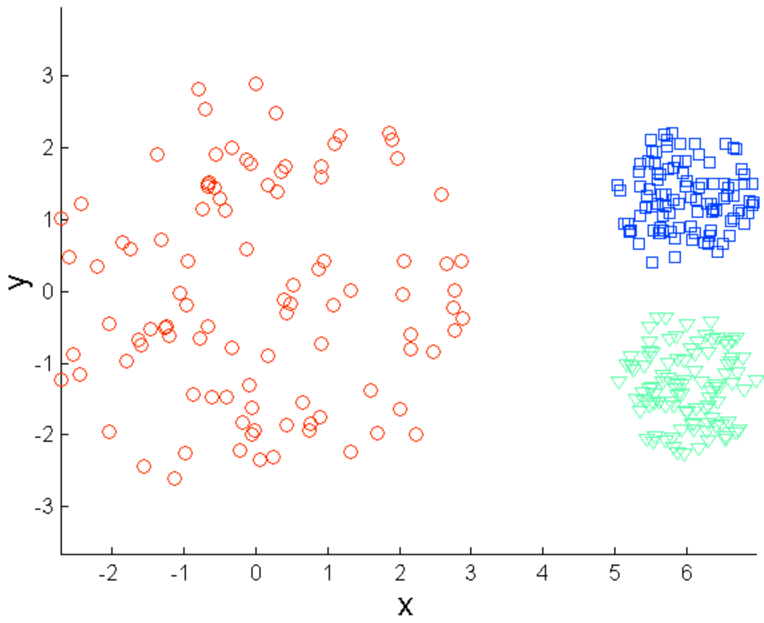

K-means Clusters

One solution is to use many clusters.

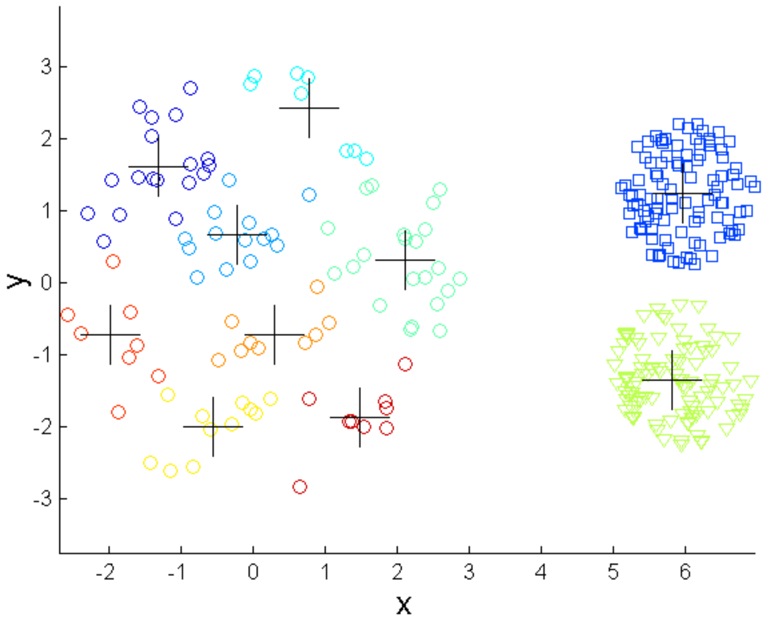
Find parts of clusters, but need to put together.

From: Tan,Steinbach, Kumar, Introduction to Data Mining, McGraw Hill 2006

# Overcoming K-means Limitations

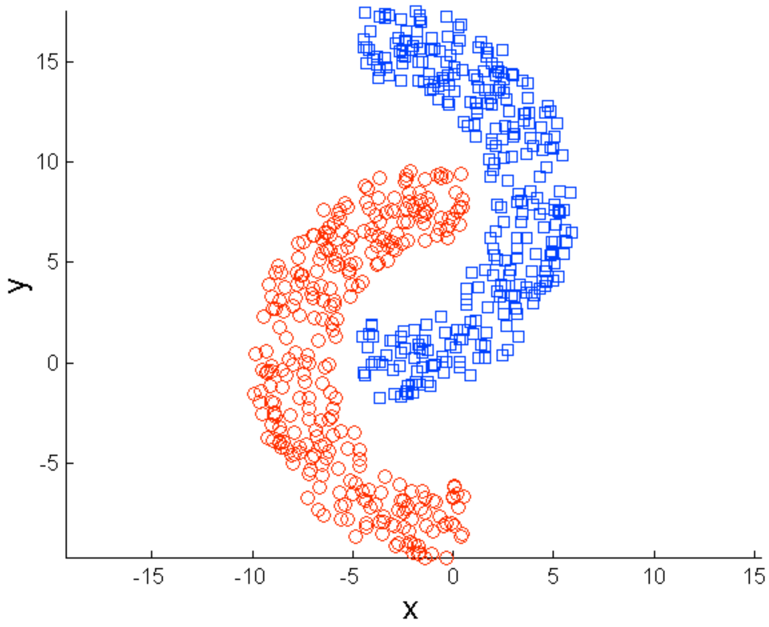


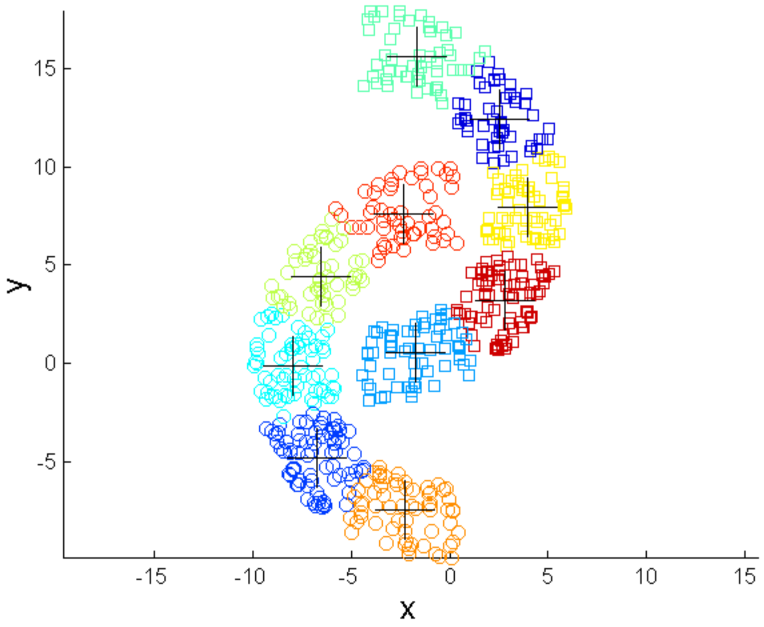

Original Points




K-means Clusters

# Overcoming K-means Limitations




Original Points

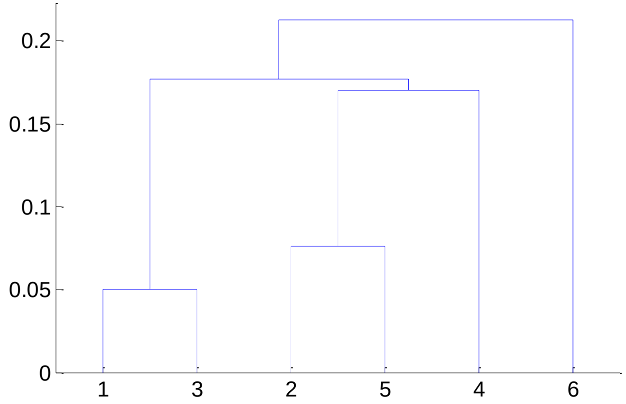
K-means Clusters

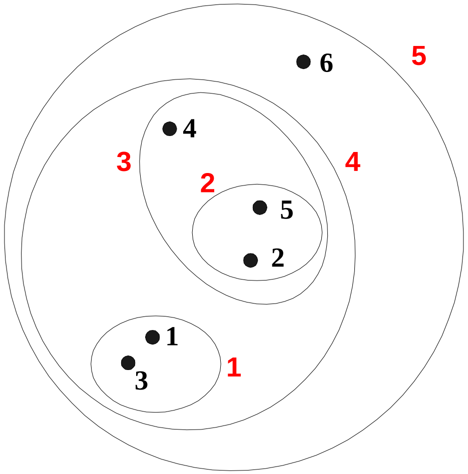


From: Tan,Steinbach, Kumar, Introduction to Data Mining, McGraw Hill 2006

# 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




From: Tan,Steinbach, Kumar, Introduction to Data Mining, McGraw Hill 2006

# Strengths of Hierarchical Clustering

- Do not have to assume any particular number of clusters
  - Any desired number of clusters can be obtained by ‘cutting’ the dendogram at the proper level

- They may correspond to meaningful taxonomies
  - Example in biological sciences (e.g., animal kingdom, phylogeny reconstruction, …)

# Hierarchical Clustering

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

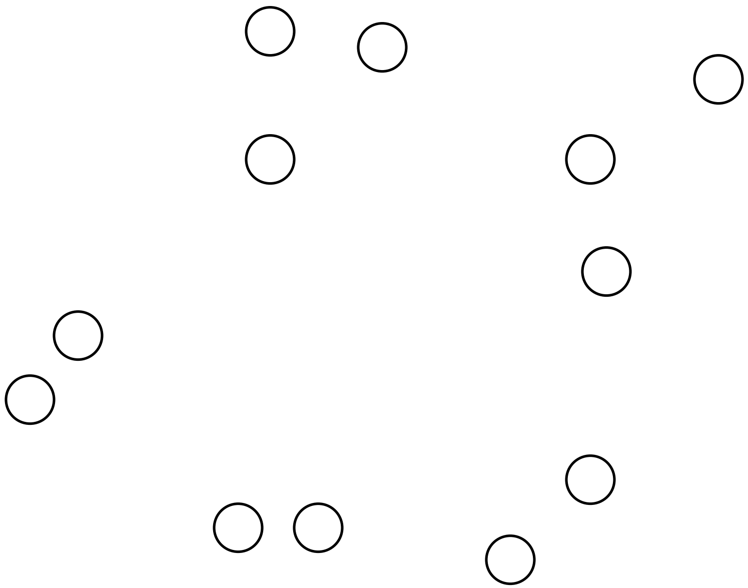
# Agglomerative Clustering Algorithm

- 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

From: Tan,Steinbach, Kumar, Introduction to Data Mining, McGraw Hill 2006

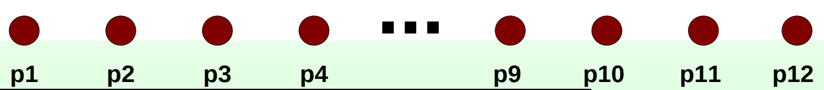
# Starting Situation

- Start with clusters of individual points and a proximity matrix



| | p1 | p2 | p3 | p4 | p5 | . . . |
|---|---|---|---|---|---|---|
| p1 | | | | | | |
| p2 | | | | | | |
| p3 | | | | | | |
| p4 | | | | | | |
| p5 | | | | | | |
| . | | | | | | |
| . | | | | | | |
| . | | | | | | |

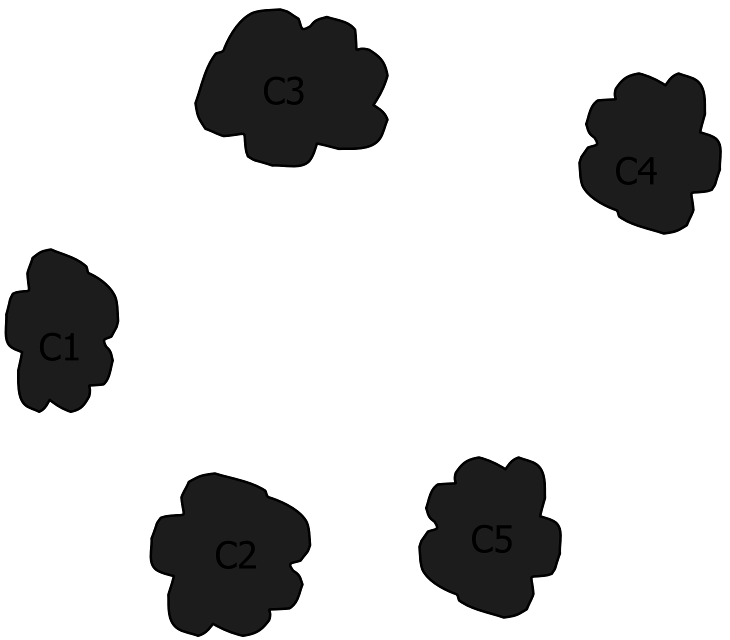
Proximity Matrix




From: Tan,Steinbach, Kumar, Introduction to Data Mining, McGraw Hill 2006

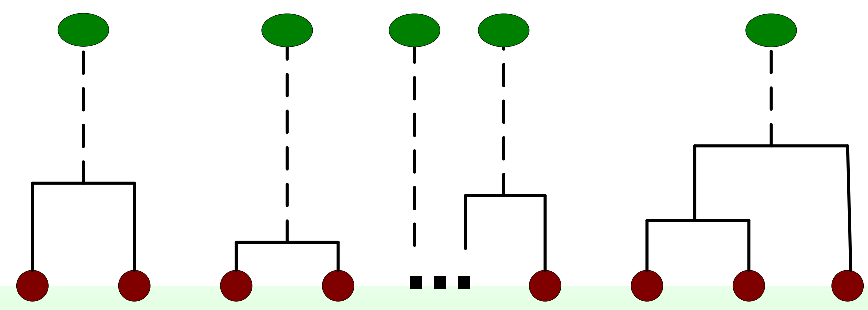
# Intermediate Situation

- After some merging steps, we have some clusters




| | C1 | C2 | C3 | C4 | C5 |
|---|---|---|---|---|---|
| C1 | | | | | |
| C2 | | | | | |
| C3 | | | | | |
| C4 | | | | | |
| C5 | | | | | |

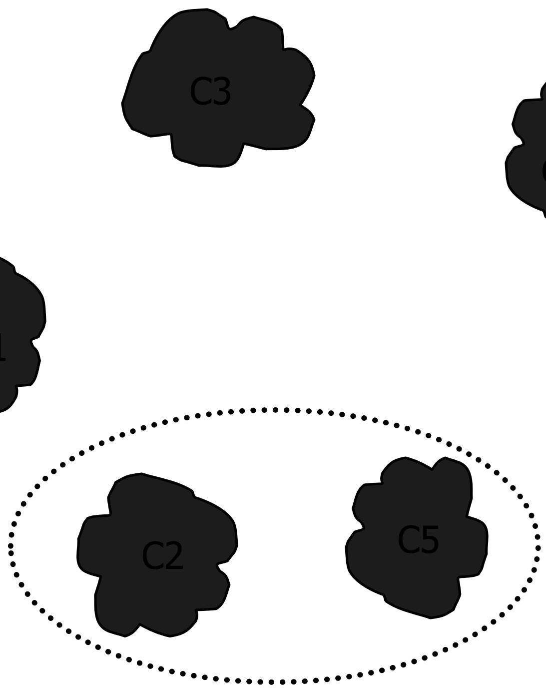
Proximity Matrix

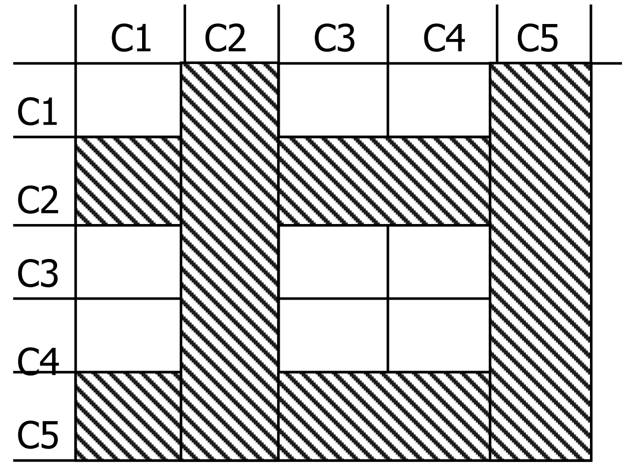



From: Tan,Steinbach, Kumar, Introduction to Data Mining, McGraw Hill 2006

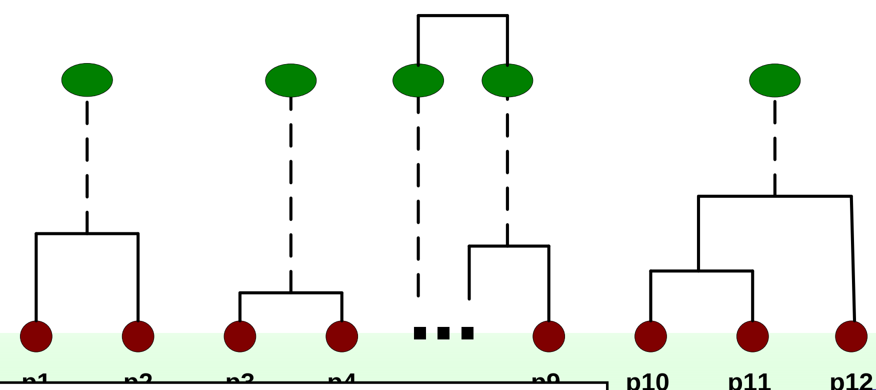
# Intermediate Situation

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



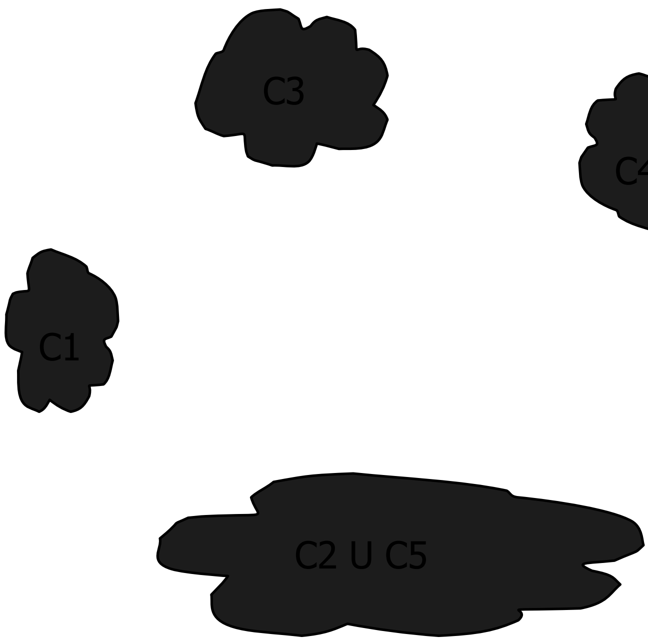

Proximity Matrix




From: Tan,Steinbach, Kumar, Introduction to Data Mining, McGraw Hill 2006

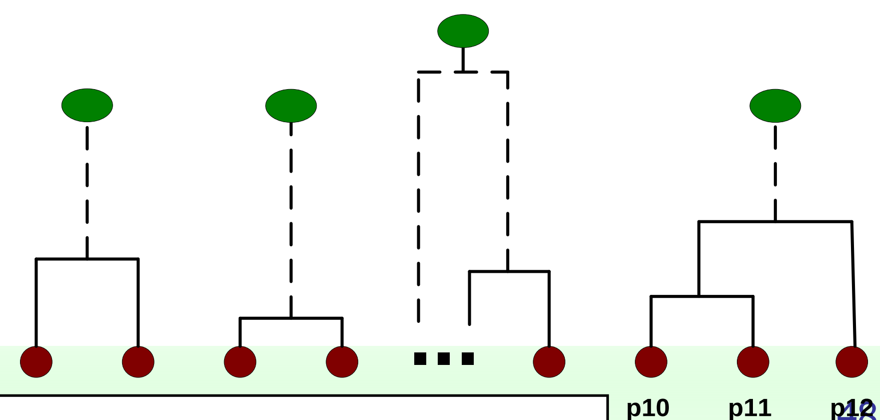
# After Merging

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



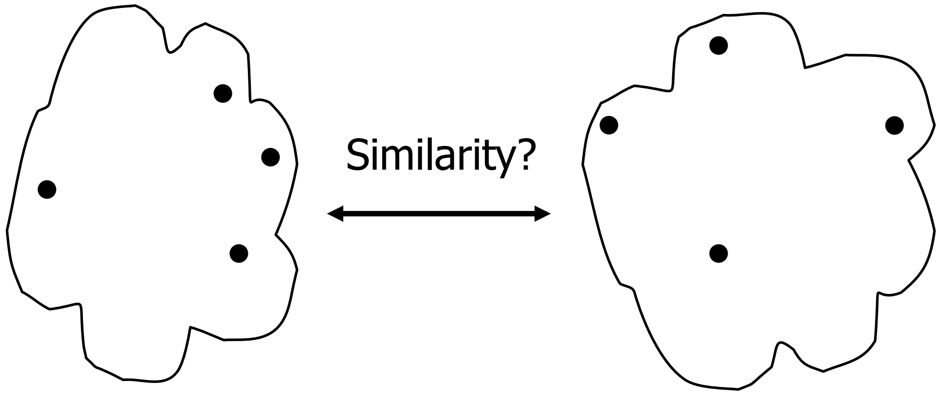

| | C1 | C2 U C5 | C3 | C4 |
|---|---|---|---|---|
| C1 | | ? | | |
| C2 U C5 | ? | ? | ? | ? |
| C3 | | ? | | |
| C4 | | ? | | |

Proximity Matrix




From: Tan,Steinbach, Kumar, Introduction to Data Mining, McGraw Hill 2006

# How to Define Inter-Cluster Similarity



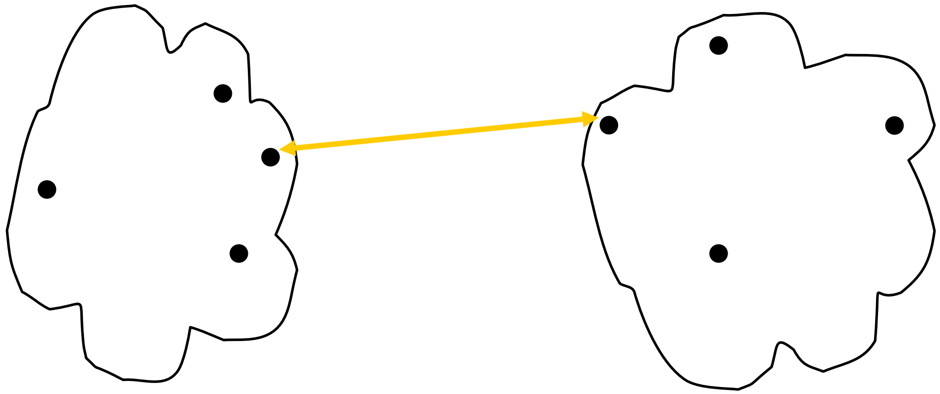

| | p1 | p2 | p3 | p4 | p5 | . . . |
|---|---|---|---|---|---|---|
| p1 | | | | | | |
| p2 | | | | | | |
| p3 | | | | | | |
| p4 | | | | | | |
| p5 | | | | | | |
| . | | | | | | |
| . | | | | | | |
| . | | | | | | |

Proximity Matrix

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

From: Tan,Steinbach, Kumar, Introduction to Data Mining, McGraw Hill 2006

# How to Define Inter-Cluster Similarity



| | p1 | p2 | p3 | p4 | p5 | . . . |
|---|---|---|---|---|---|---|
| p1 | | | | | | |
| p2 | | | | | | |
| p3 | | | | | | |
| p4 | | | | | | |
| p5 | | | | | | |
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| . | | | | | | |

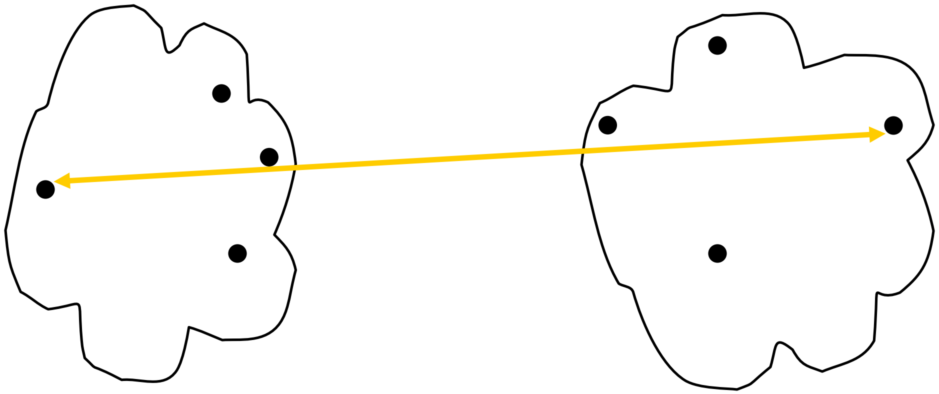
Proximity Matrix

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



From: Tan,Steinbach, Kumar, Introduction to Data Mining, McGraw Hill 2006

# How to Define Inter-Cluster Similarity



| | p1 | p2 | p3 | p4 | p5 | . . . |
|---|---|---|---|---|---|---|
| p1 | | | | | | |
| p2 | | | | | | |
| p3 | | | | | | |
| p4 | | | | | | |
| p5 | | | | | | |
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| . | | | | | | |

Proximity Matrix

- MIN
- MAX
- Group Average
- Distance Between Centroids
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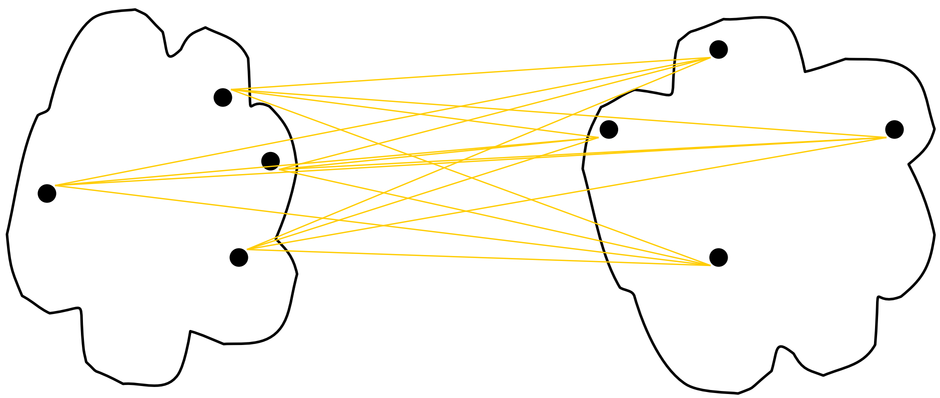
  - Ward's Method uses squared error



From: Tan,Steinbach, Kumar, Introduction to Data Mining, McGraw Hill 2006

# How to Define Inter-Cluster Similarity

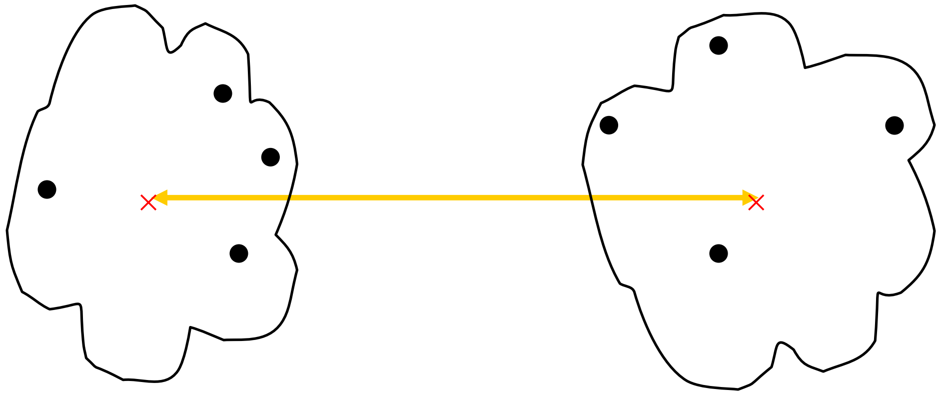


| | p1 | p2 | p3 | p4 | p5 | . . . |
|---|---|---|---|---|---|---|
| p1 | | | | | | |
| p2 | | | | | | |
| p3 | | | | | | |
| p4 | | | | | | |
| p5 | | | | | | |
| . . . | | | | | | |

Proximity Matrix

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

# How to Define Inter-Cluster Similarity



| | p1 | p2 | p3 | p4 | p5 | . . . |
|---|---|---|---|---|---|---|
| p1 | | | | | | |
| p2 | | | | | | |
| p3 | | | | | | |
| p4 | | | | | | |
| p5 | | | | | | |
| . | | | | | | |
| . | | | | | | |
| . | | | | | | |

Proximity Matrix

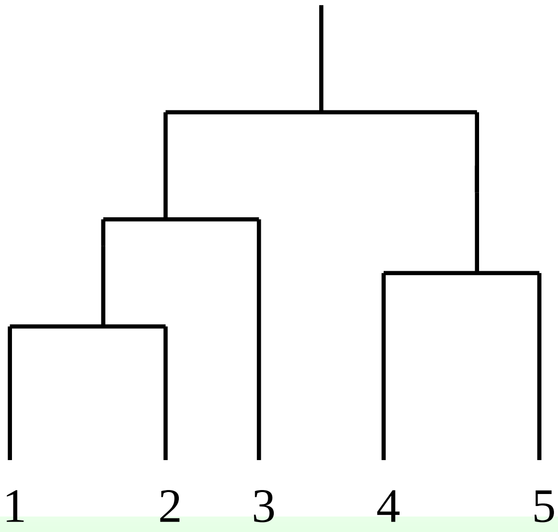
- MIN
- MAX
- Group Average
- Distance Between Centroids
- Other methods driven by an objective function
  - Ward's Method uses squared error

From: Tan,Steinbach, Kumar, Introduction to Data Mining, McGraw Hill 2006

# Cluster Similarity: MIN or Single Link

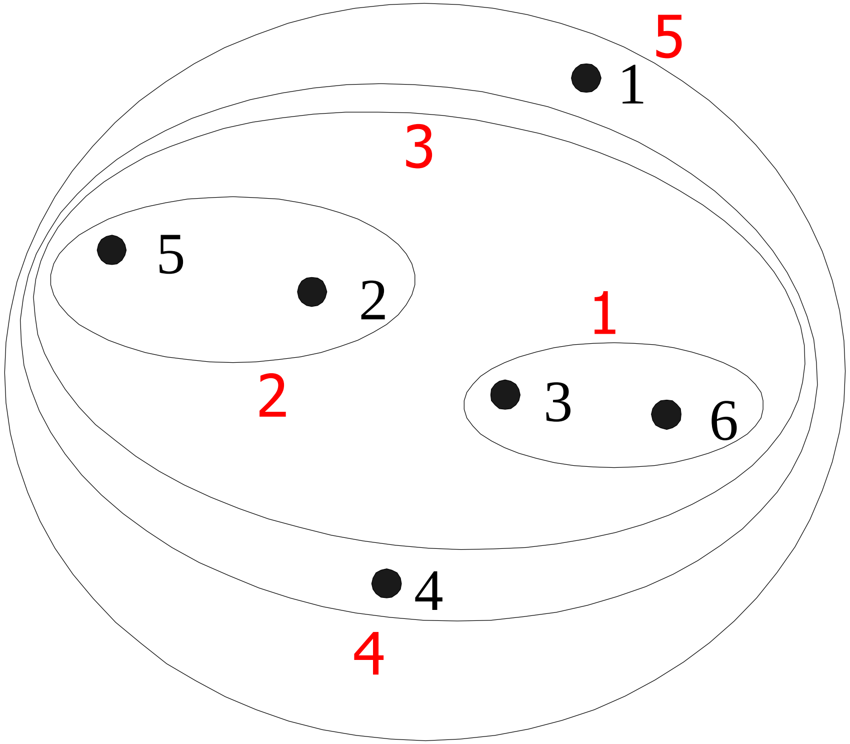
- Similarity of two clusters is based on the two most similar (closest) points in the different clusters
  - Determined by one pair of points, i.e., by one link in the proximity graph.

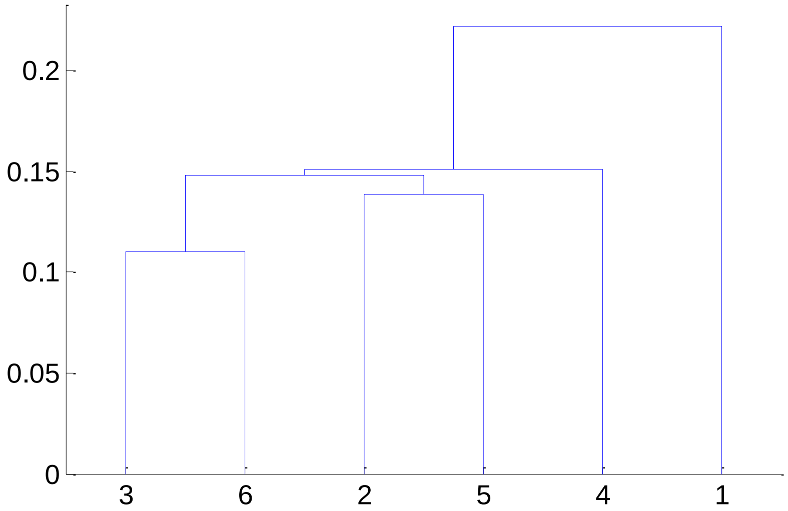
| | I1 | I2 | I3 | I4 | I5 |
|---|---|---|---|---|---|
| I1 | 1.00 | 0.90 | 0.10 | 0.65 | 0.20 |
| I2 | 0.90 | 1.00 | 0.70 | 0.60 | 0.50 |
| I3 | 0.10 | 0.70 | 1.00 | 0.40 | 0.30 |
| I4 | 0.65 | 0.60 | 0.40 | 1.00 | 0.80 |
| I5 | 0.20 | 0.50 | 0.30 | 0.80 | 1.00 |




From: Tan,Steinbach, Kumar, Introduction to Data Mining, McGraw Hill 2006

# Hierarchical Clustering: MIN



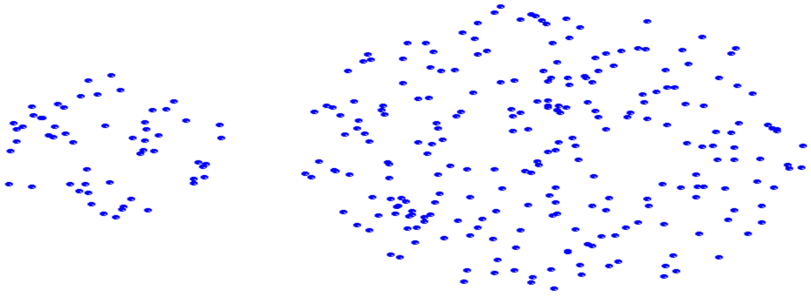




Nested Clusters

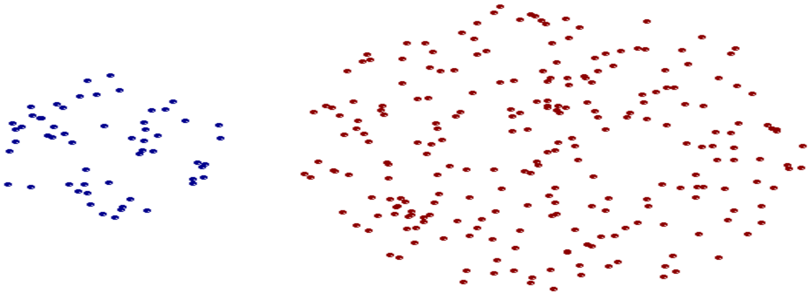
Dendrogram

From: Tan,Steinbach, Kumar, Introduction to Data Mining, McGraw Hill 2006

# Strength of MIN



Original Points

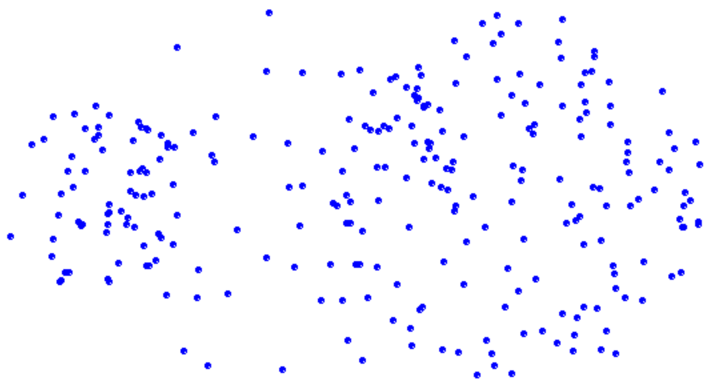


Two Clusters

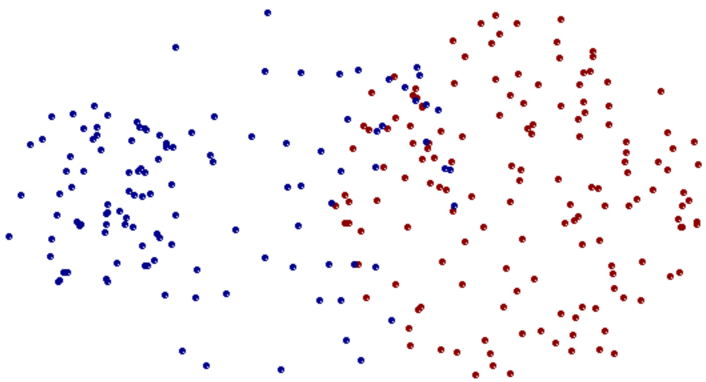
- Can handle non-elliptical shapes

From: Tan,Steinbach, Kumar, Introduction to Data Mining, McGraw Hill 2006

# Limitations of MIN



Original Points



Two Clusters

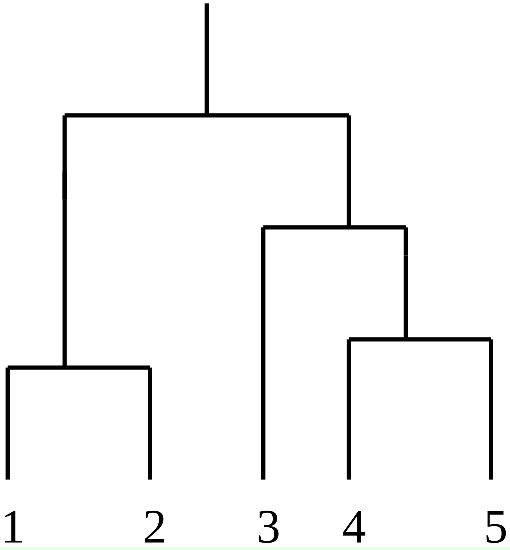
- Sensitive to noise and outliers

From: Tan,Steinbach, Kumar, Introduction to Data Mining, McGraw Hill 2006

# Cluster Similarity: MAX or Complete Linkage

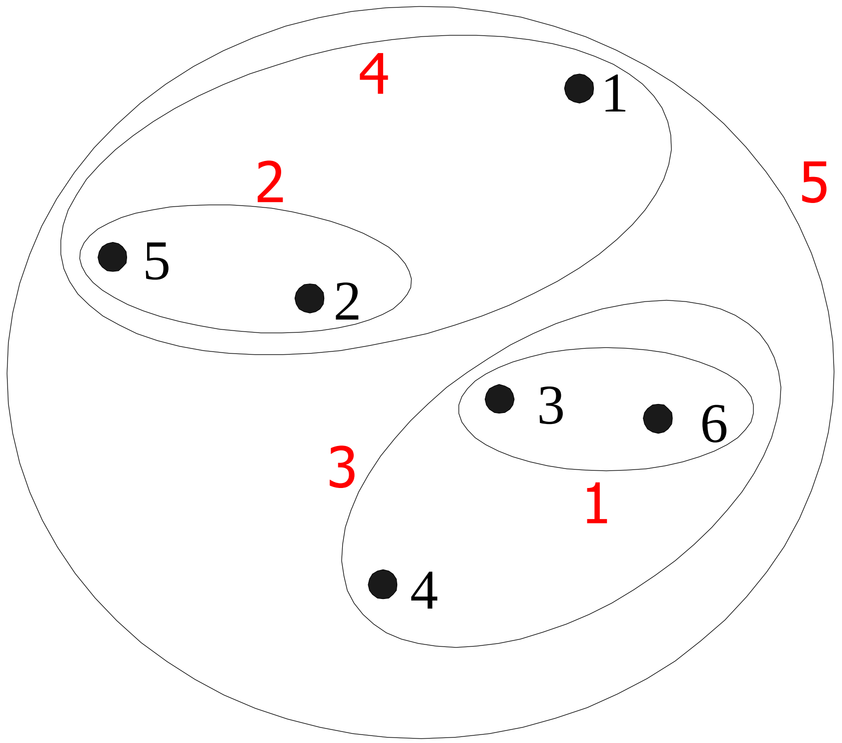
- Similarity of two clusters is based on the two least similar (most distant) points in the different clusters
  - Determined by all pairs of points in the two clusters

| | I1 | I2 | I3 | I4 | I5 |
|---|---|---|---|---|---|
| I1 | 1.00 | 0.90 | 0.10 | 0.65 | 0.20 |
| I2 | 0.90 | 1.00 | 0.70 | 0.60 | 0.50 |
| I3 | 0.10 | 0.70 | 1.00 | 0.40 | 0.30 |
| I4 | 0.65 | 0.60 | 0.40 | 1.00 | 0.80 |
| I5 | 0.20 | 0.50 | 0.30 | 0.80 | 1.00 |

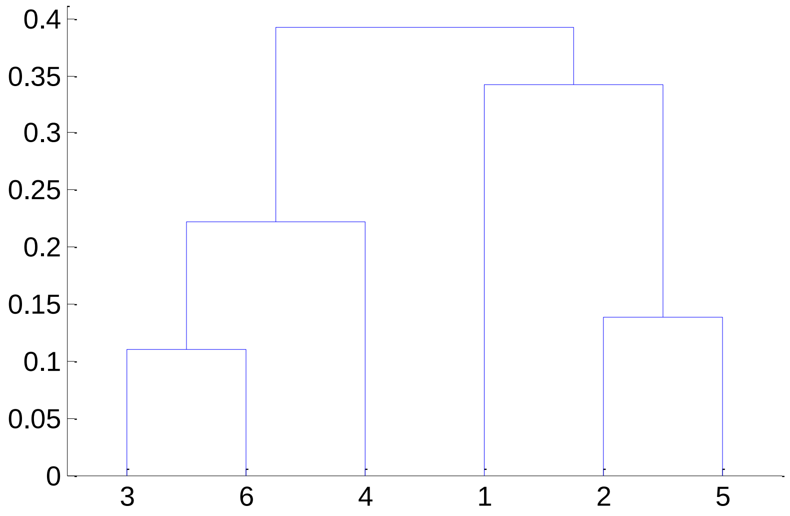



From: Tan,Steinbach, Kumar, Introduction to Data Mining, McGraw Hill 2006

# Hierarchical Clustering: MAX

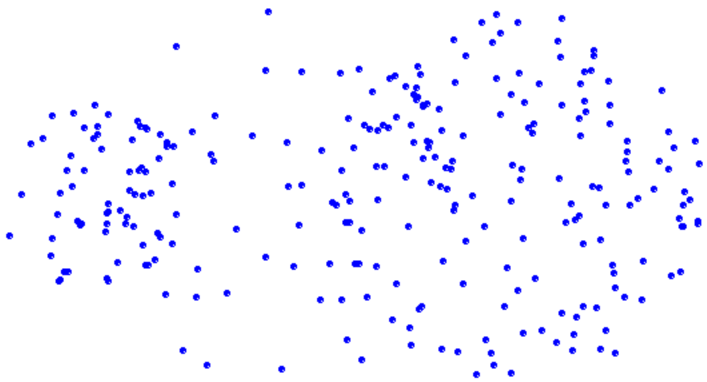



Nested Clusters

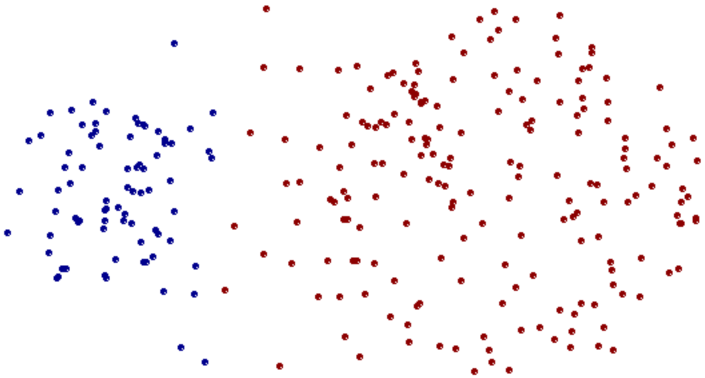



Dendrogram

# Strength of MAX



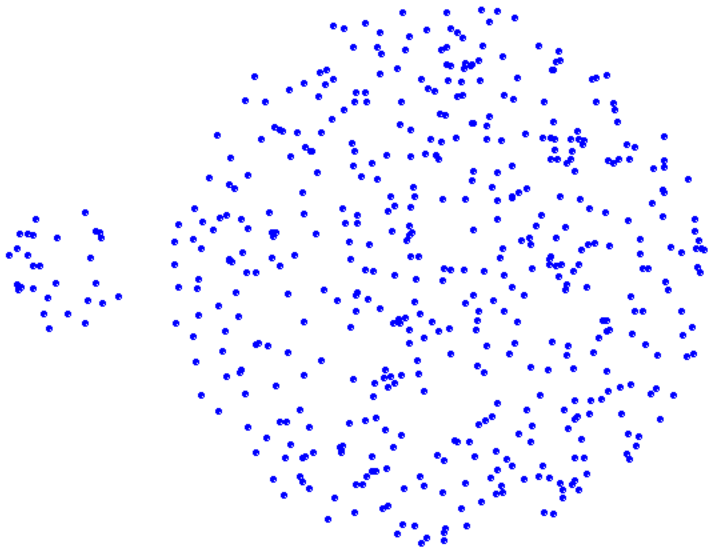
Original Points



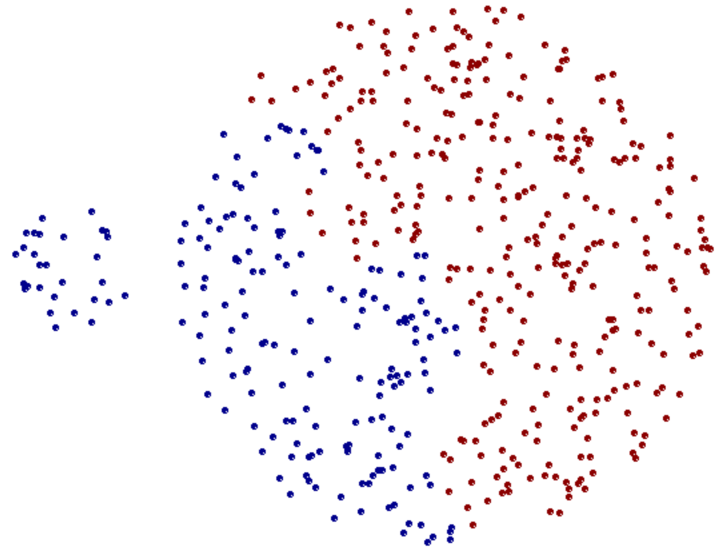
Two Clusters

- Less susceptible to noise and outliers

# Limitations of MAX



Original Points



Two Clusters

- Tends to break large clusters
- Biased towards globular clusters

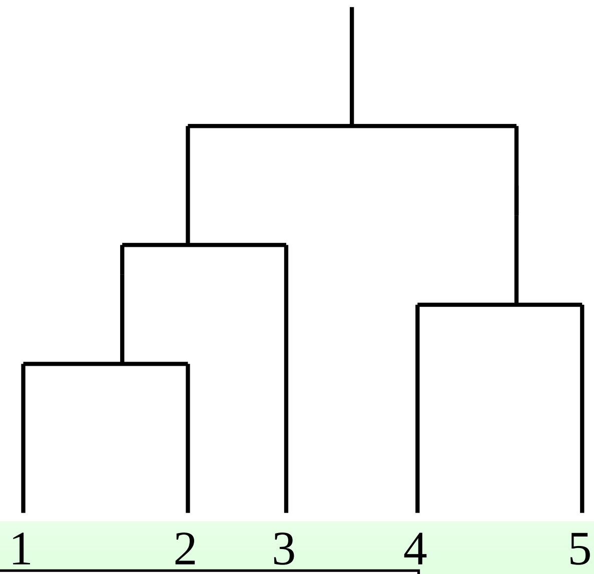
# Cluster Similarity: Group Average

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

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

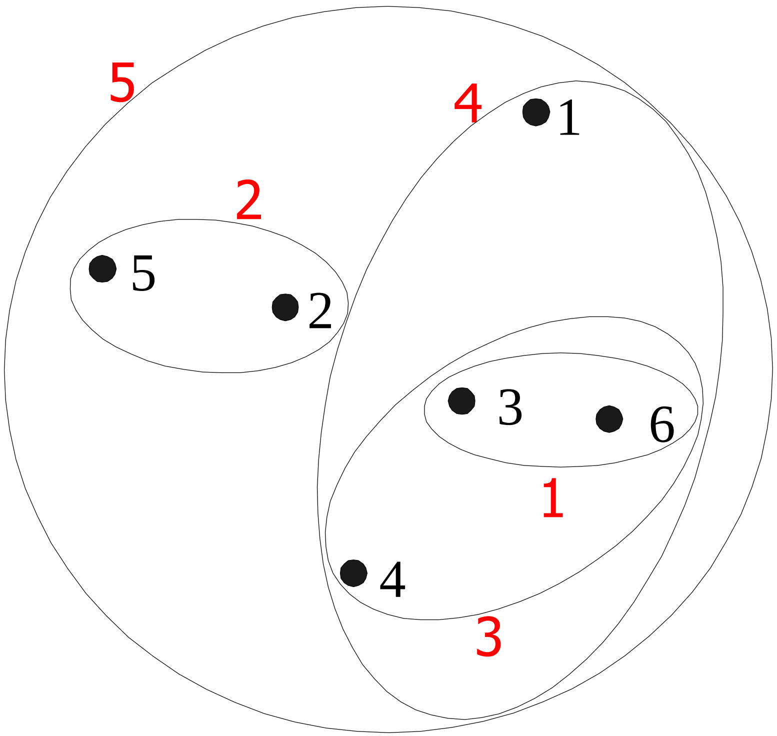
- Need to use average connectivity for scalability since total proximity favors large clusters

| | I1 | I2 | I3 | I4 | I5 |
|---|---|---|---|---|---|
| I1 | 1.00 | 0.90 | 0.10 | 0.65 | 0.20 |
| I2 | 0.90 | 1.00 | 0.70 | 0.60 | 0.50 |
| I3 | 0.10 | 0.70 | 1.00 | 0.40 | 0.30 |
| I4 | 0.65 | 0.60 | 0.40 | 1.00 | 0.80 |
| I5 | 0.20 | 0.50 | 0.30 | 0.80 | 1.00 |

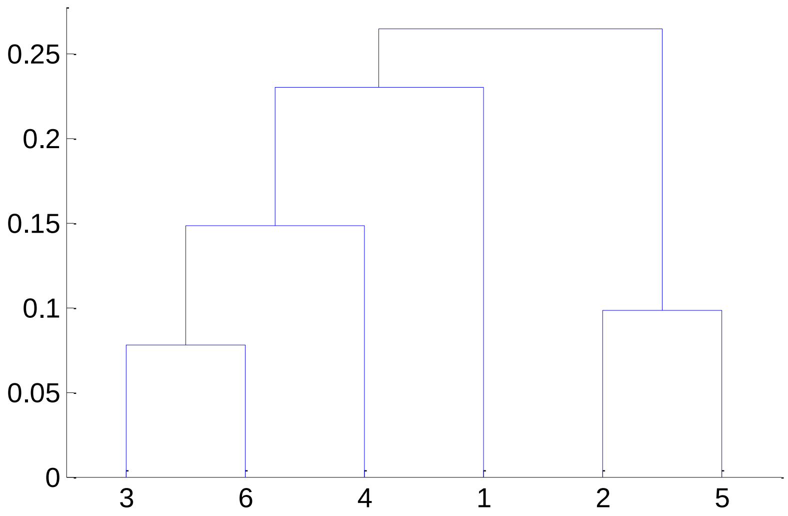



From: Tan,Steinbach, Kumar, Introduction to Data Mining, McGraw Hill 2006

# Hierarchical Clustering: Group Average




Nested Clusters




Dendrogram

# Hierarchical Clustering: Group Average

- Compromise between Single and Complete Link

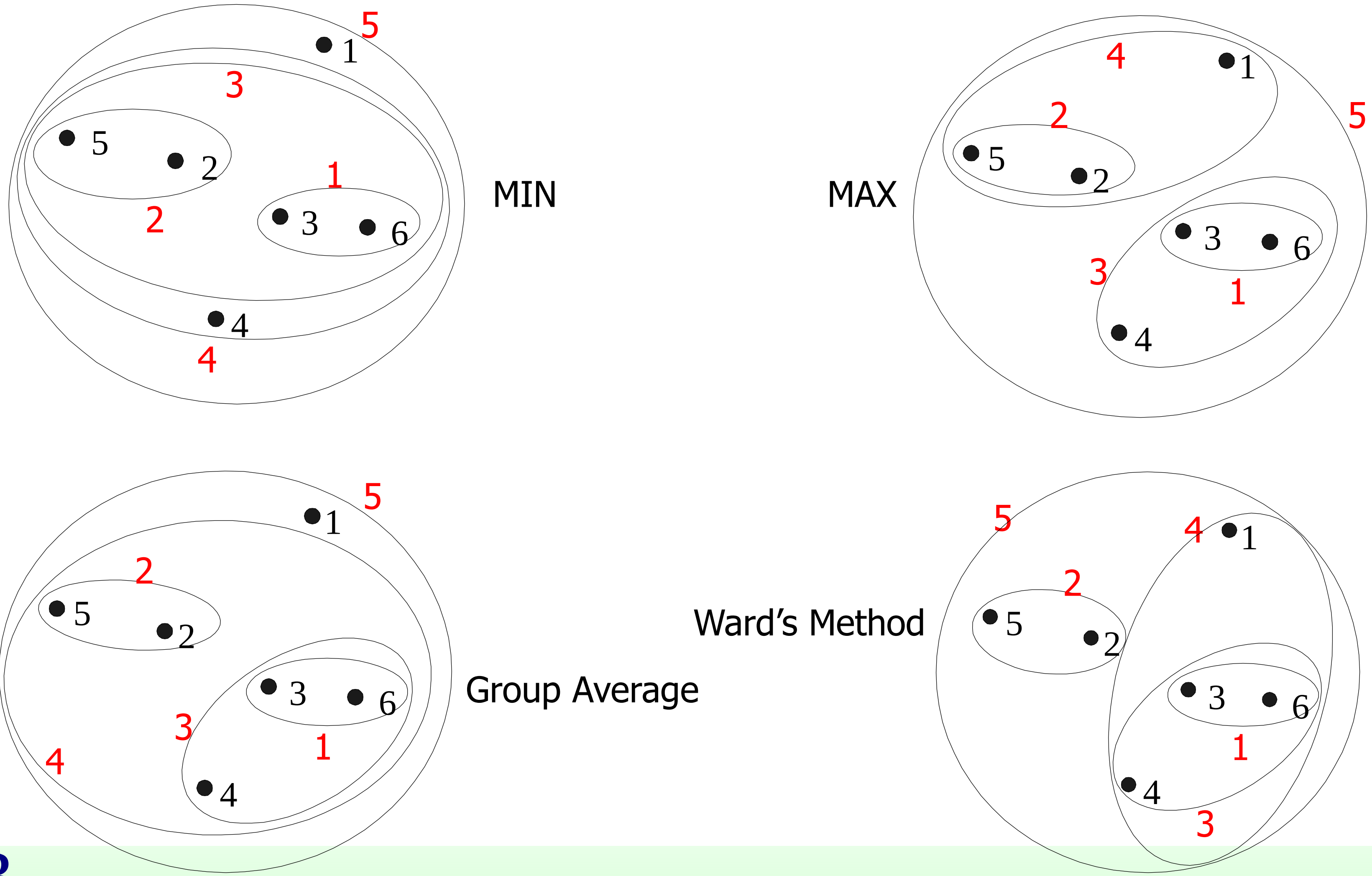
- Strengths
  - Less susceptible to noise and outliers

- 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




From: Tan,Steinbach, Kumar, Introduction to Data Mining, McGraw Hill 2006

# Hierarchical Clustering: Time and Space requirements

- $O(N^2)$ space since it uses the proximity matrix.
  - N is the number of points.

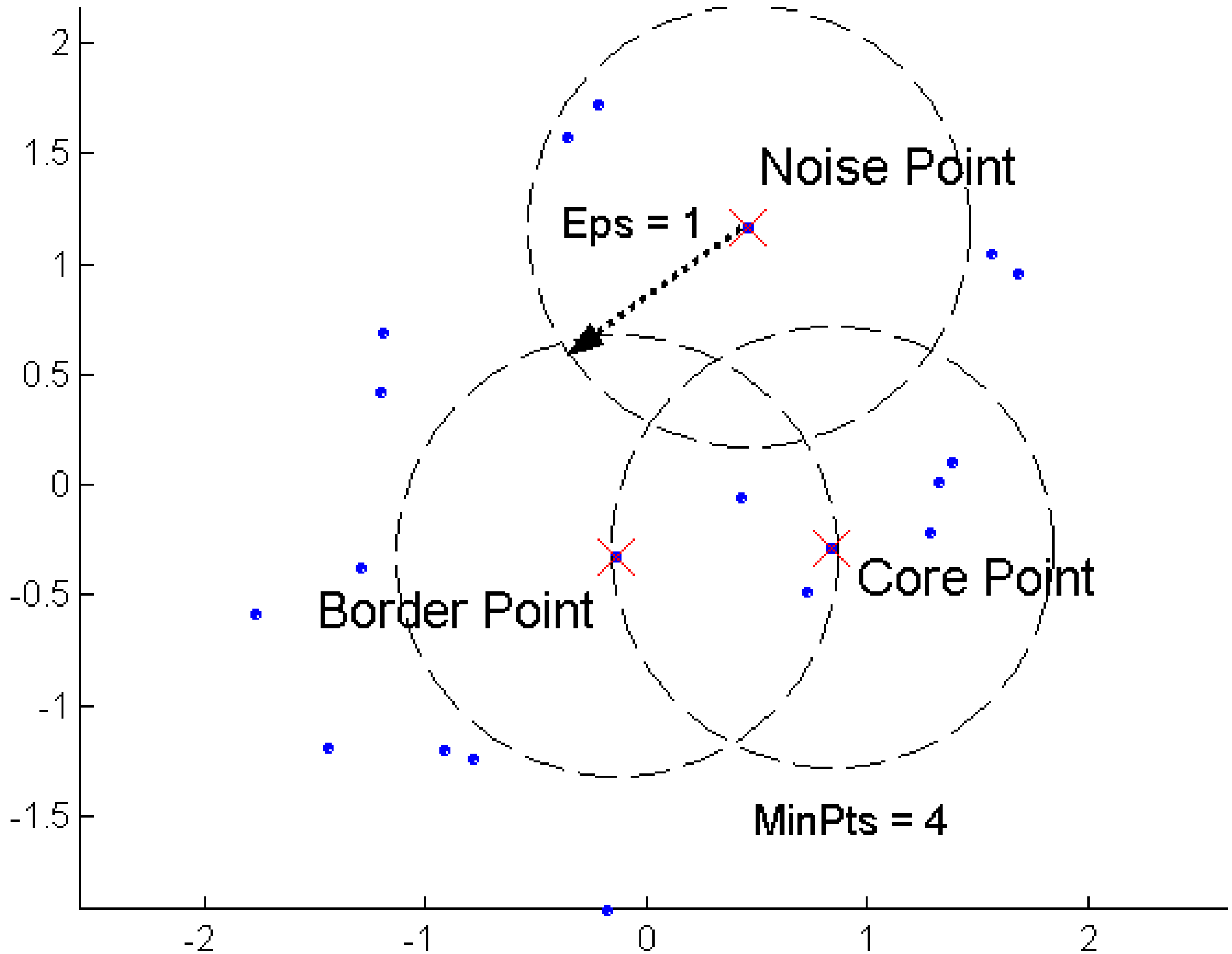
- $O(N^3)$ time in many cases
  - There are N steps and at each step the size, $N^2$, proximity matrix must be updated and searched
  - Complexity can be reduced to $O(N^2 \log(N))$ time for some approaches

# 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.

From: Tan,Steinbach, Kumar, Introduction to Data Mining, McGraw Hill 2006

# DBSCAN: Core, Border, and Noise Points




From: Tan,Steinbach, Kumar, Introduction to Data Mining, McGraw Hill 2006

# DBSCAN Algorithm

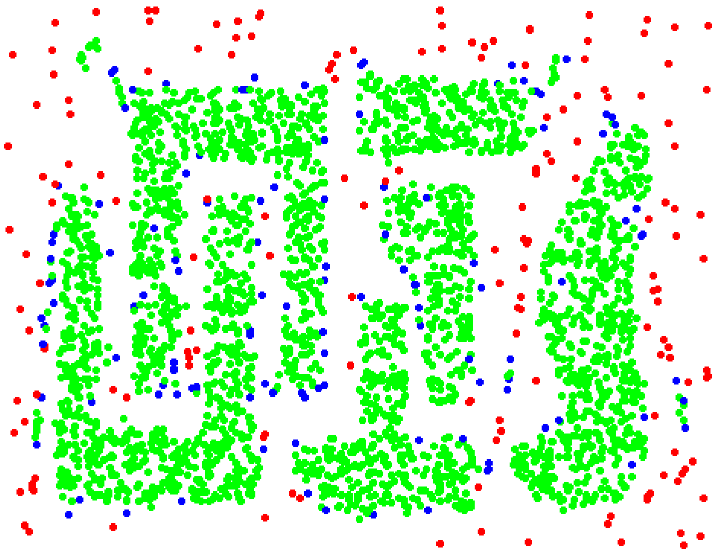
- Eliminate noise points
- Perform clustering on the remaining points

$current\_cluster\_label \leftarrow 1$
**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**

From: Tan,Steinbach, Kumar, Introduction to Data Mining, McGraw Hill 2006

# DBSCAN: Core, Border, and Noise Points

Original Points



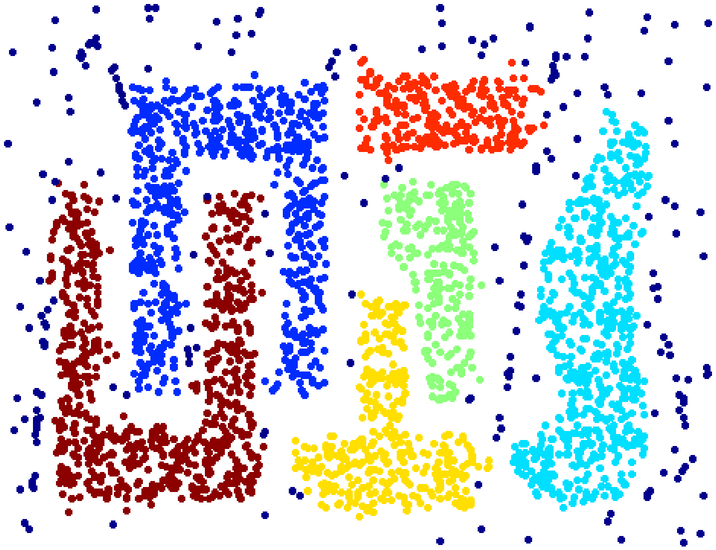
Point types: core, border and noise

Eps = 10, MinPts = 4

From: Tan,Steinbach, Kumar, Introduction to Data Mining, McGraw Hill 2006

# When DBSCAN Works Well

Original Points

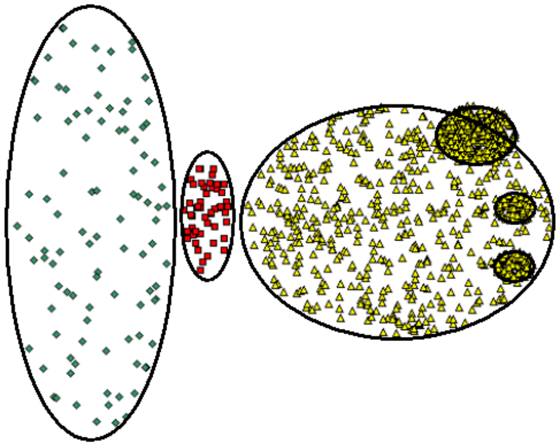


Clusters

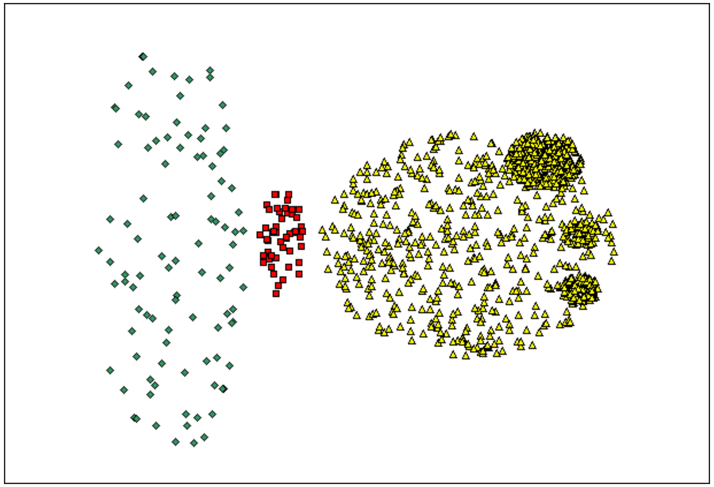
- Resistant to Noise
- Can handle clusters of different shapes and sizes

From: Tan,Steinbach, Kumar, Introduction to Data Mining, McGraw Hill 2006

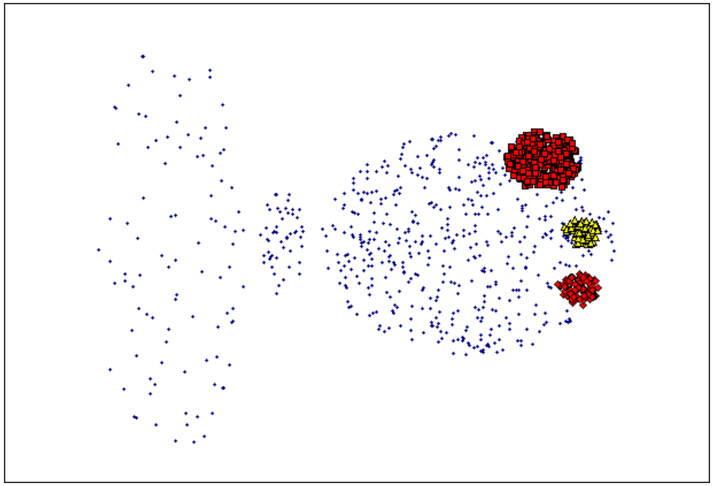
# When DBSCAN Does NOT Work Well



Original Points



(MinPts=4, Eps=9.75).



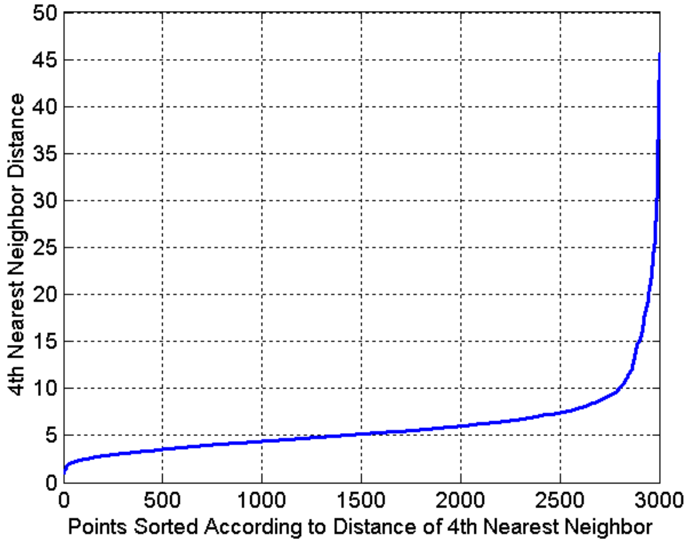
(MinPts=4, Eps=9.62)

- Varying densities
- High-dimensional data

From: Tan,Steinbach, Kumar, Introduction to Data Mining, McGraw Hill 2006

# 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




From: Tan,Steinbach, Kumar, Introduction to Data Mining, McGraw Hill 2006

# Measures of Cluster Validity

- The validation of clustering structures is the most difficult task
- To evaluate the “goodness” of the resulting clusters, some numerical measures can be exploited
- Numerical measures are classified into two main classes
  - External Index: Used to measure the extent to which cluster labels match externally supplied class labels.
    - e.g., entropy, purity
  - Internal Index: Used to measure the goodness of a clustering structure *without* respect to external information.
    - e.g., Sum of Squared Error (SSE), cluster cohesion, cluster separation, Rand-Index, adjusted rand-index, Silhouette index

# 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 $purity = \sum_{i=1}^{K} \frac{m_i}{m} purity_j$.

From: Tan,Steinbach, Kumar, Introduction to Data Mining, McGraw Hill 2006

# Internal Measures: Cohesion and Separation

- **Cluster Cohesion**: Measures how closely related are objects in a cluster
  - Cohesion is measured by the within cluster sum of squares (SSE)

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

- **Cluster Separation**: Measure how distinct or well-separated a cluster is from other clusters
  - Separation is measured by the between cluster sum of squares

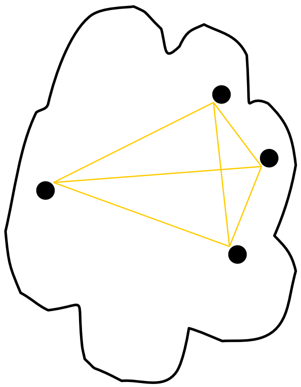
$$BSS = \sum_{i} |C_i| (m - m_i)^2$$



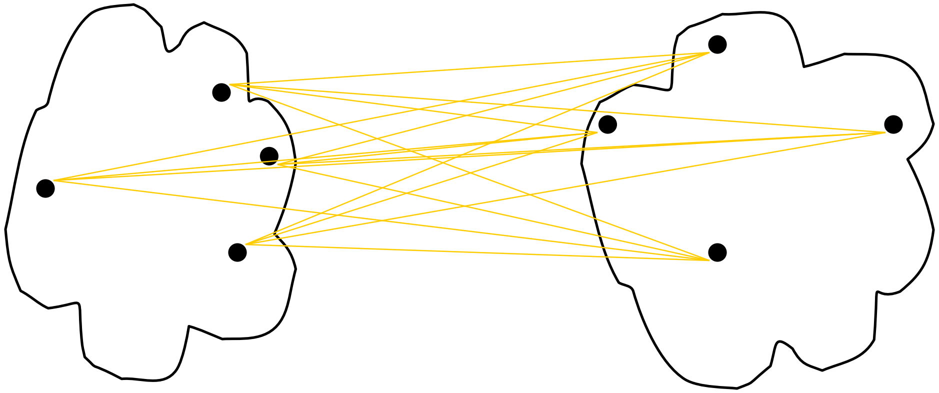
From: Tan,Steinbach, Kumar, Introduction to Data Mining, McGraw Hill 2006

# 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

# Evaluating cluster quality: Silhouette

- To ease the interpretation and validation of consistency within clusters of data
  - a succinct measure to evaluate how well each object lies within its cluster
- For each object *i*
  - *a(i):* the average dissimilarity of *i* with all other data within the same cluster (the smaller the value, the better the assignment)
  - *b(i):* is the lowest average dissimilarity of *i* to any other cluster, of which *i* is not a member

$$s(i) = \frac{b(i) - a(i)}{\max\{a(i), b(i)\}} \qquad s(i) = \begin{cases} 1 - a(i)/b(i), & a(i) < b(i) \\ 0, & a(i) = b(i) \\ b(i)/a(i) - 1 & a(i) > b(i) \end{cases}$$

  - The average s(i) over all data of the dataset measures how appropriately the data has been clustered
  - The average s(i) over all data of a cluster measures how tightly grouped all the data in the cluster are

# 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