Clustering fundamentals

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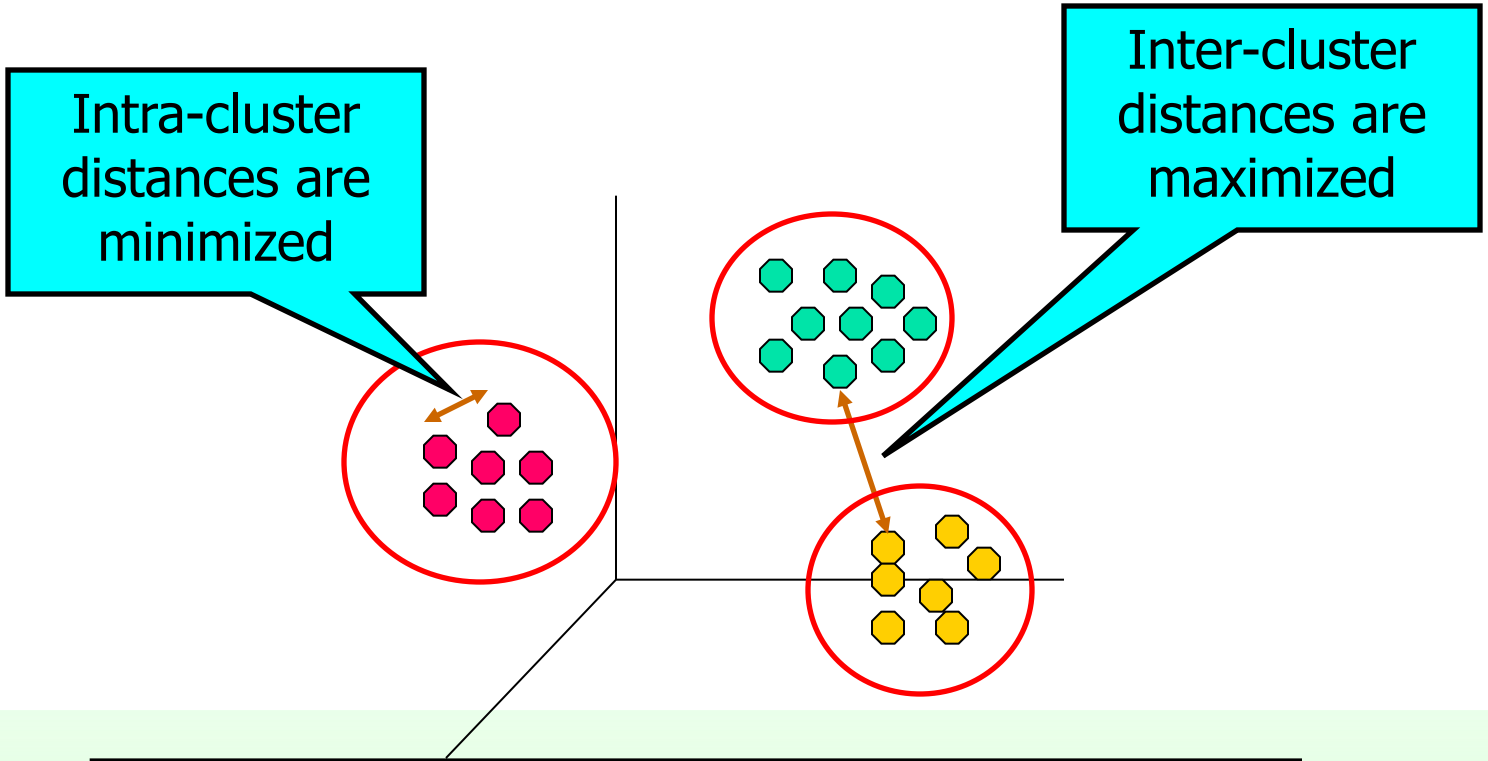
What is Cluster Analysis?

- 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



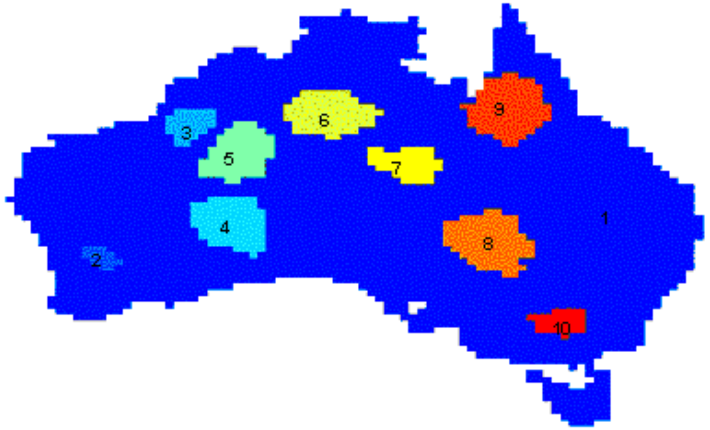
From: Tan,Steinbach, Kumar, Introduction to Data Mining, McGraw Hill 2006

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

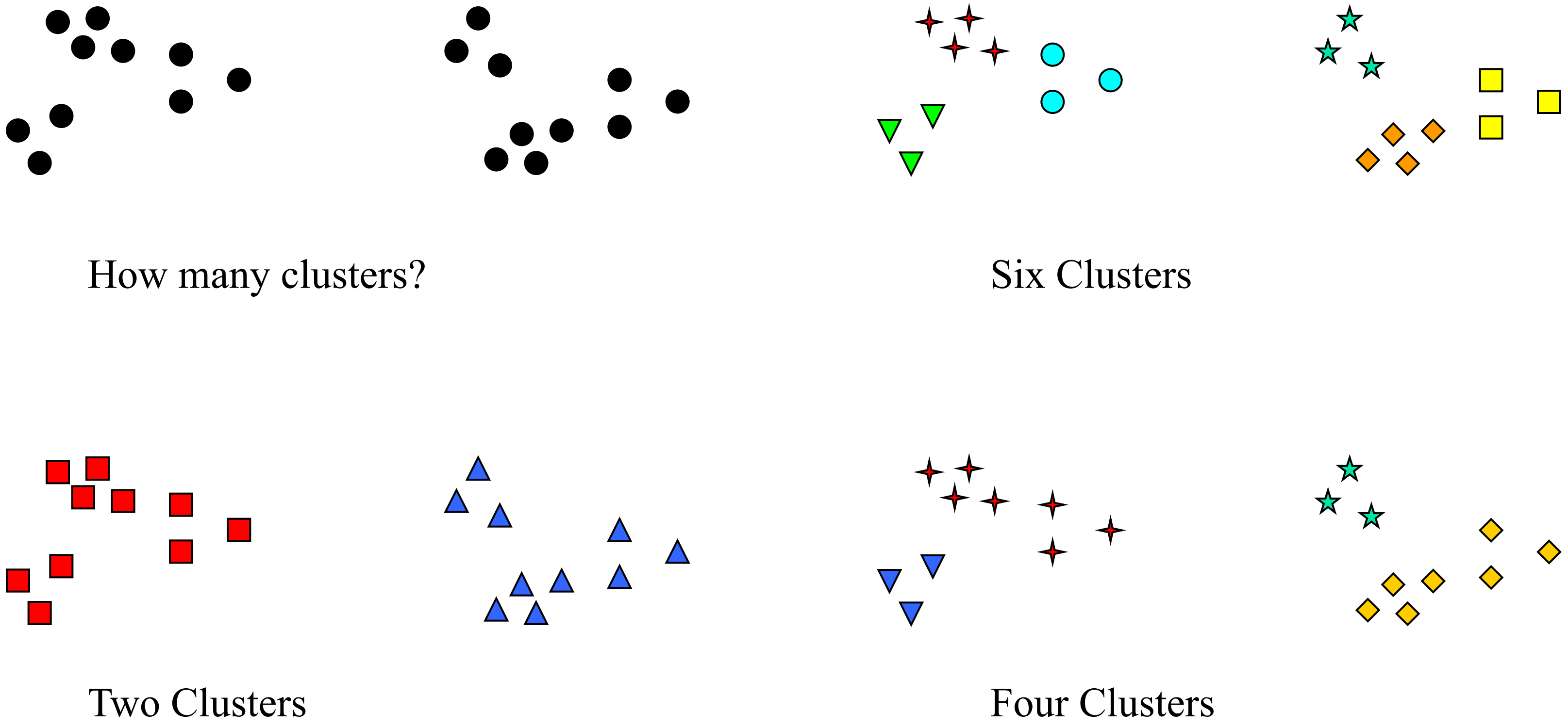
- **Summarization**
  - Reduce the size of large data sets



Clustering precipitation in Australia

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

Notion of a Cluster can be Ambiguous



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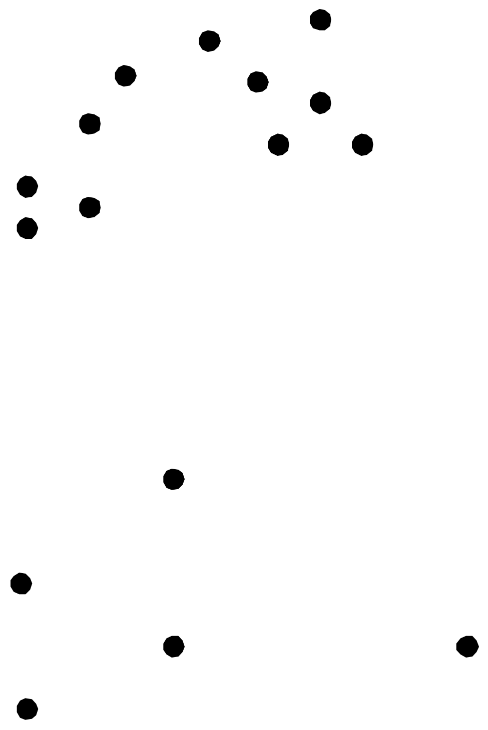
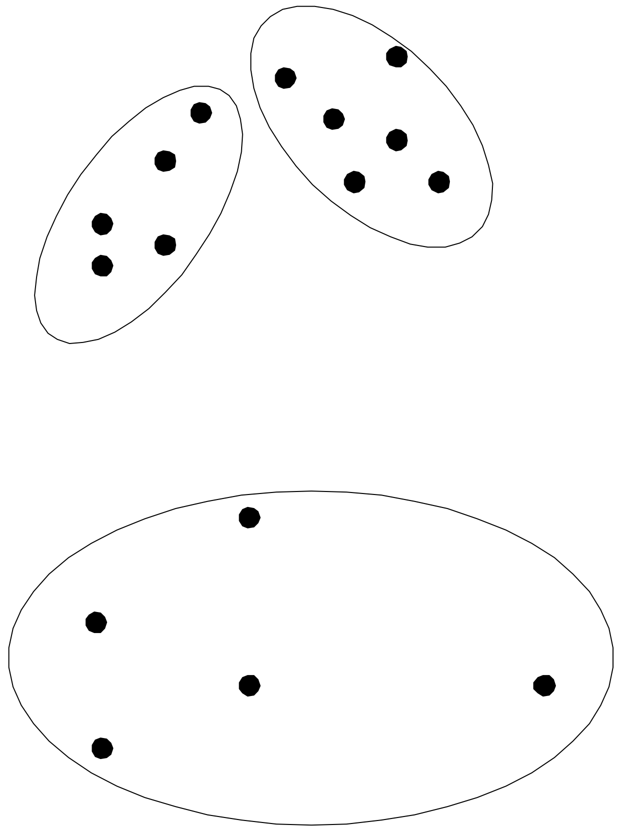
Types of Clusterings

- A clustering is a set of clusters
- Important distinction between hierarchical and partitional sets of clusters
- Partitional Clustering
  - Divides data objects into non-overlapping subsets (clusters) such that each data object is in exactly one subset
- Hierarchical clustering
  - A set of nested clusters organized as a hierarchical tree

Partitional Clustering

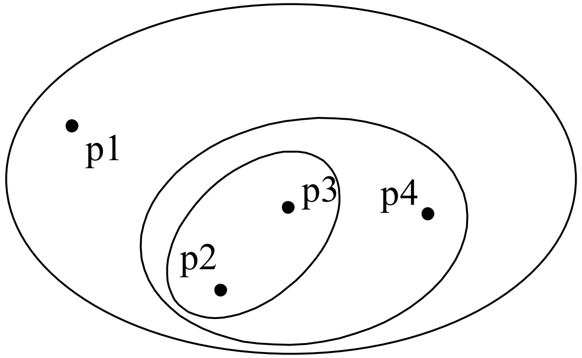


Original Points

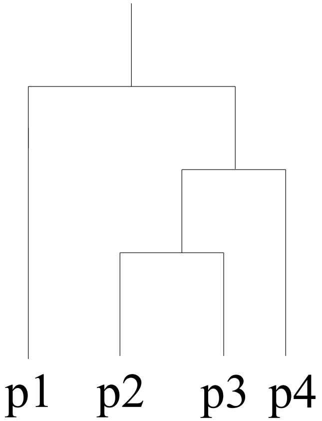


A Partitional Clustering

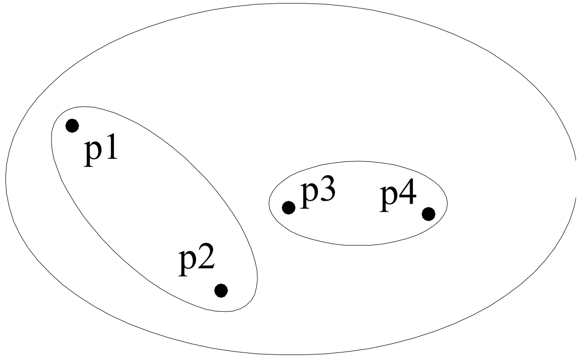
Hierarchical Clustering



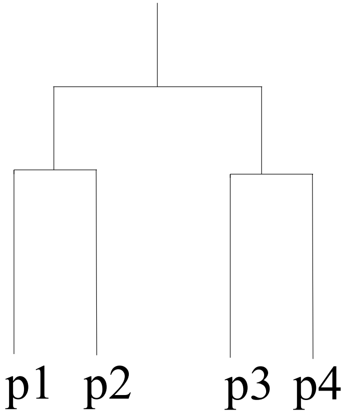
Traditional Hierarchical Clustering



Traditional Dendrogram



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

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

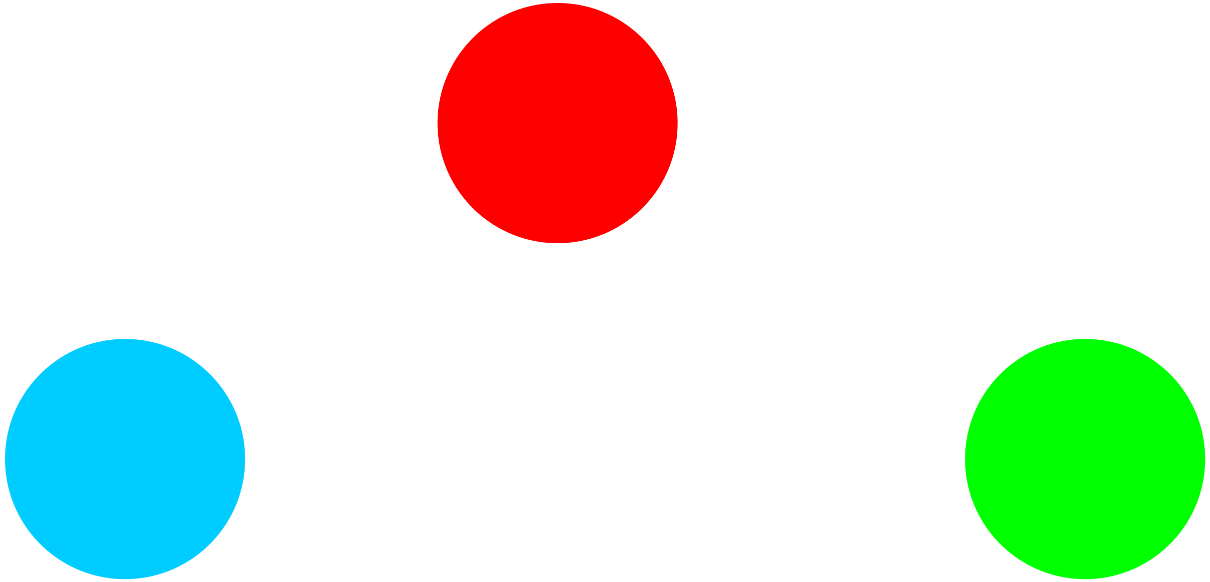
Types of Clusters

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

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

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

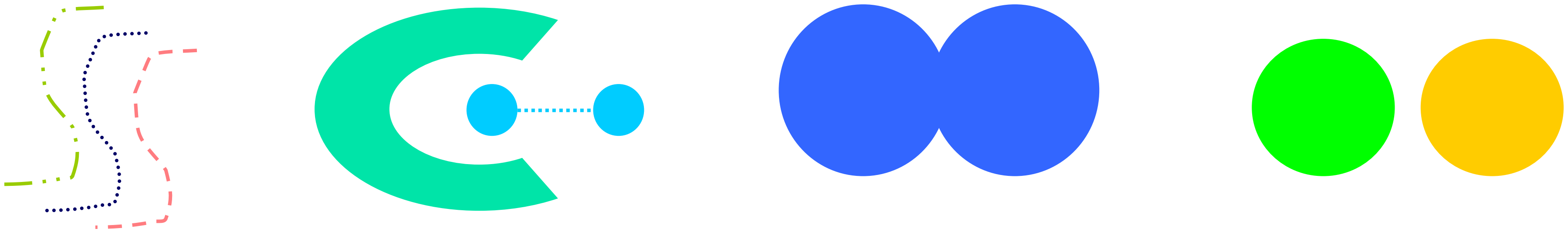
- Center-based
  - A cluster is a set of objects such that an object in a cluster is closer (more similar) to the "center" of a cluster, than to the center of any other cluster
  - The center of a cluster is often a centroid, the average of all the points in the cluster, or a medoid, the most "representative"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

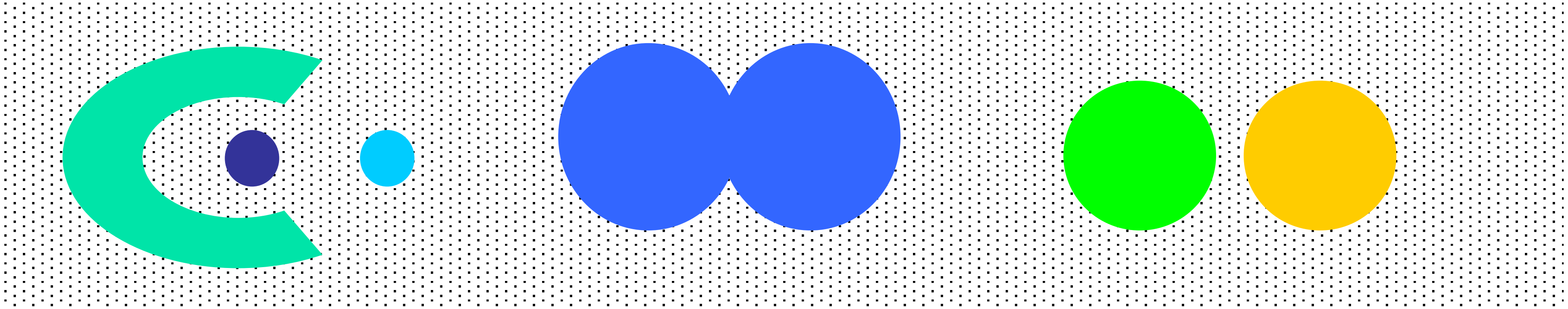


8 contiguous clusters

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.

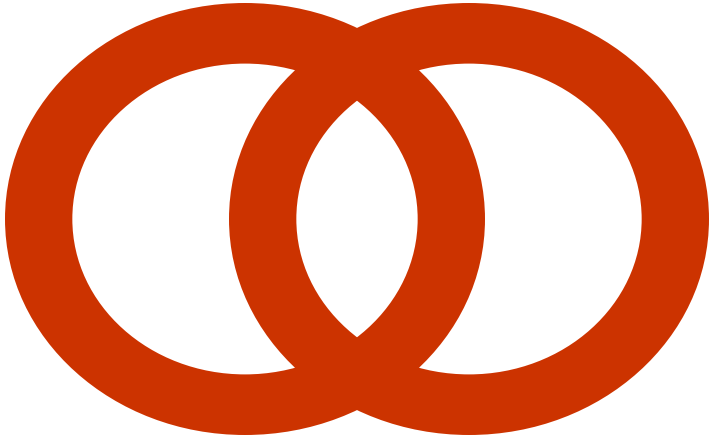


6 density-based clusters

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.



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

```
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
```

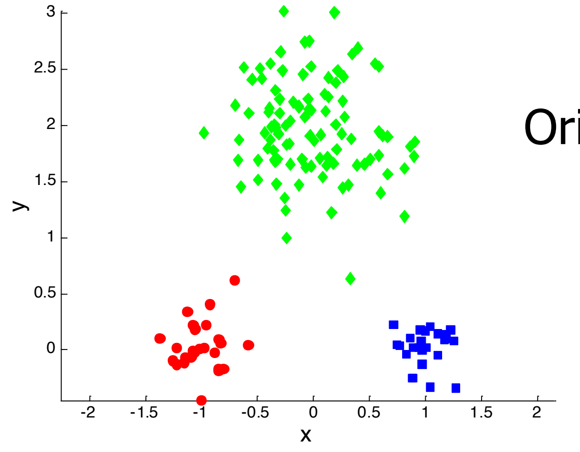
From: Tan,Steinbach, Kumar, Introduction to Data Mining, McGraw Hill 2006

K-means Clustering – Details

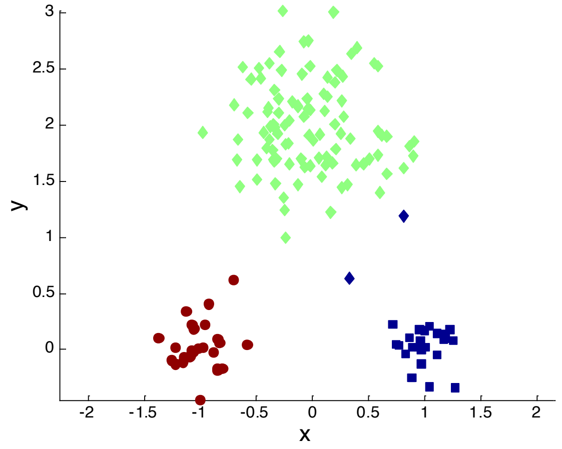
- Initial centroids are often chosen randomly.
  - Clusters produced vary from one run to another.
- The centroid is (typically) the mean of the points in the cluster.
- ‘Closeness’ is measured by Euclidean distance, cosine similarity, correlation, etc.
- K-means will converge for common similarity measures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

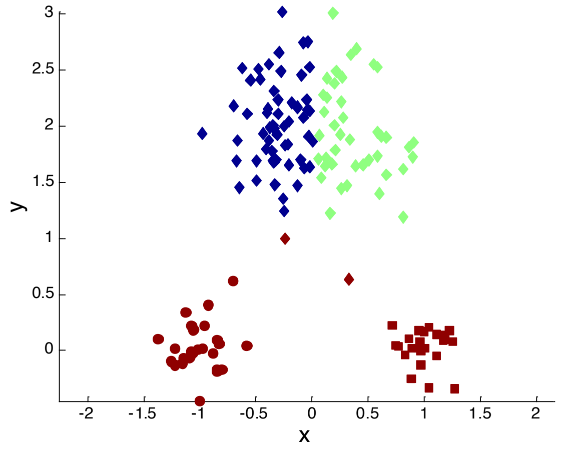
Two different K-means Clusterings



Original Points



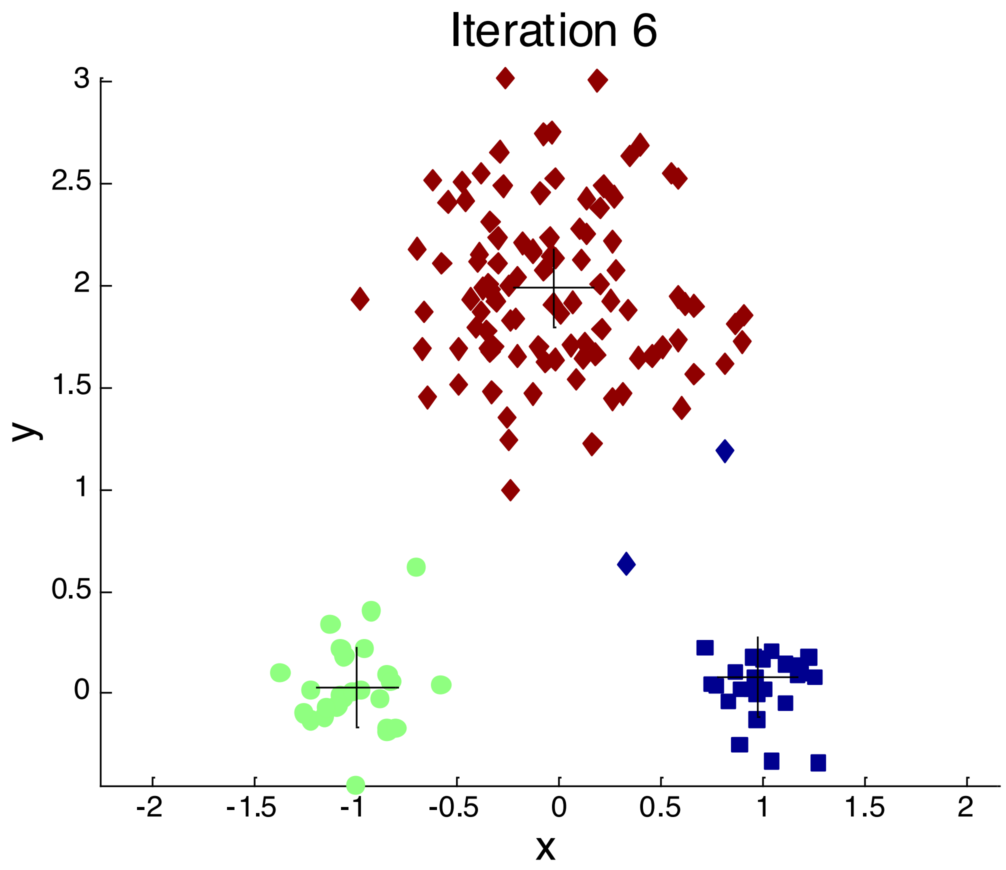
Optimal Clustering



Sub-optimal Clustering

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

Importance of Choosing Initial Centroids



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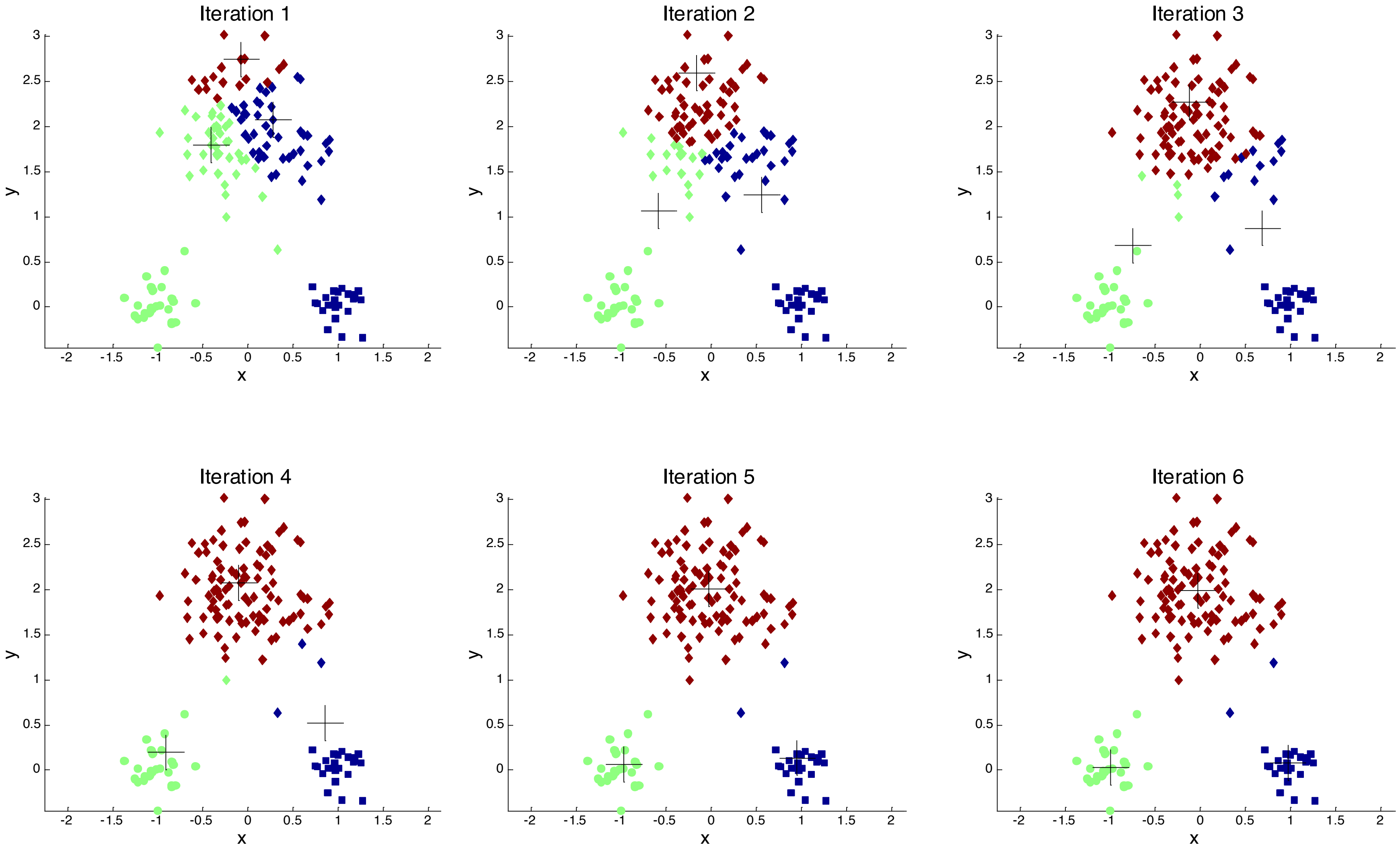

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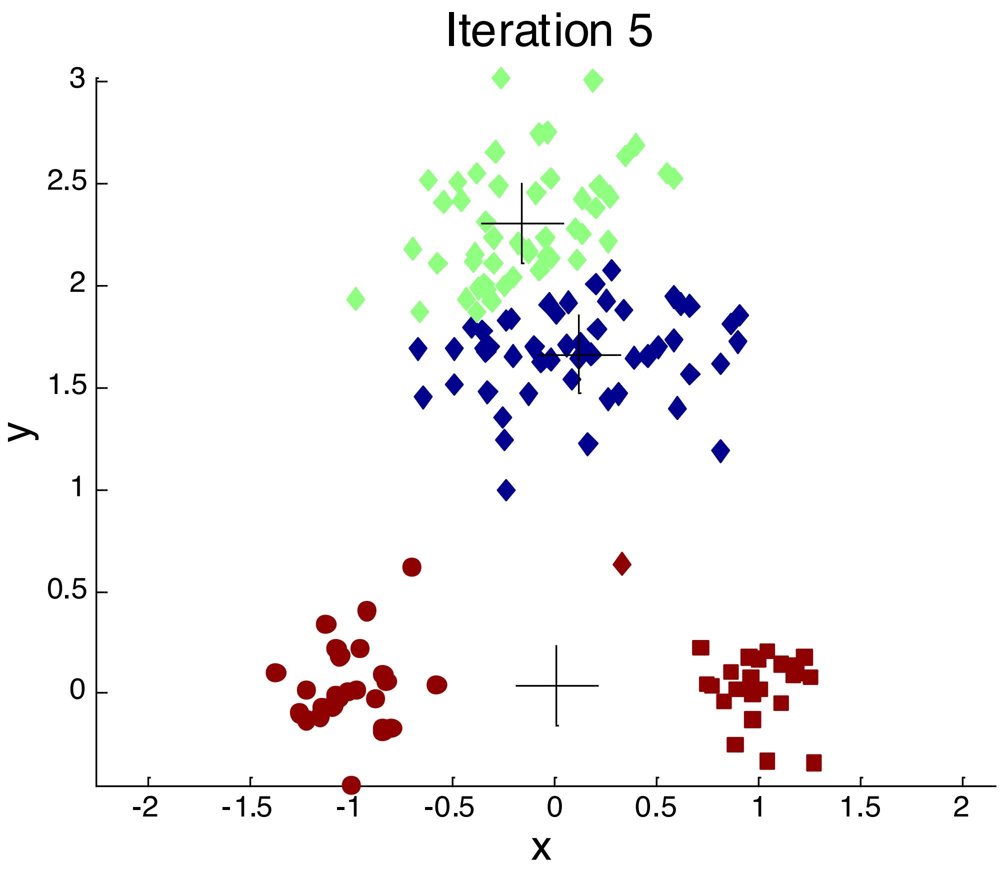

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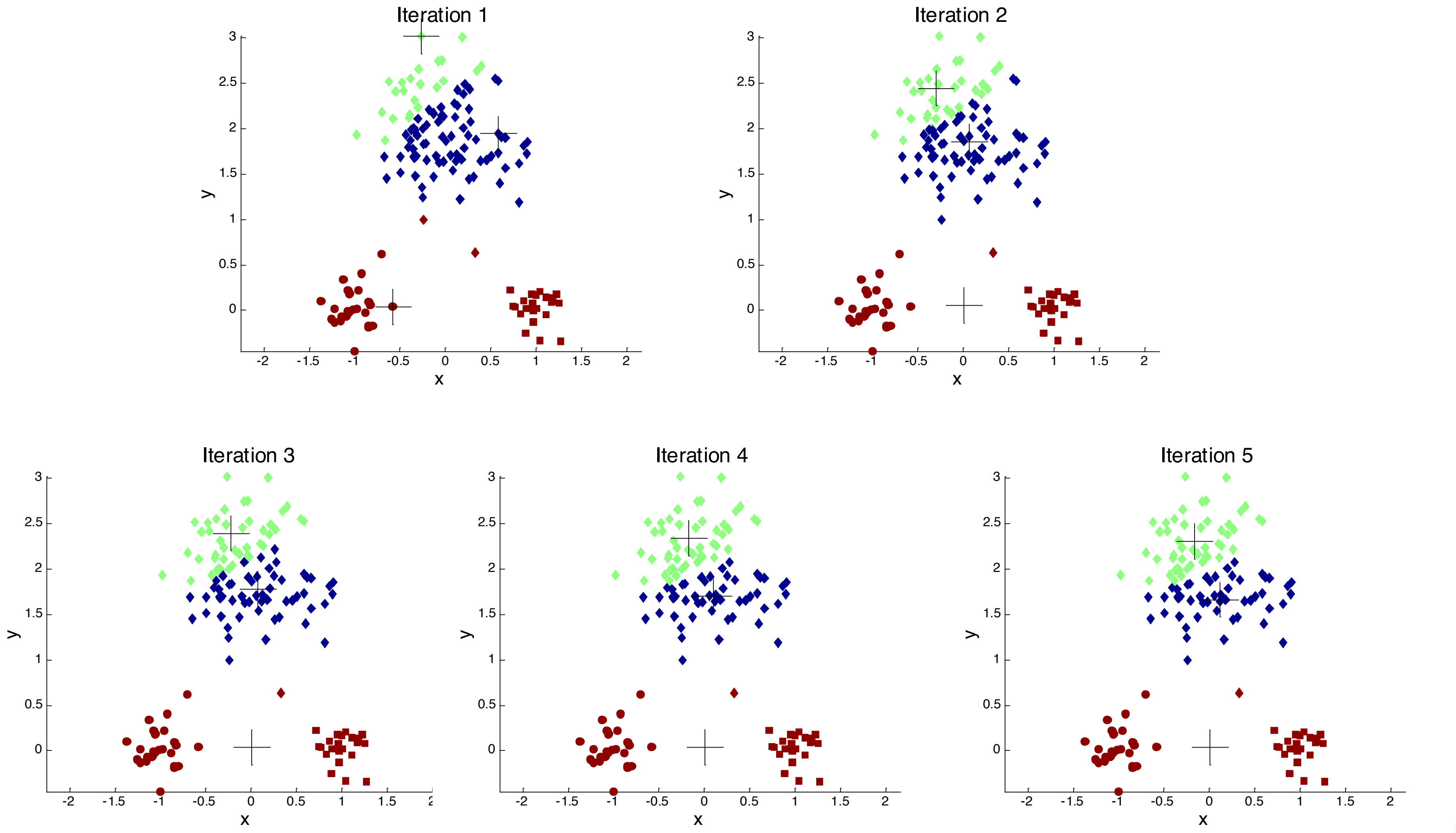

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Evaluating K-means Clusters

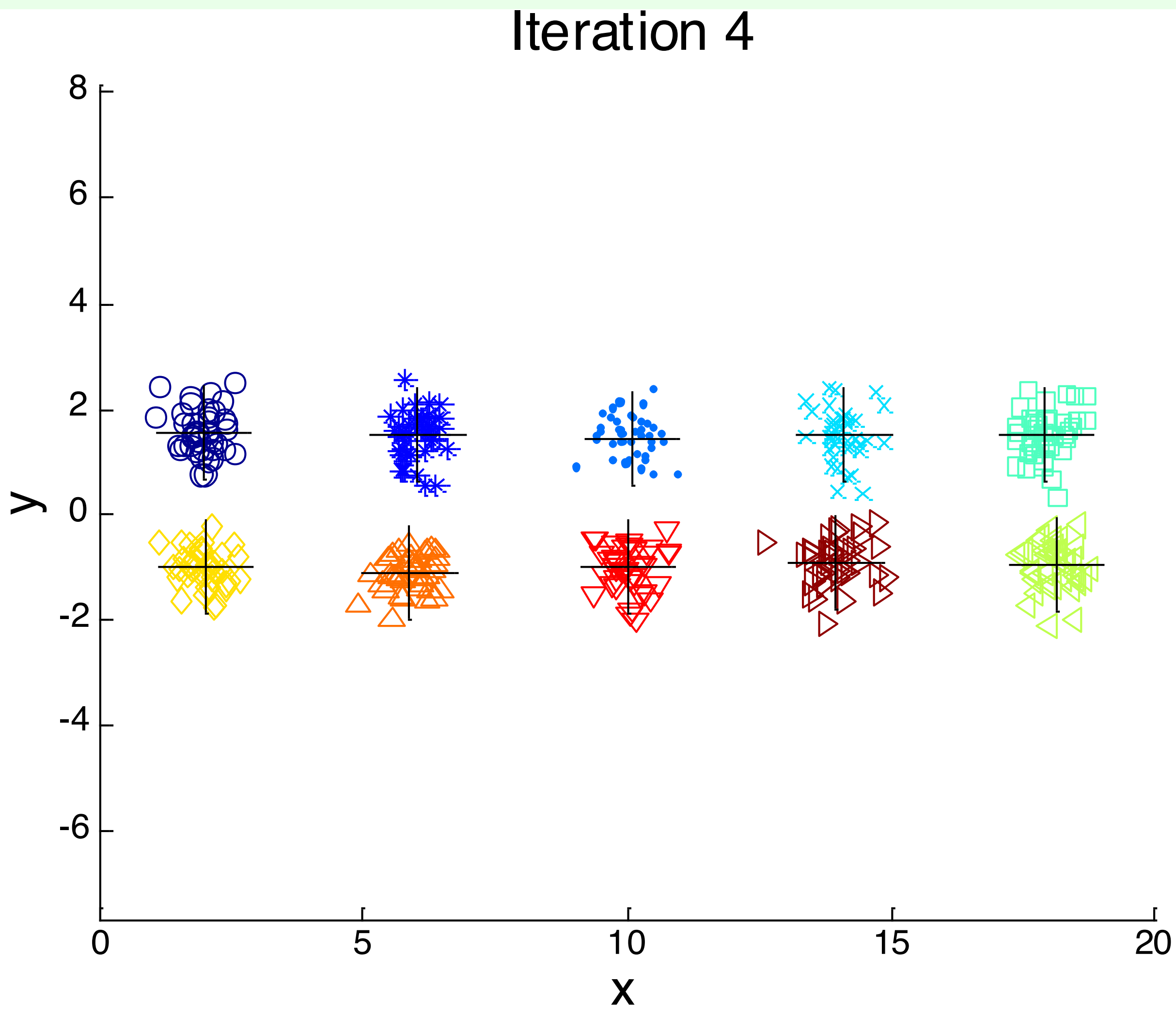
- Most common measure is Sum of Squared Error (SSE)
  - For each point, the error is the distance to the nearest cluster
  - To get SSE, we square these errors and sum them.

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

  - x is a data point in cluster C_i and m_i is the representative 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

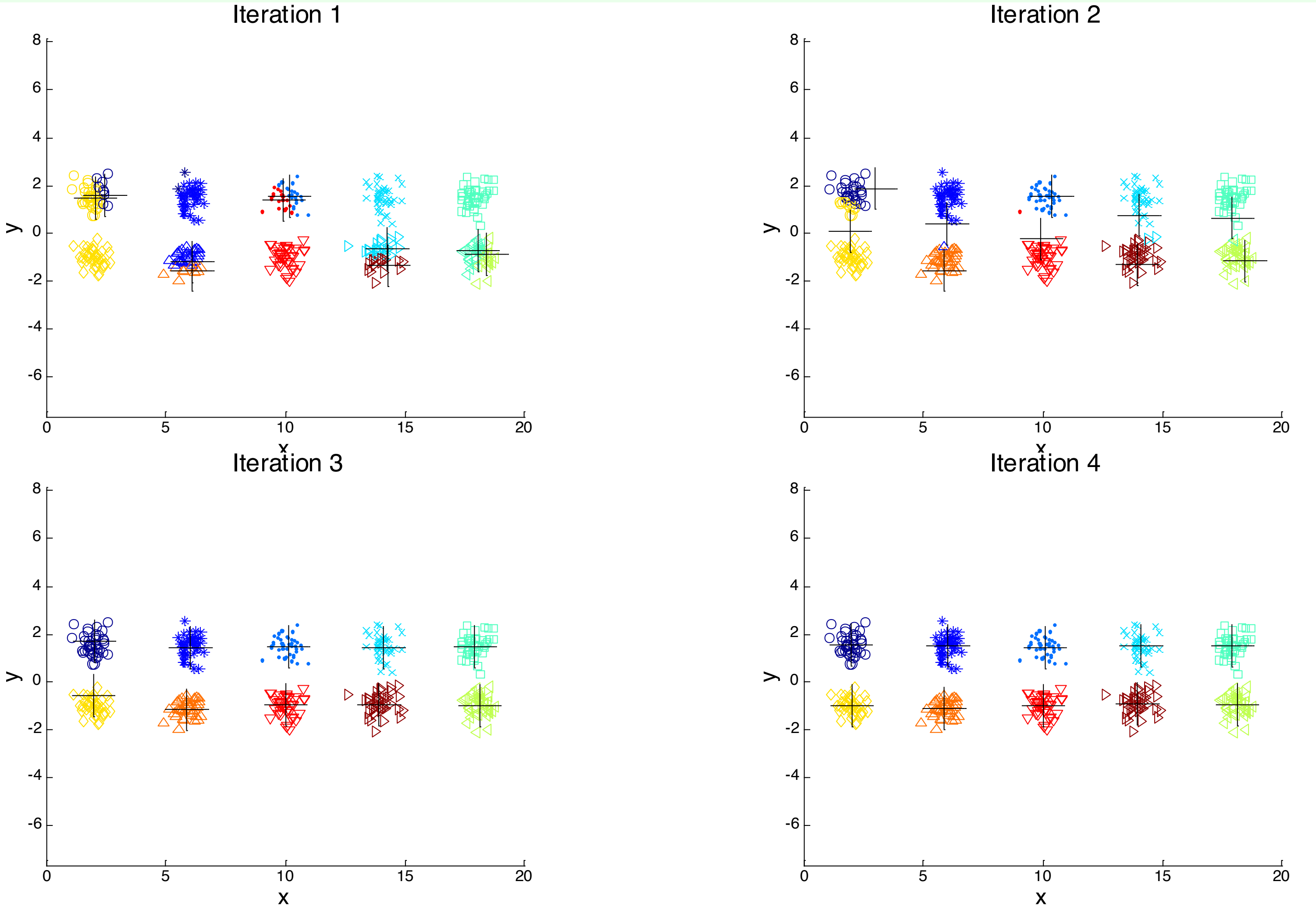
10 Clusters Example



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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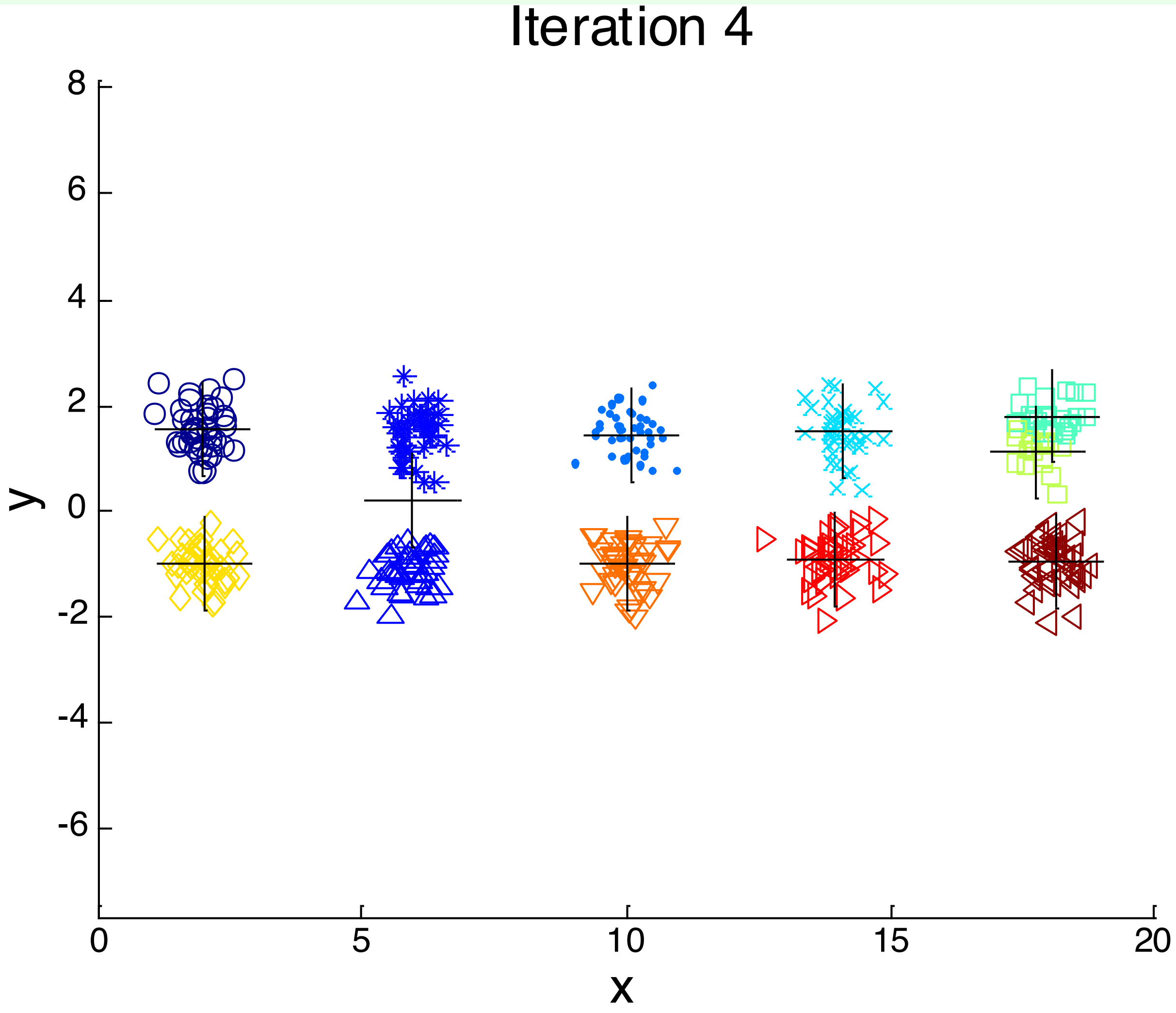
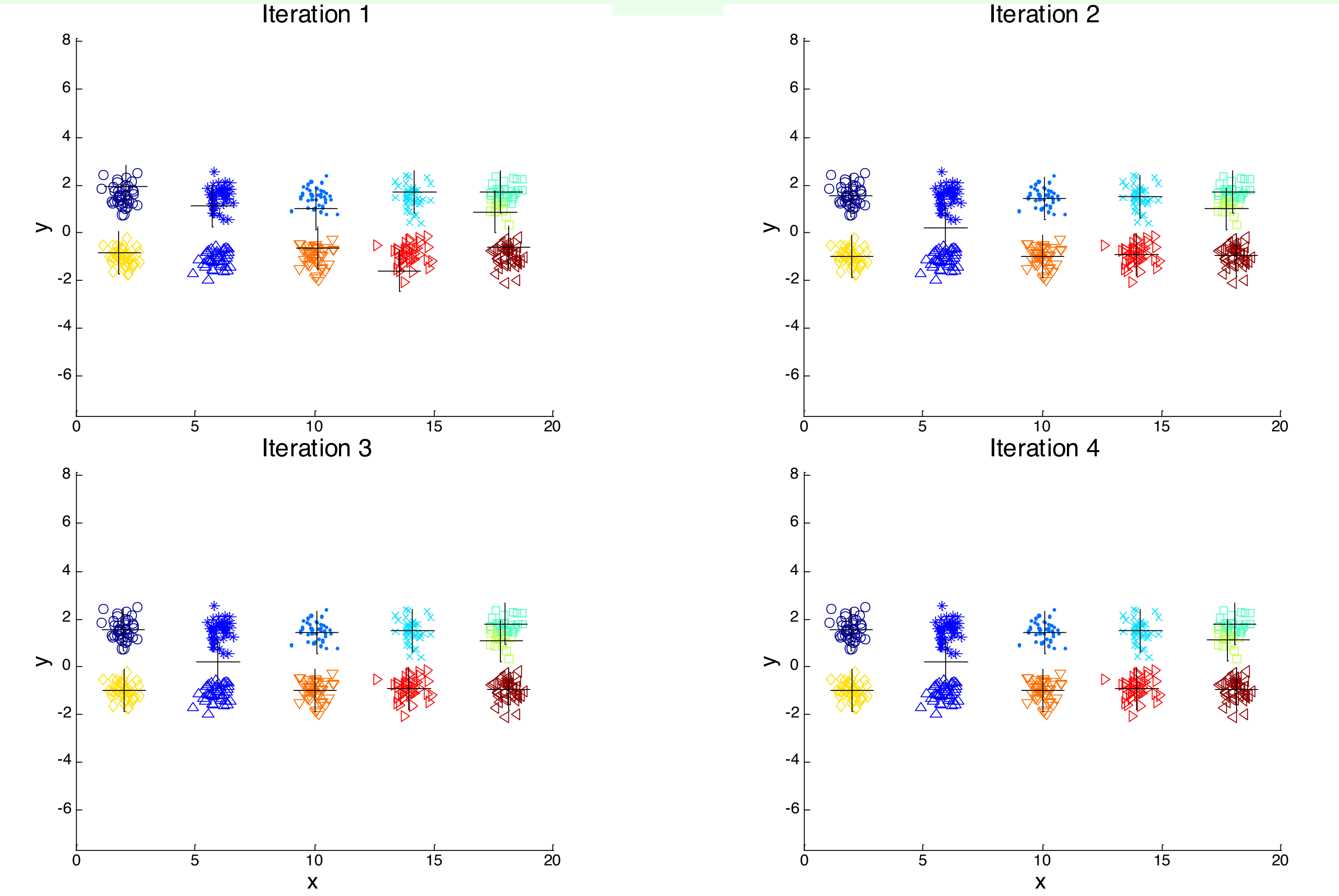


Starting with some pairs of clusters having three initial centroids, while other have only one.

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.

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

Solutions to Initial Centroids Problem

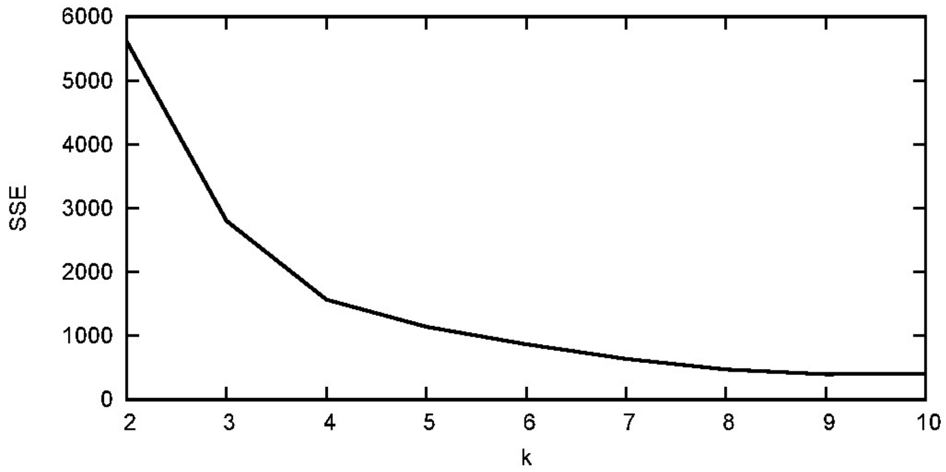
- Multiple runs
  - Helps, but probability is not on your side
- Sample and use hierarchical clustering to determine initial centroids
- Select more than k initial centroids and then select among these initial centroids
  - Select most widely separated
- Postprocessing
- Bisecting K-means
  - Not as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

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

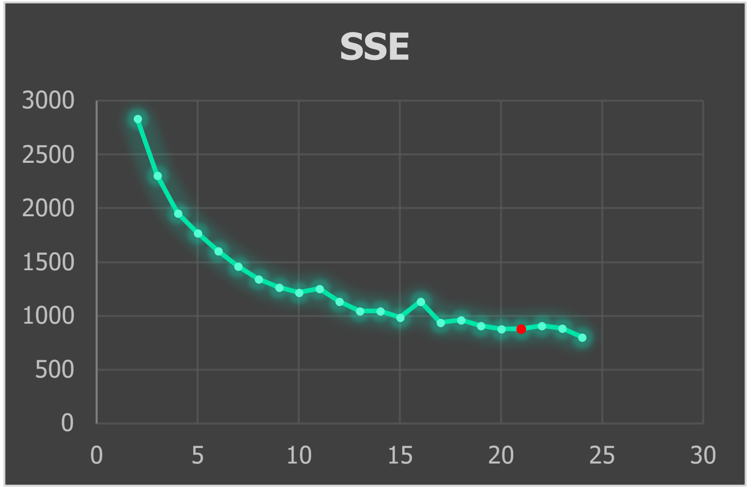
K-means parameter setting

- 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



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

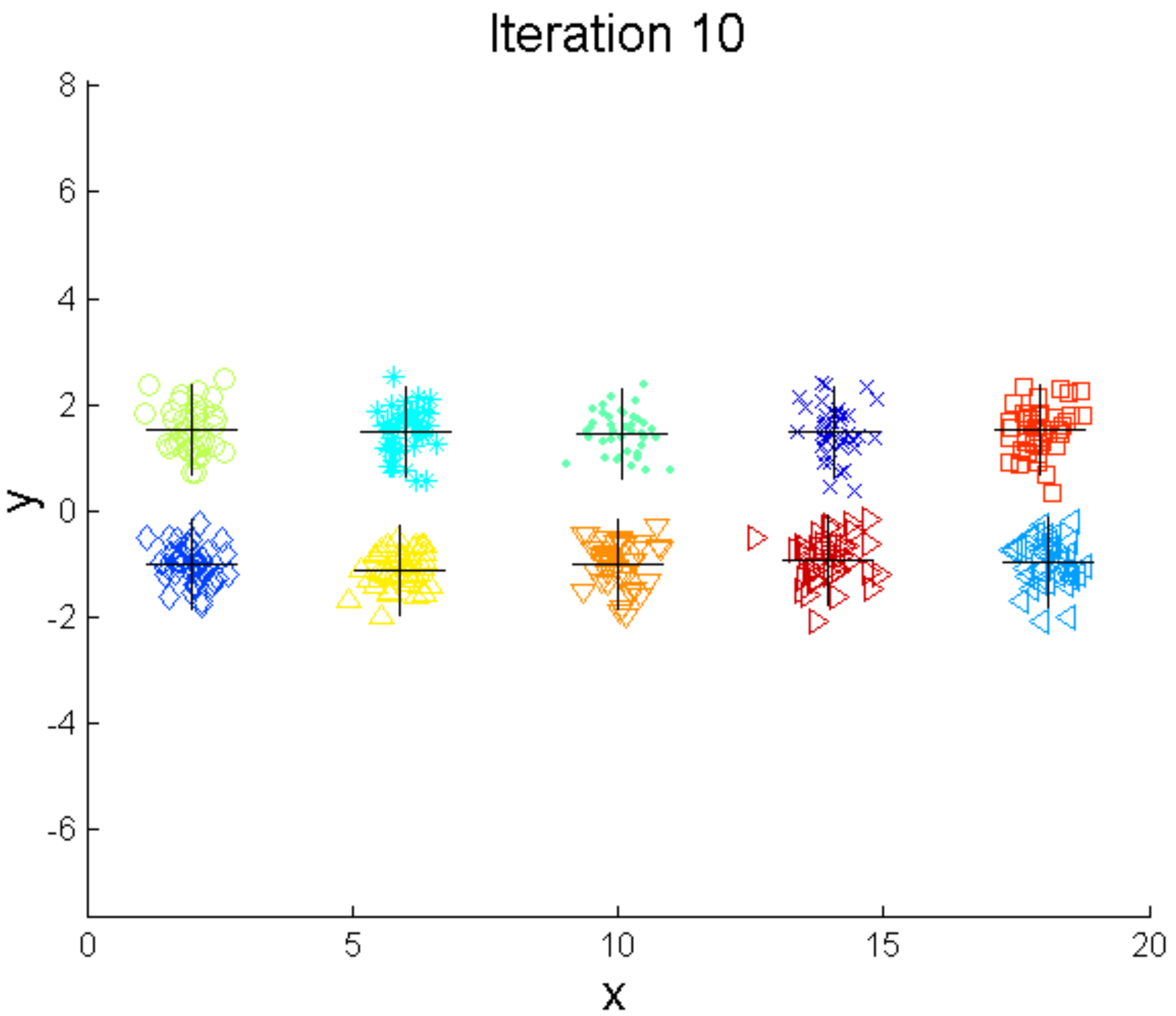
From: Tan,Steinbach, Kumar, Introduction to Data Mining, McGraw Hill 2006

- Bisecting K-means 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



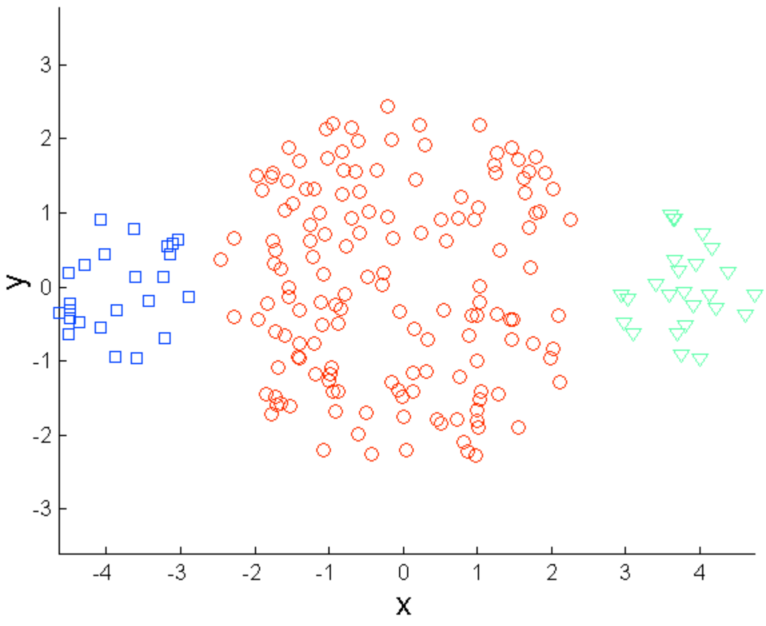
From: Tan,Steinbach, Kumar, Introduction to Data Mining, McGraw Hill 2006

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



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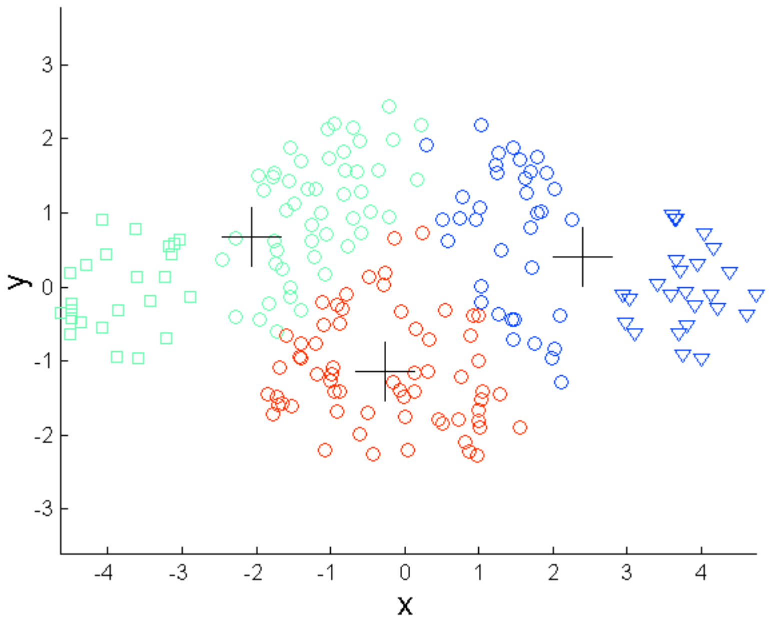
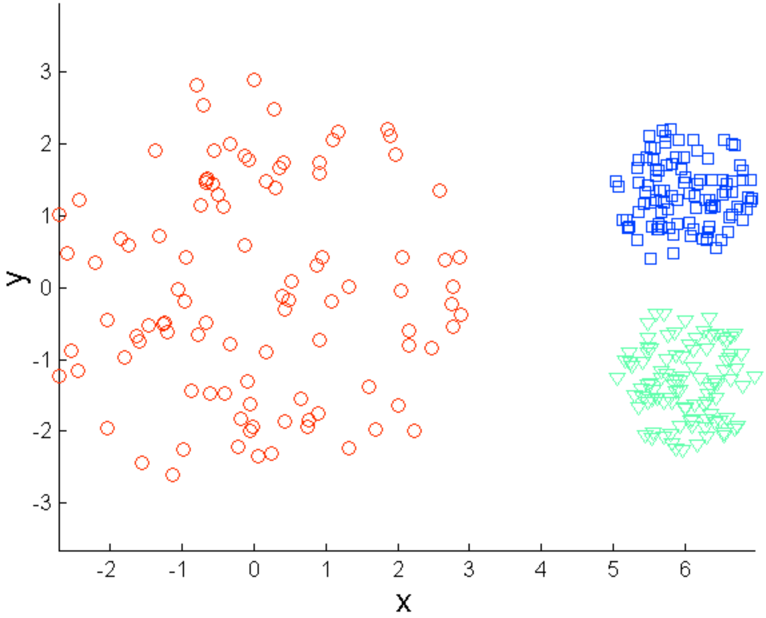


K-means (3 Clusters)

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

Limitations of K-means: Differing Density



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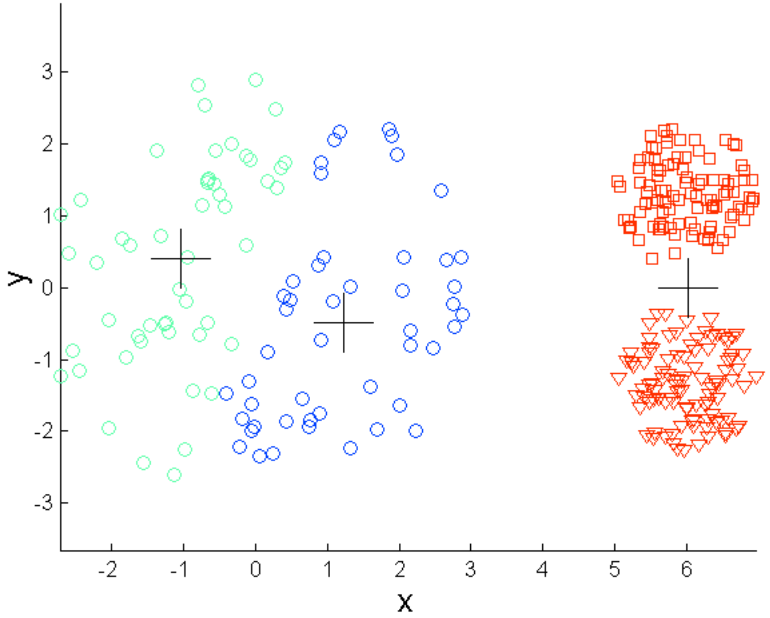

K-means (3 Clusters)

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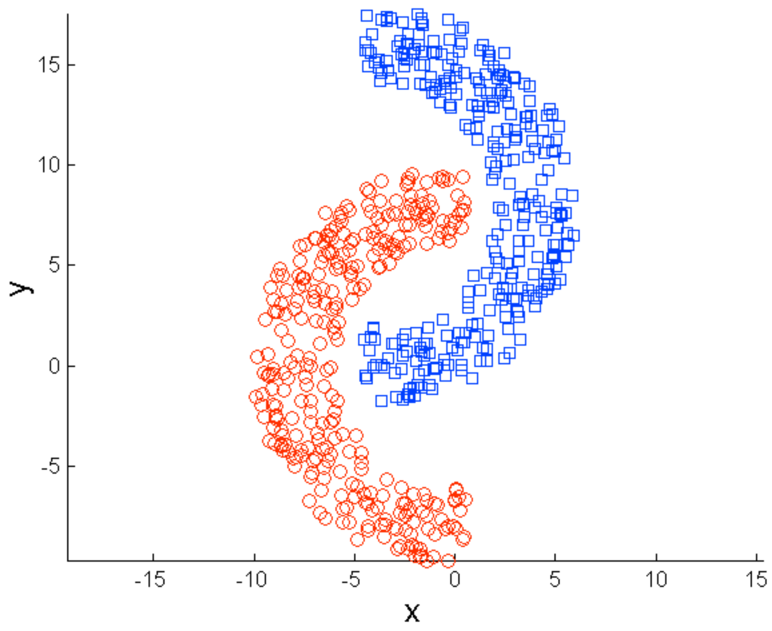
Limitations of K-means: Non-globular Shapes



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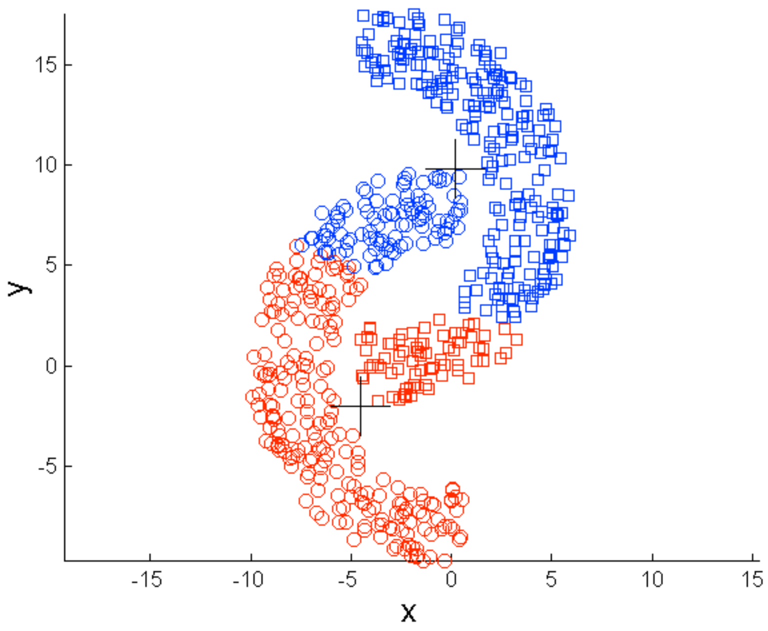
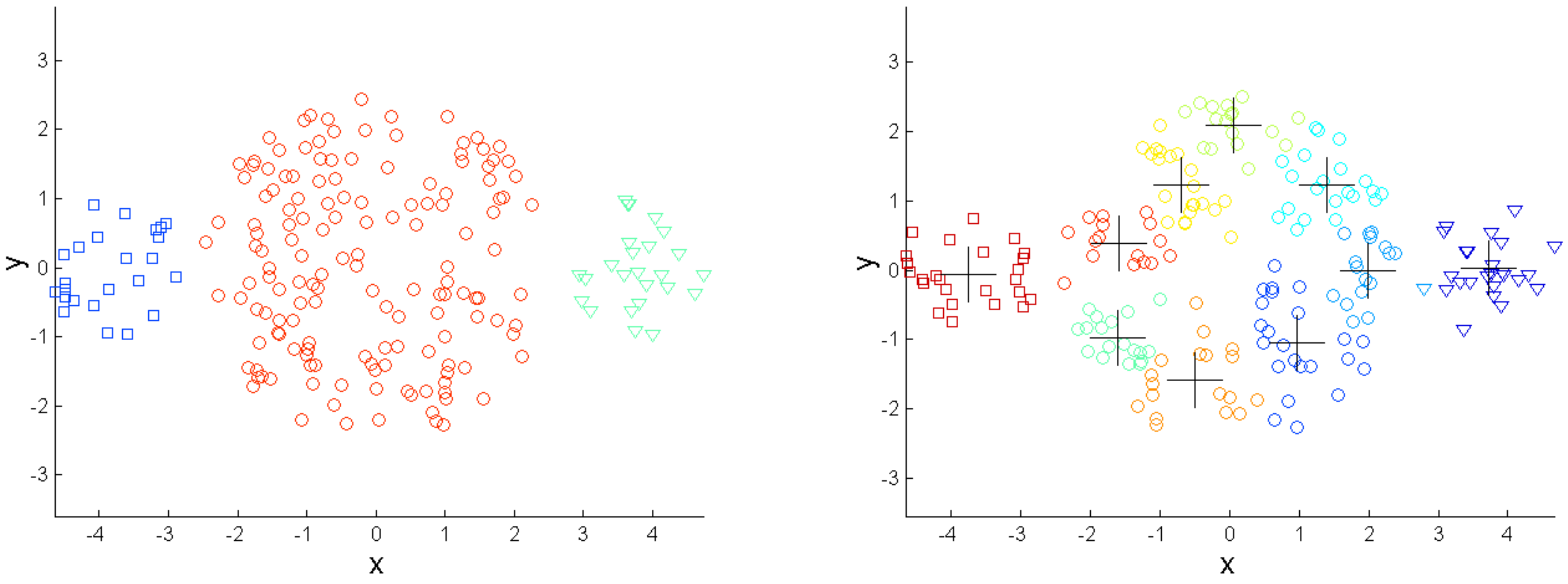


K-means (2 Clusters)

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

Overcoming K-means Limitations



Original Points

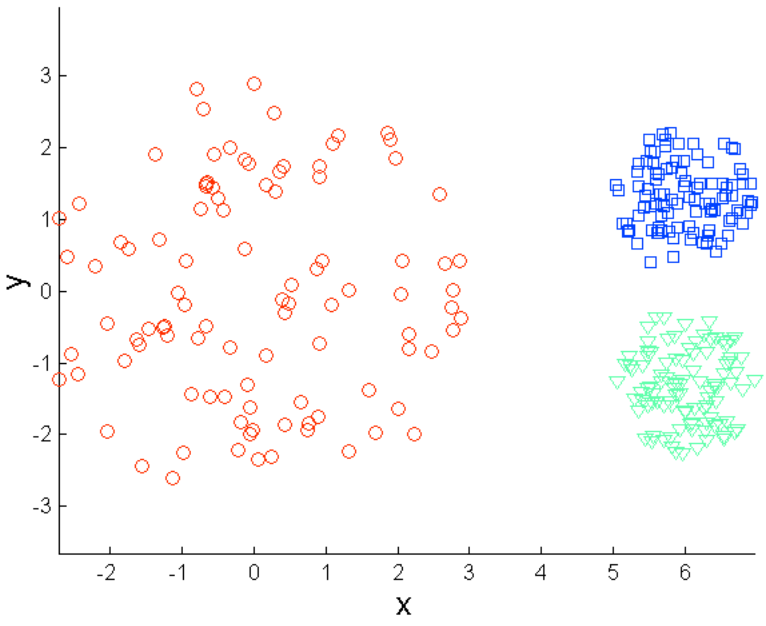
K-means Clusters

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



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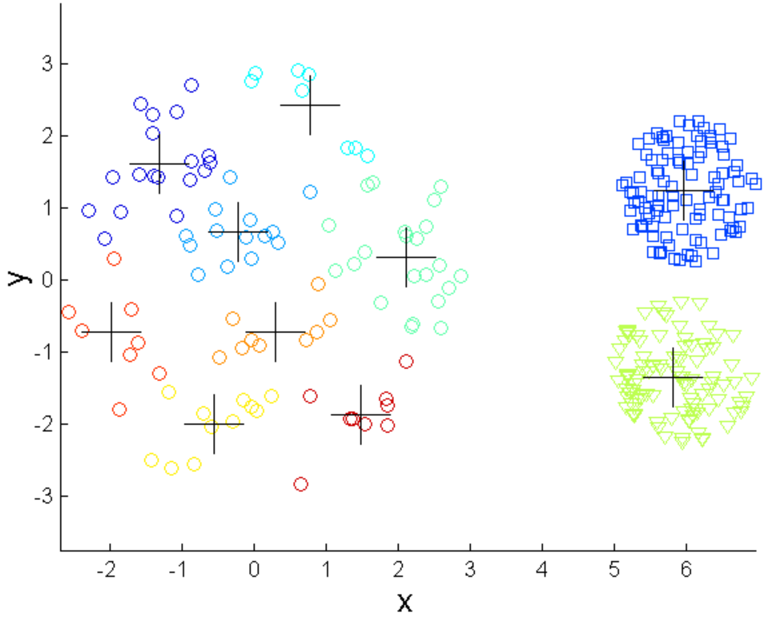

K-means Clusters

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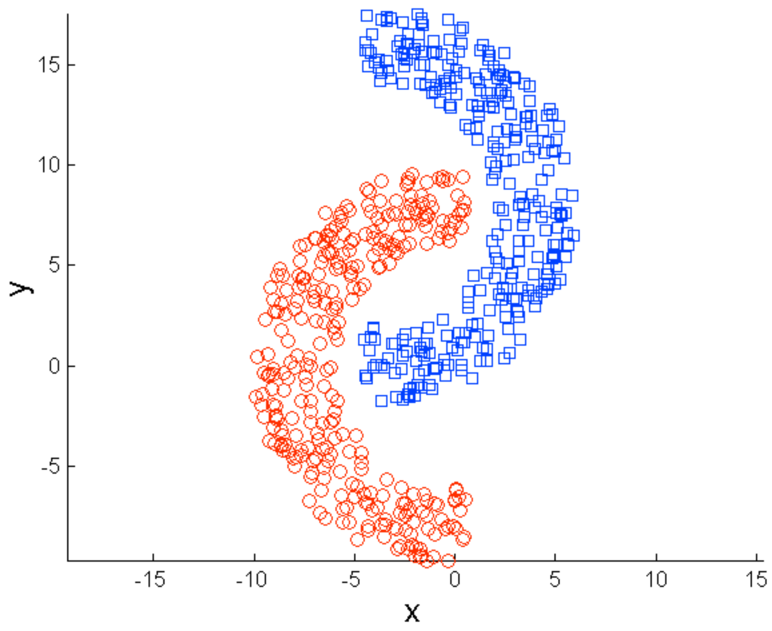
Overcoming K-means Limitations



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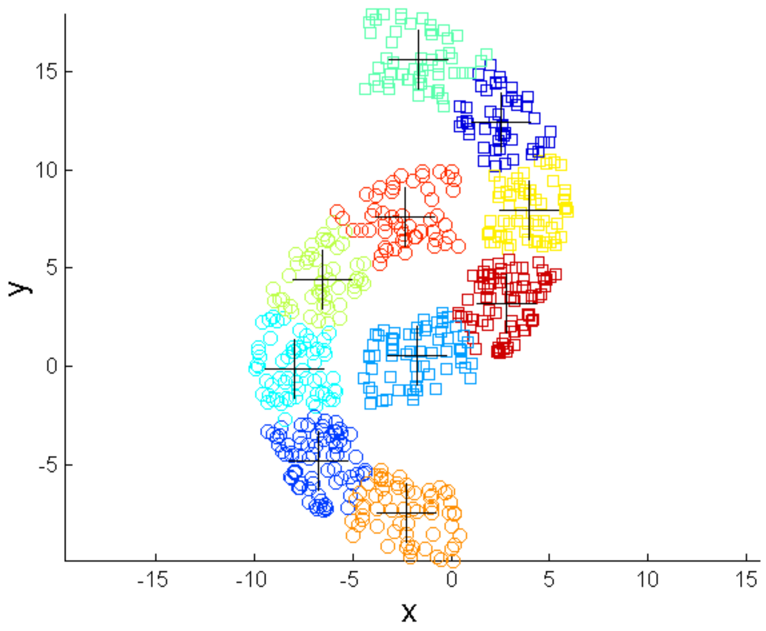
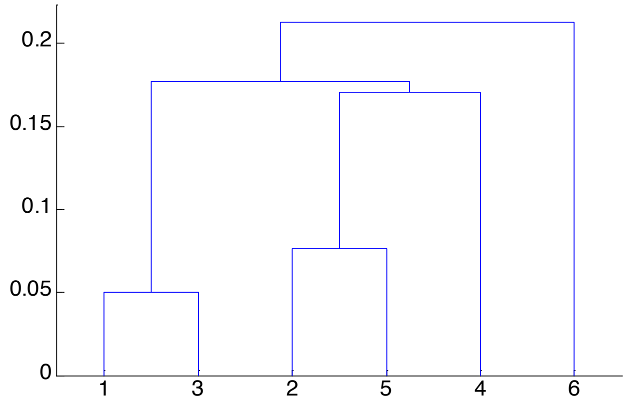


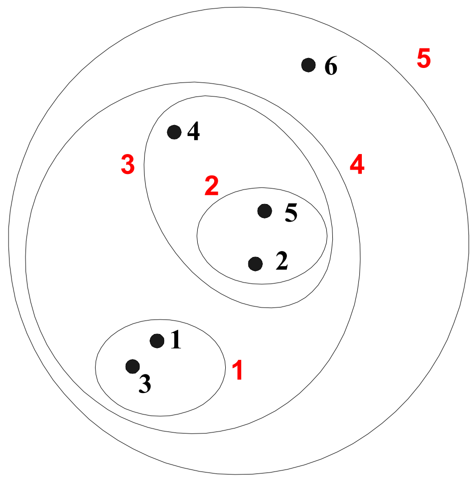
K-means Clusters

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

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

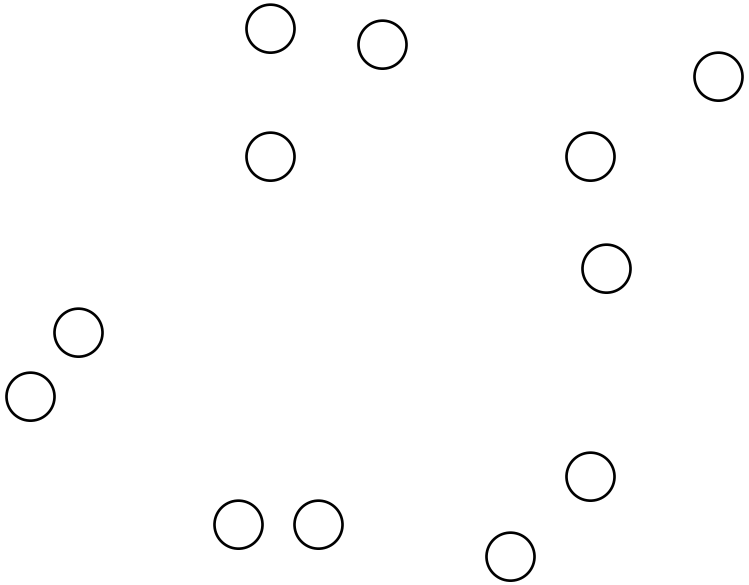
Agglomerative Clustering Algorithm

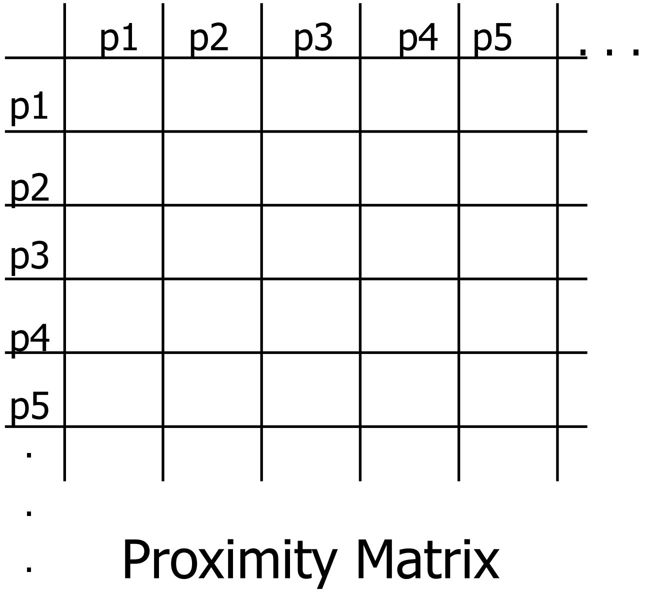
- More popular hierarchical clustering technique
- Basic algorithm is straightforward
  1. Compute the proximity matrix
  2. Let each data point be a cluster
  3. **Repeat**
  4. Merge the two closest clusters
  5. Update the proximity matrix
  6. **Until** only a single cluster remains
- Key operation 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

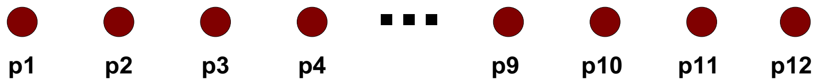
Starting Situation

- Start with clusters of individual points and a proximity matrix





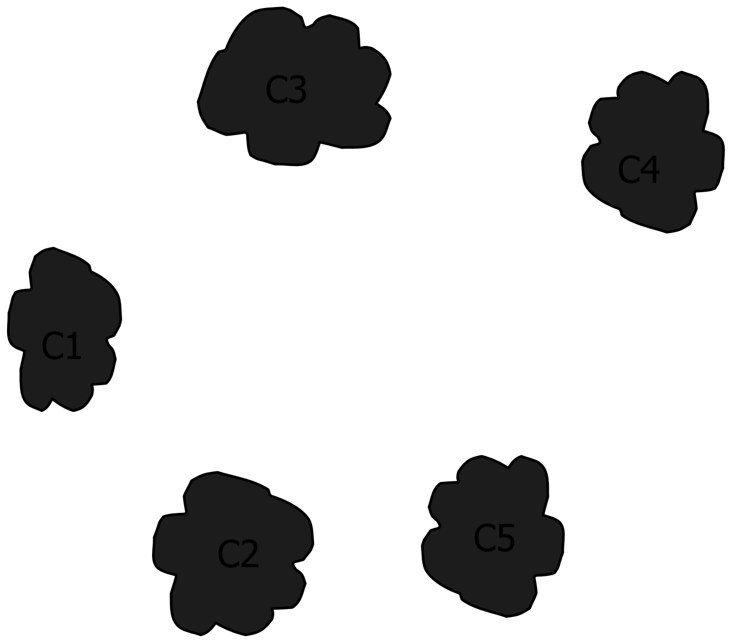
Proximity Matrix



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

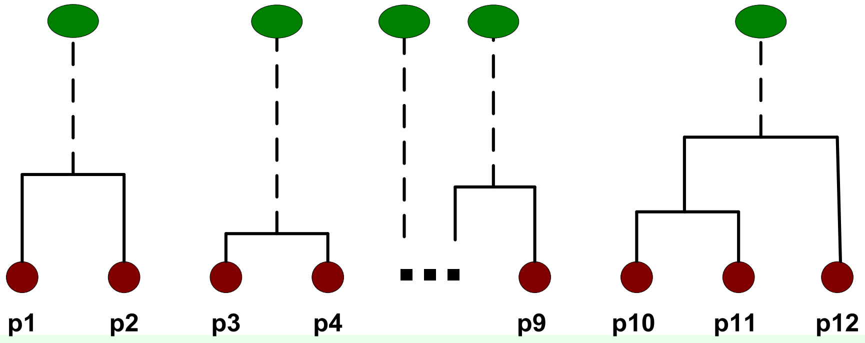
Intermediate Situation

- After some merging steps, we have some clusters



	C1	C2	C3	C4	C5
C1					
C2					
C3					
C4					
C5					

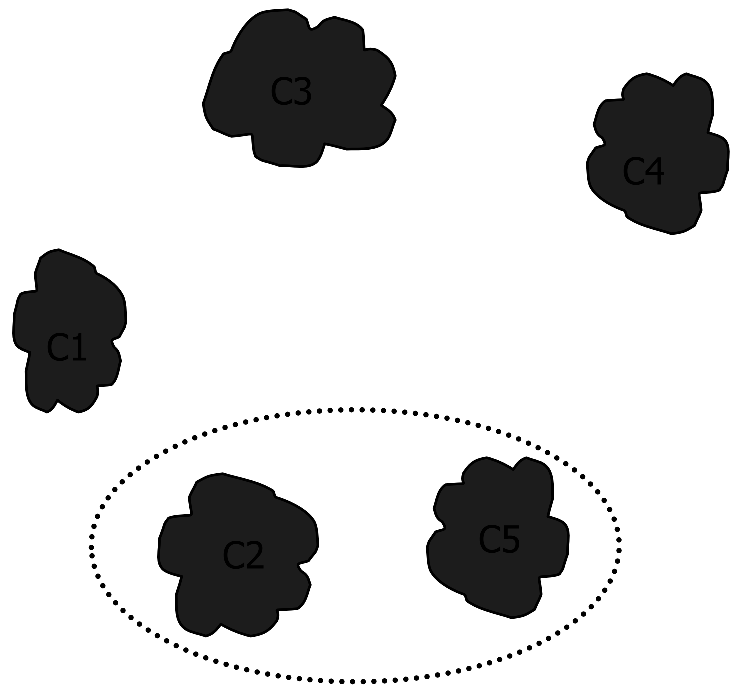
Proximity Matrix

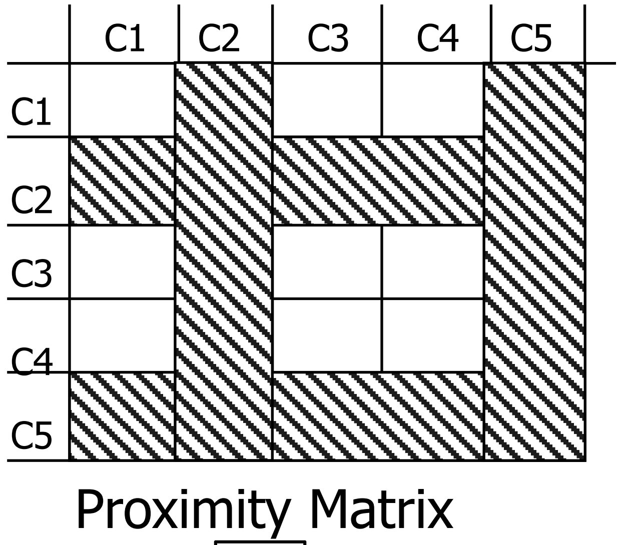


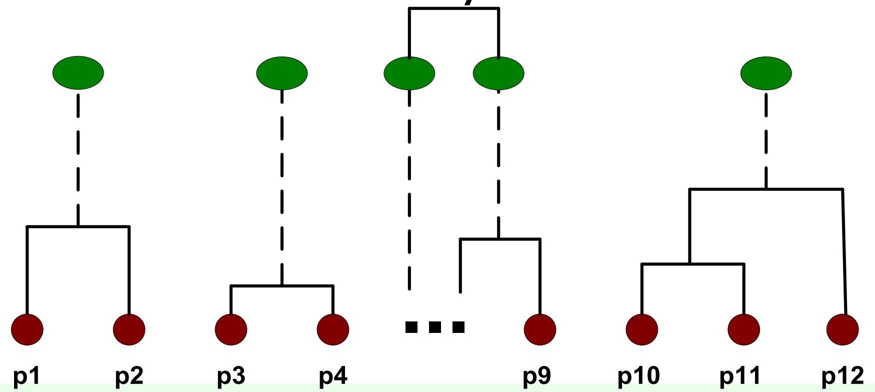
From: Tan,Steinbach, Kumar, Introduction to Data Mining, McGraw Hill 2006

Intermediate Situation

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



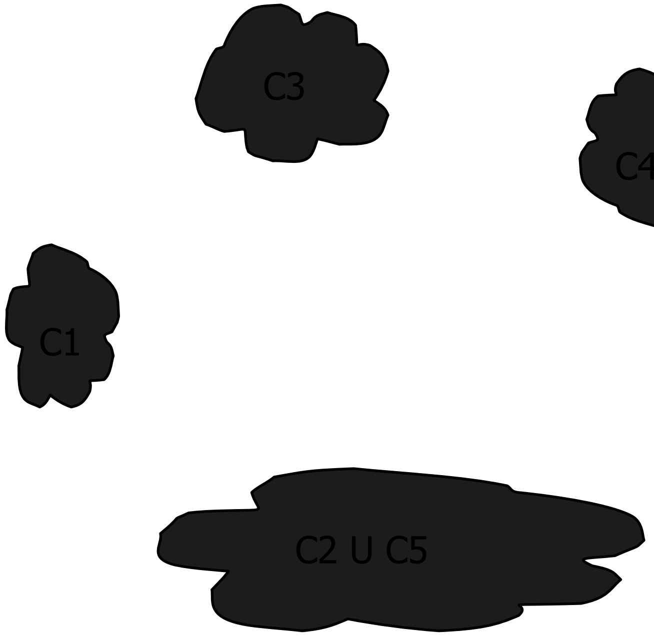




From: Tan,Steinbach, Kumar, Introduction to Data Mining, McGraw Hill 2006

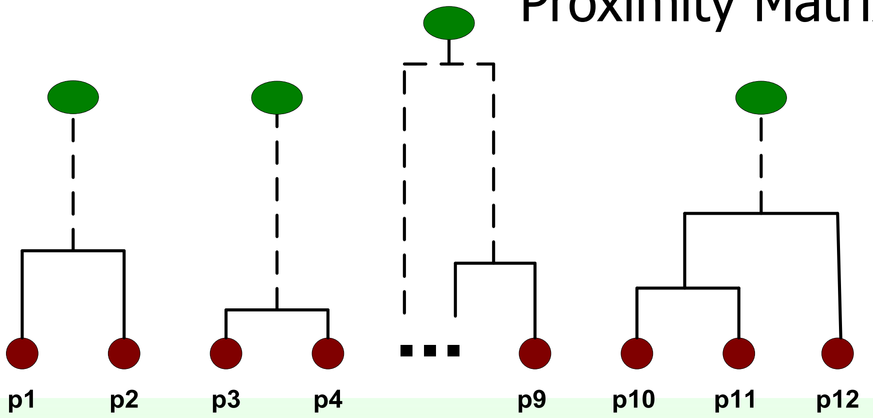
After Merging

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



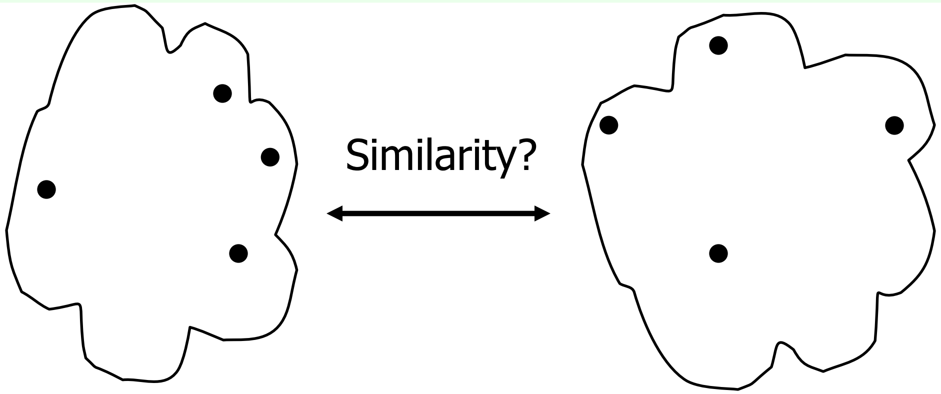
	C1	C2 U C5	C3	C4
C1		?		
C2 U C5	?	?	?	?
C3		?		
C4		?		

Proximity Matrix



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

How to Define Inter-Cluster Similarity



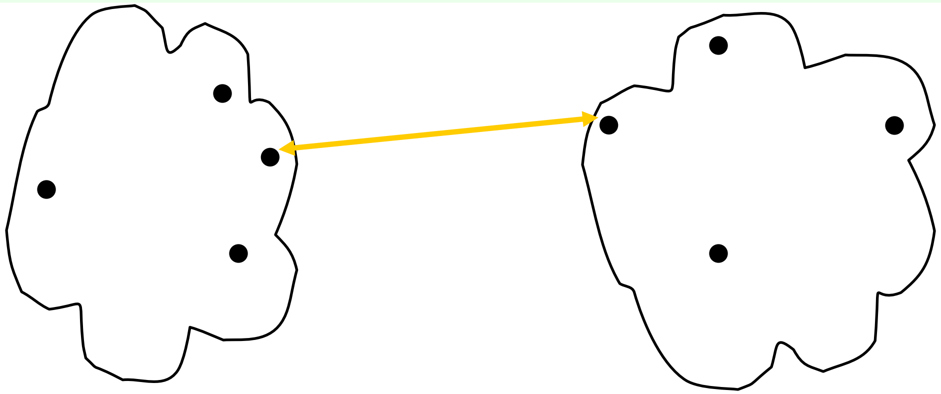
	p1	p2	p3	p4	p5	. . .
p1						
p2						
p3						
p4						
p5						
.						
.						
.						

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						
.						
.						
.						

Proximity Matrix

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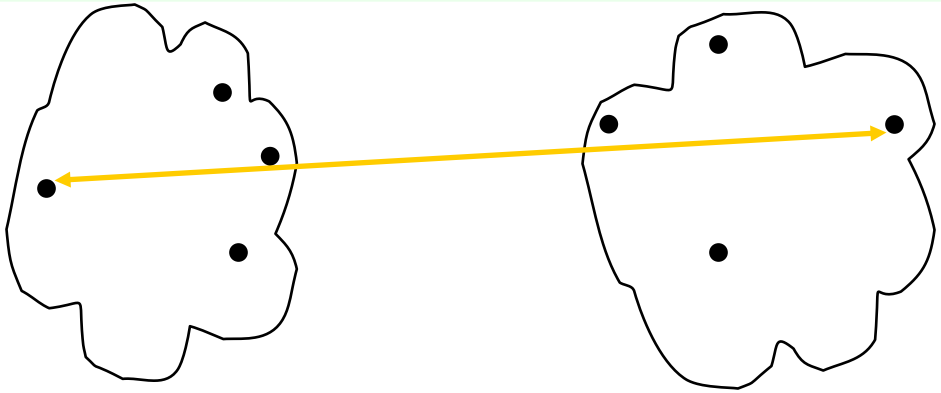
How to Define Inter-Cluster Similarity



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

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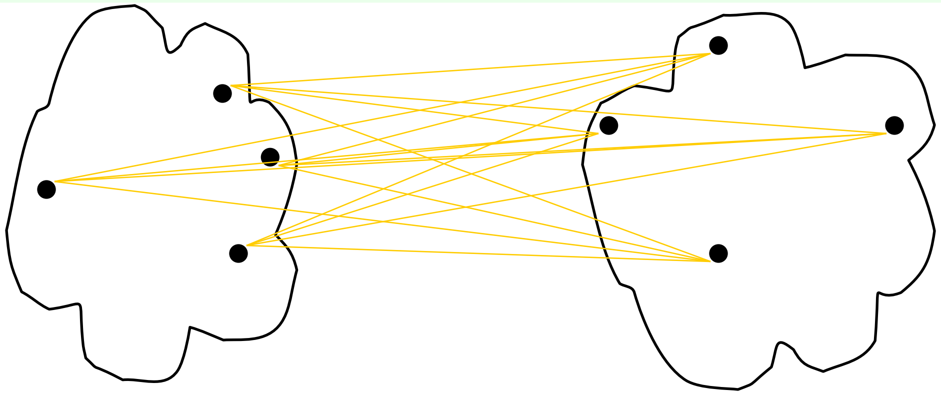
How to Define Inter-Cluster Similarity



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

Proximity Matrix

- MIN
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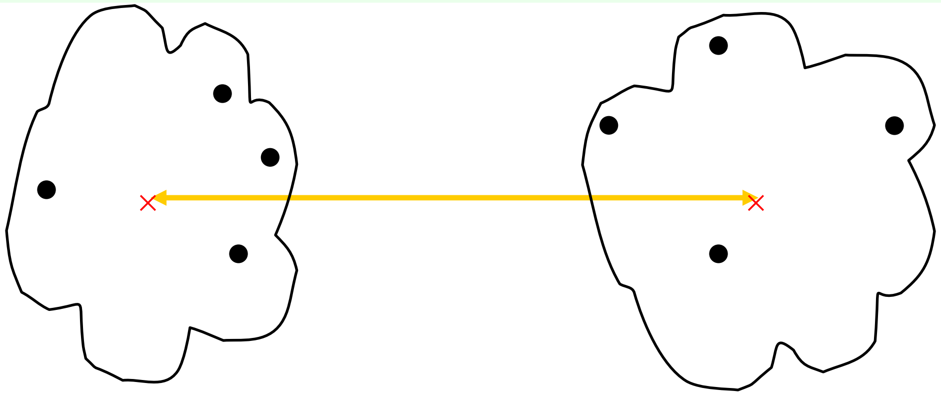
How to Define Inter-Cluster Similarity



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

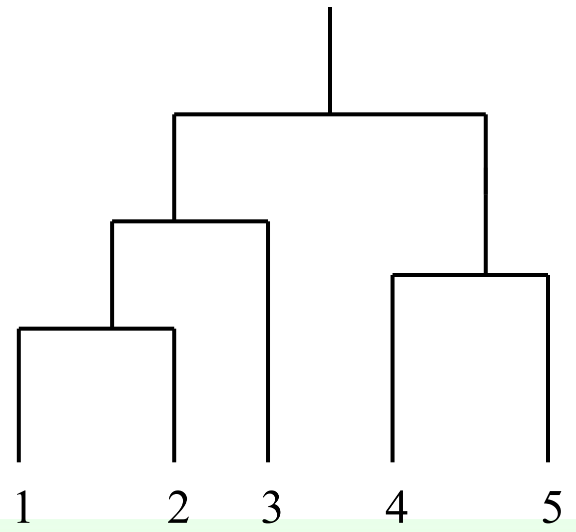
Proximity Matrix

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

Cluster Similarity: MIN or Single Link

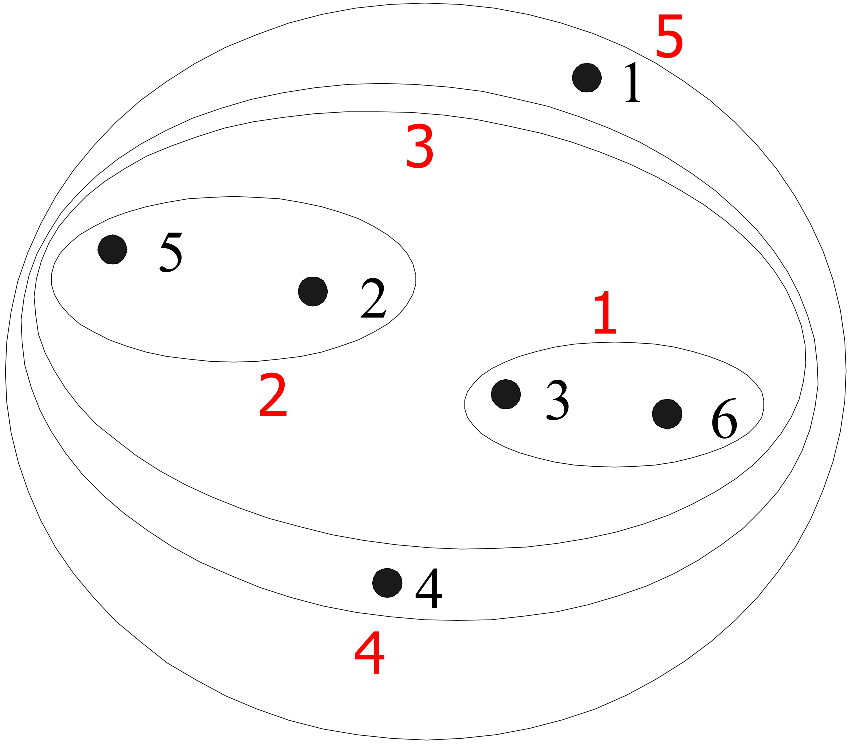
- Similarity of two clusters is based on the two most similar (closest) points in the different clusters
  - Determined by one pair of points, i.e., by one link in the proximity graph.

	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

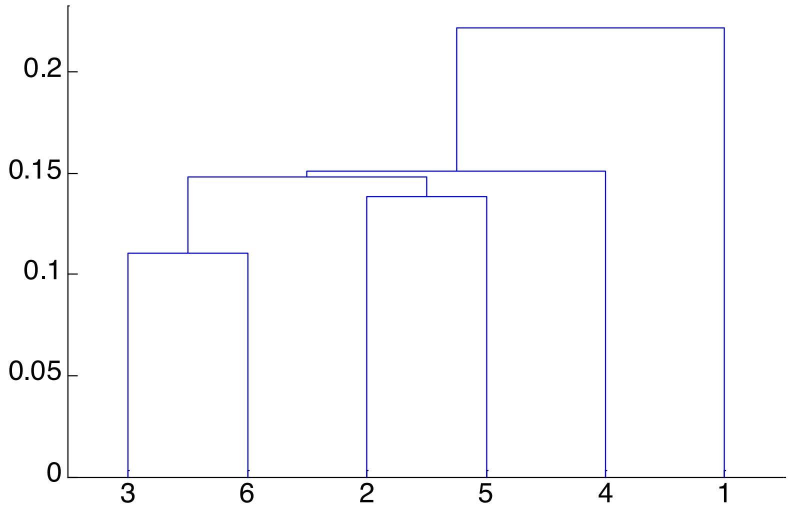


From: Tan,Steinbach, Kumar, Introduction to Data Mining, McGraw Hill 2006

Hierarchical Clustering: MIN



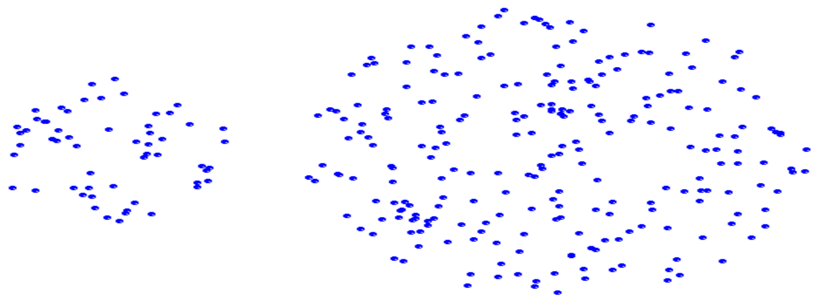
Nested Clusters



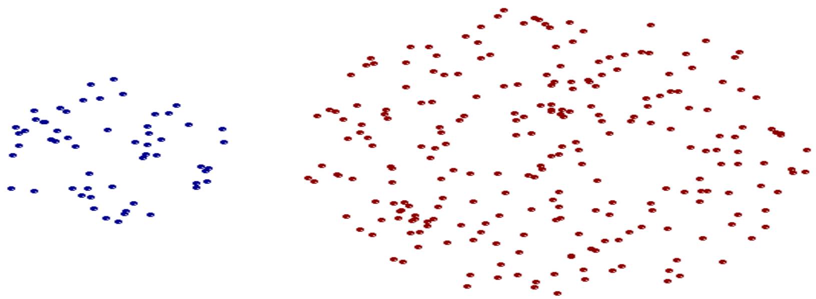
Dendrogram

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

Strength of MIN



Original Points

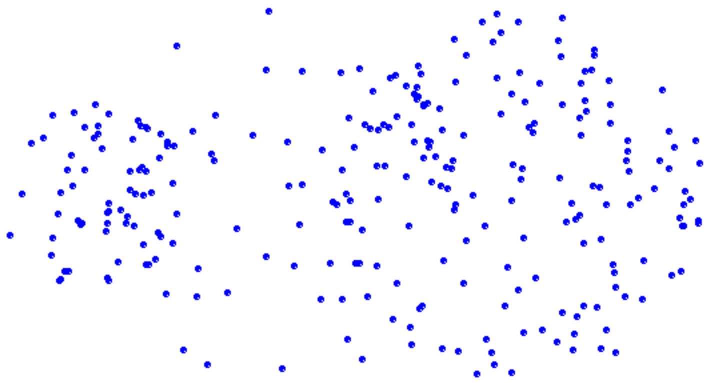


Two Clusters

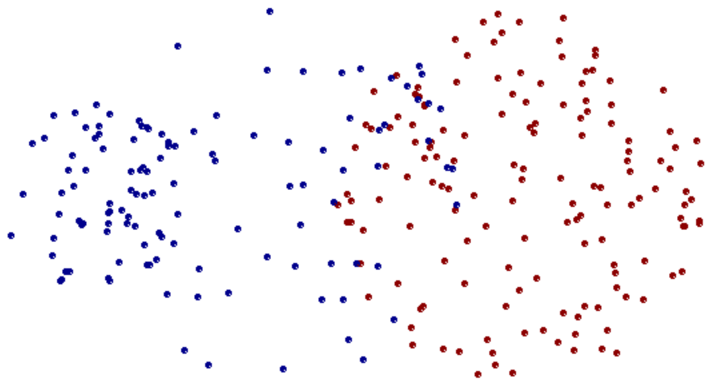
- Can handle non-elliptical shapes

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

Limitations of MIN



Original Points



Two Clusters

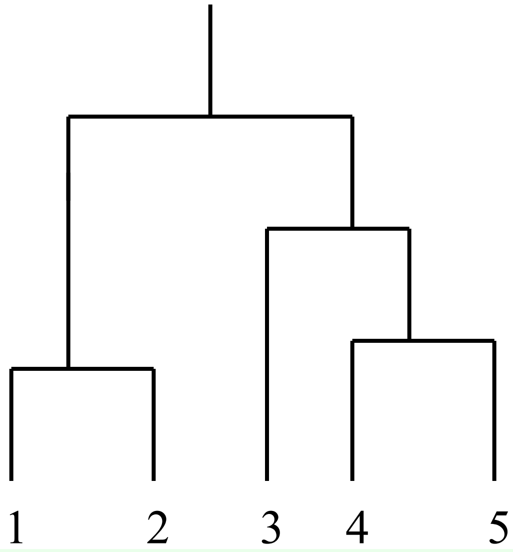
- Sensitive to noise and outliers

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

Cluster Similarity: MAX or Complete Linkage

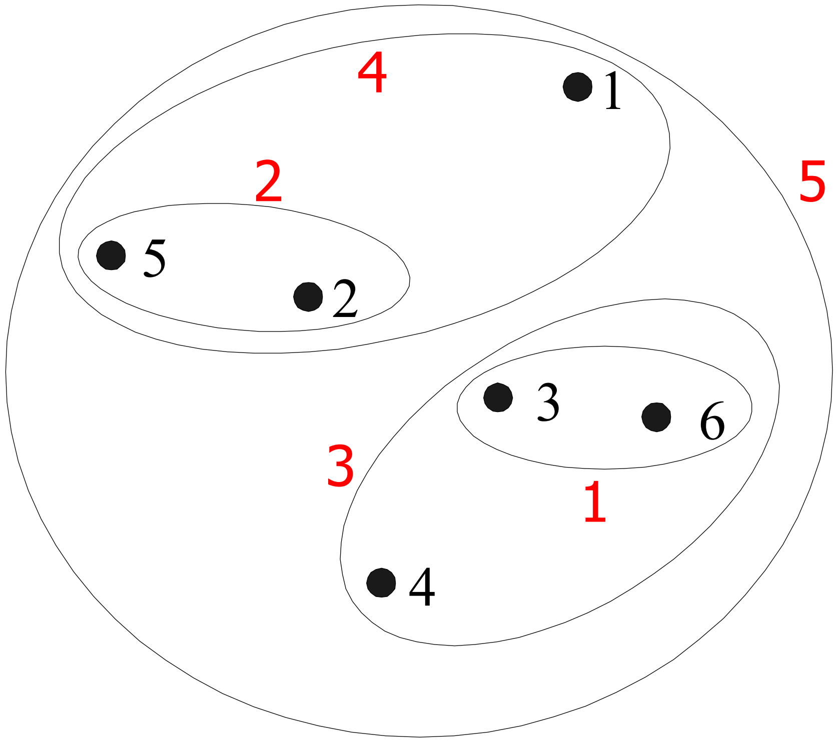
- Similarity of two clusters is based on the two least similar (most distant) points in the different clusters
  - Determined by all pairs of points in the two clusters

	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

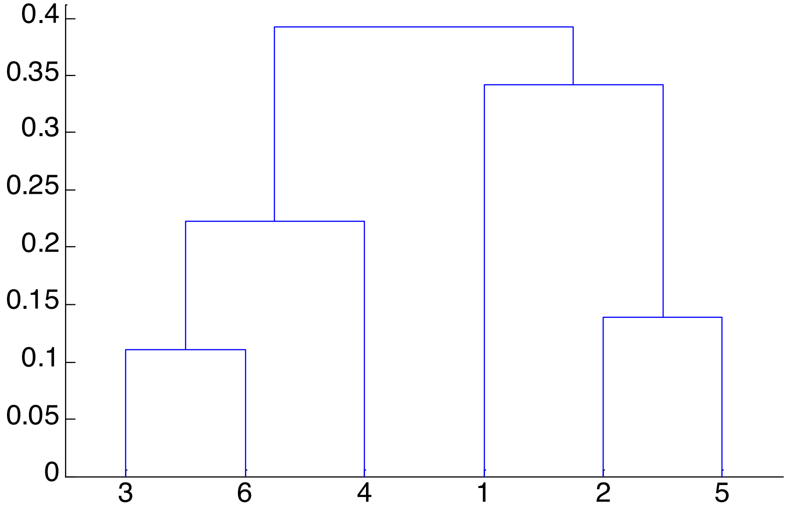


From: Tan,Steinbach, Kumar, Introduction to Data Mining, McGraw Hill 2006

Hierarchical Clustering: MAX



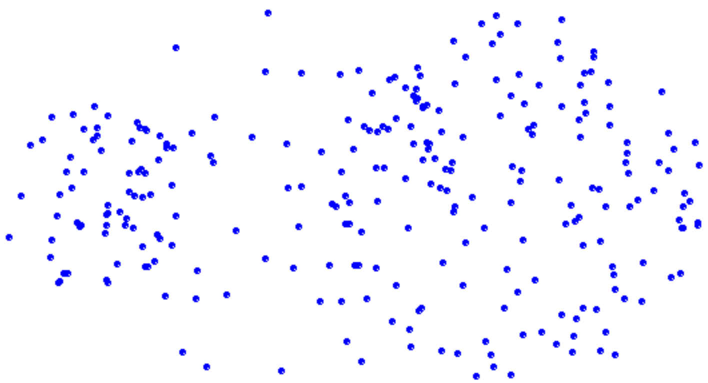
Nested Clusters



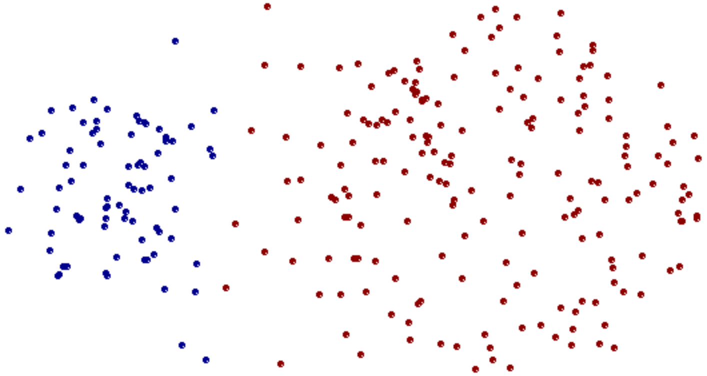
Dendrogram

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

Strength of MAX



Original Points

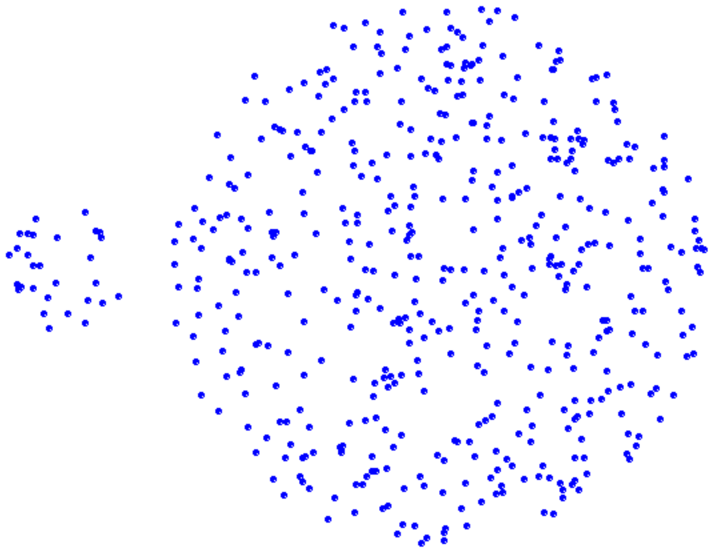


Two Clusters

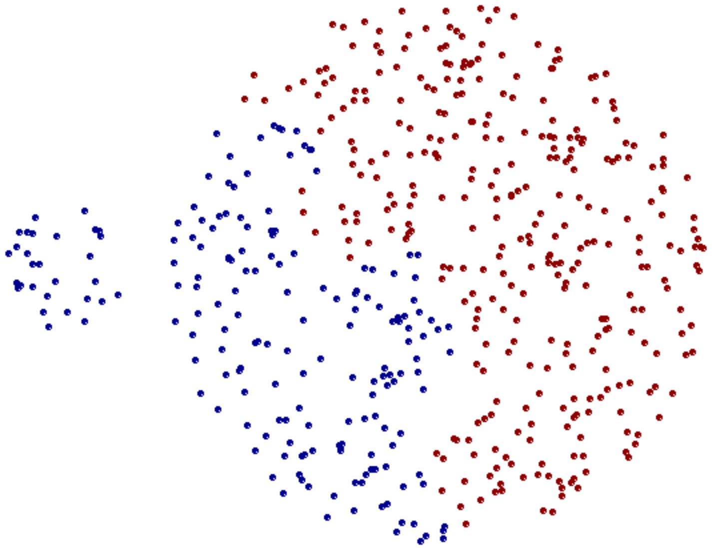
- Less susceptible to noise and outliers

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

Limitations of MAX



Original Points



Two Clusters

- Tends to break large clusters
- Biased towards globular clusters

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

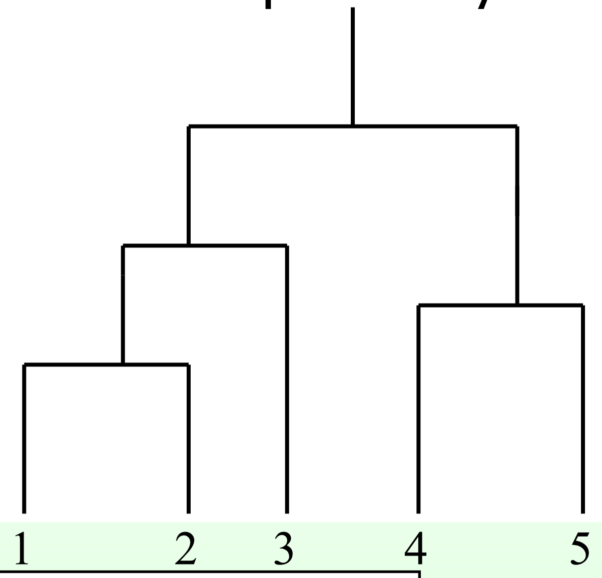
Cluster Similarity: Group Average

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

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

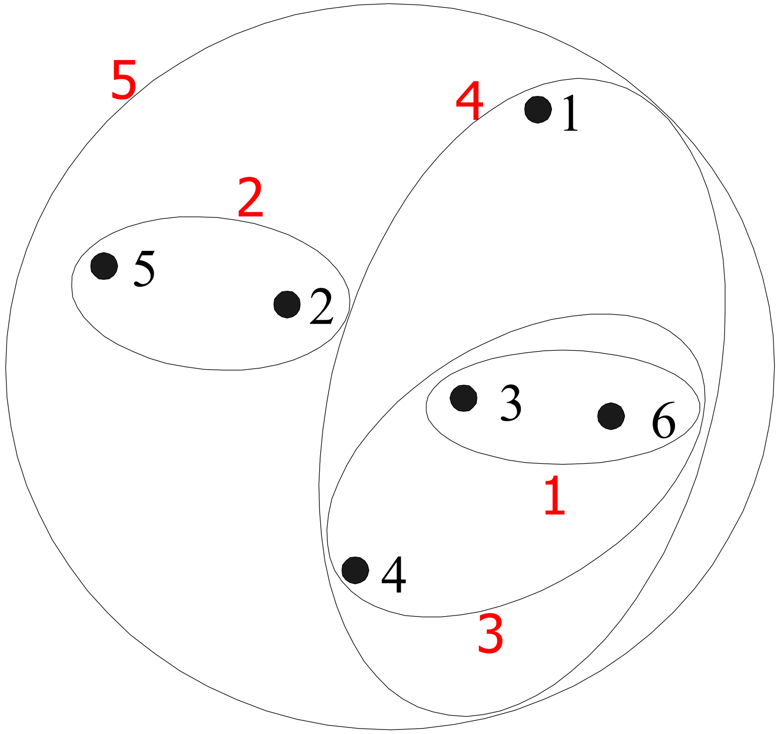
- Need to use average connectivity for scalability since total proximity favors large clusters

	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

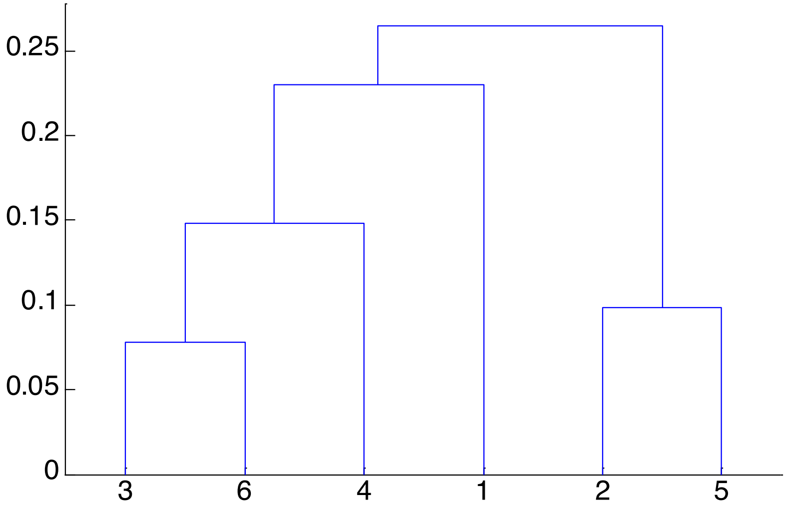


From: Tan,Steinbach, Kumar, Introduction to Data Mining, McGraw Hill 2006

Hierarchical Clustering: Group Average



Nested Clusters



Dendrogram

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

Hierarchical Clustering: Group Average

- Compromise between Single and Complete Link

- Strengths
  - Less susceptible to noise and outliers

- Limitations
  - Biased towards globular clusters

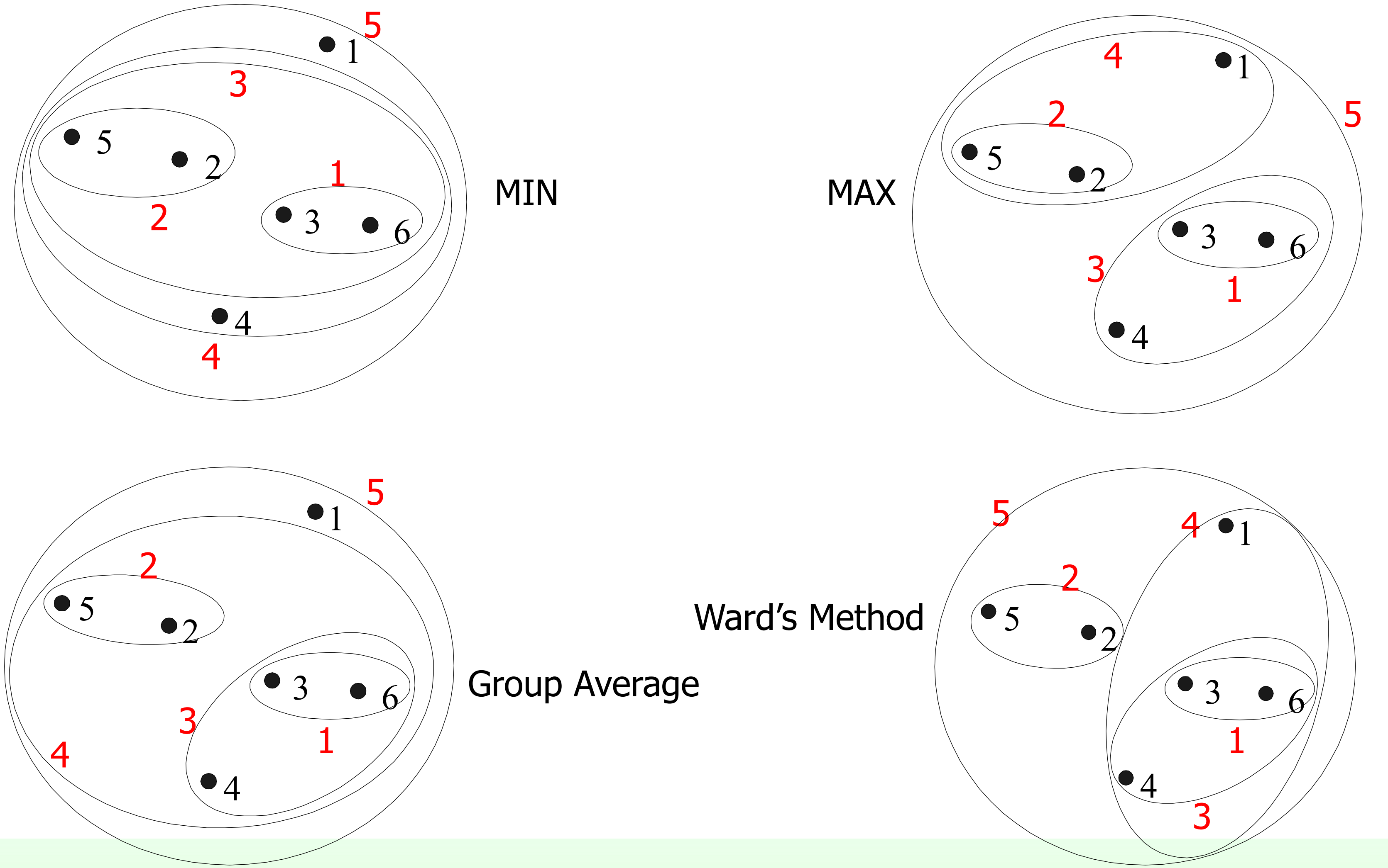
From: Tan,Steinbach, Kumar, Introduction to Data Mining, McGraw Hill 2006

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

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

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.

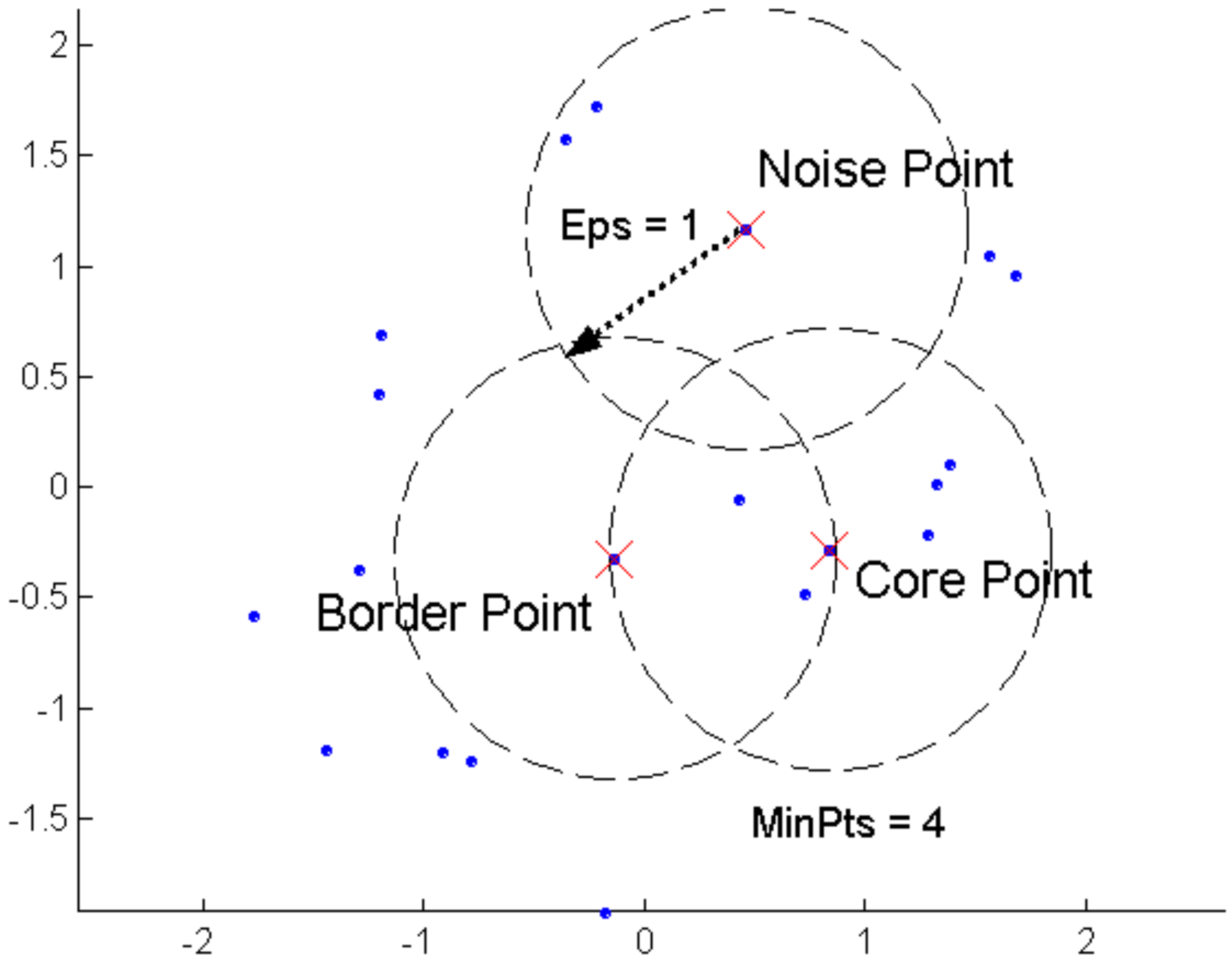
- $O(N^3)$ time in many cases
  - There are N steps and at each step the size, N^2, proximity matrix must be updated and searched
  - Complexity can be reduced to $O(N^2 \log(N))$ time for some approaches

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

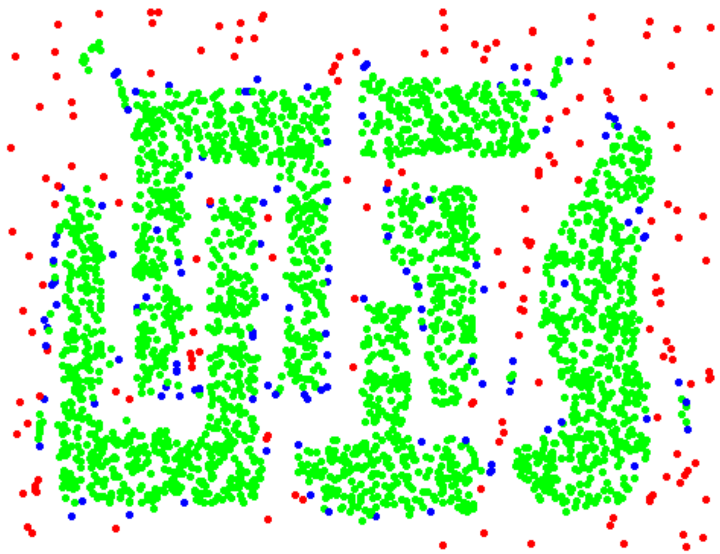
  end for

end for

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

DBSCAN: Core, Border, and Noise Points

Original Points



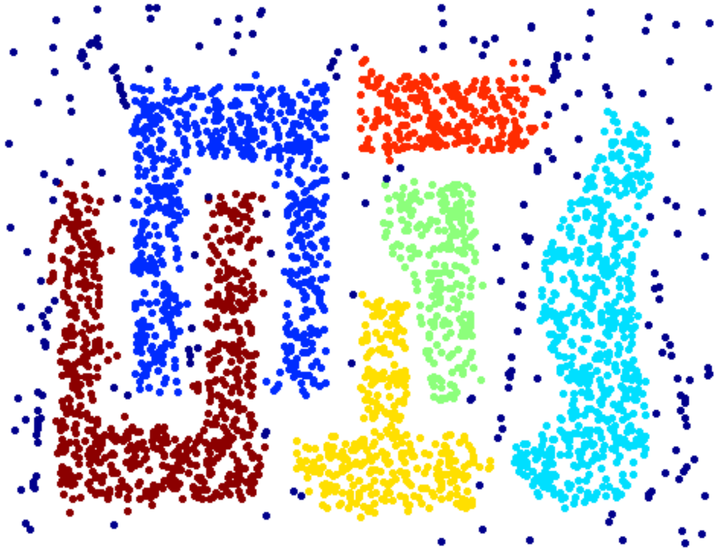
Point types: core, border and noise

Eps = 10, MinPts = 4

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

When DBSCAN Works Well

Original Points

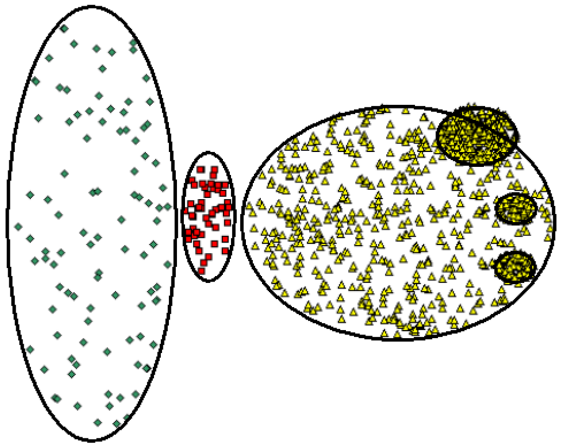


Clusters

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

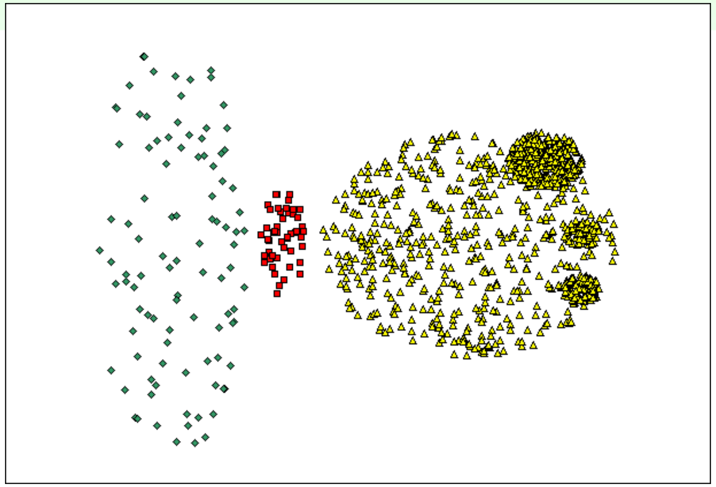
From: Tan,Steinbach, Kumar, Introduction to Data Mining, McGraw Hill 2006

When DBSCAN Does NOT Work Well

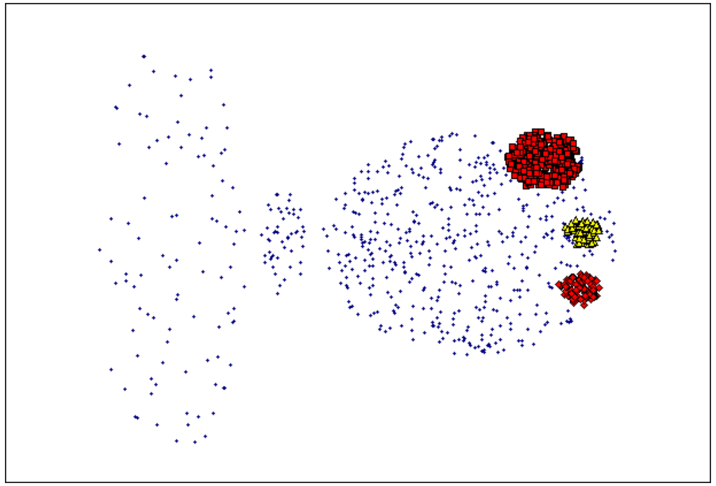


Original Points

- Varying densities
- High-dimensional data



(MinPts=4, Eps=9.75).

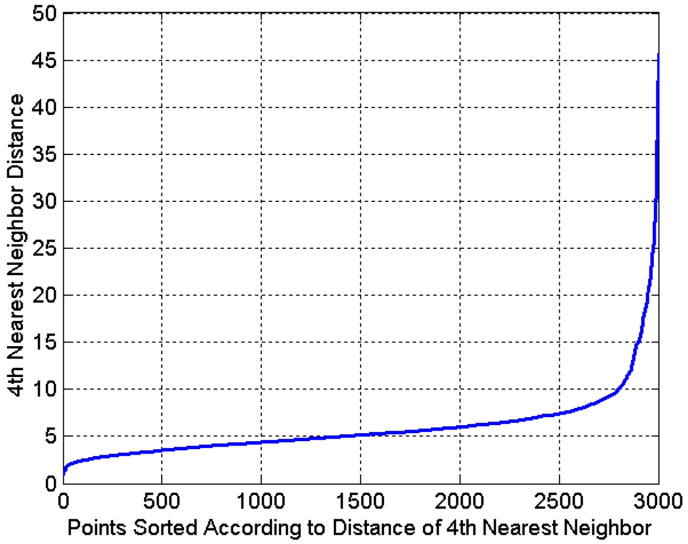


(MinPts=4, Eps=9.62)

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

Cluster Validity

Data Base and Data Mining Group of Politecnico di Torino

Elena Baralis, Tania Cerquitelli
Politecnico di Torino

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"!

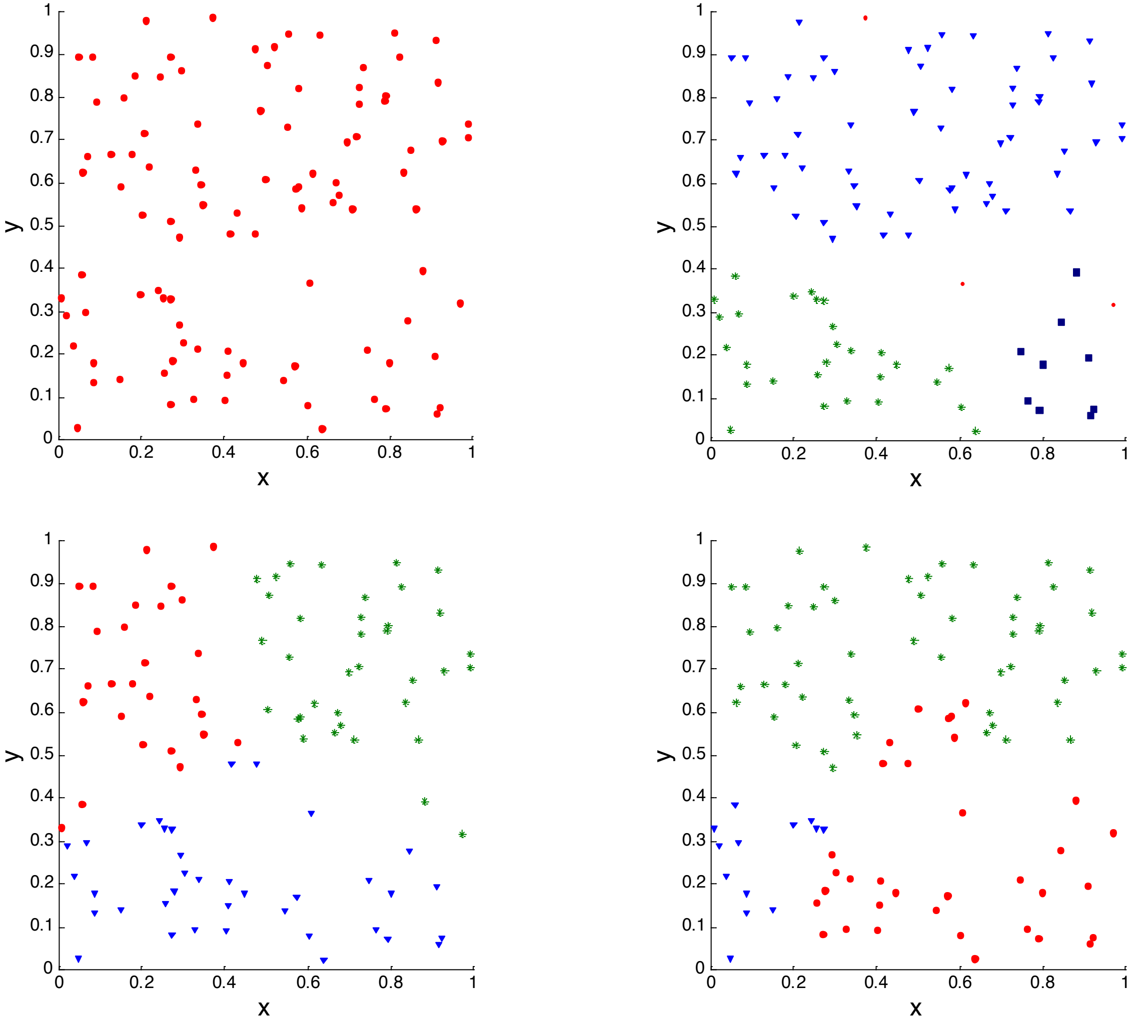
- Then why do we want to evaluate them?
  - To avoid finding patterns in noise
  - To compare clustering algorithms
  - To compare two sets of clusters
  - To compare two clusters

From: Tan, Steinbach, Karpatne, Kumar, Introduction to Data Mining 2nd Ed., McGraw Hill 2018

Clusters found in Random Data

Random Points | **DBSCAN**

K-means | **Complete Link**



From: Tan, Steinbach, Karpatne, Kumar, Introduction to Data Mining 2nd Ed., McGraw Hill 2018

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.

From: Tan, Steinbach, Karpatne, Kumar, Introduction to Data Mining 2nd Ed., McGraw Hill 2018

Measures of Cluster Validity

- Numerical measures are applied to judge various aspects of cluster validity
- Numerical measures can be classified into three 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
  - 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

From: Tan, Steinbach, Karpatne, Kumar, Introduction to Data Mining 2nd Ed., McGraw Hill 2018

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)

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

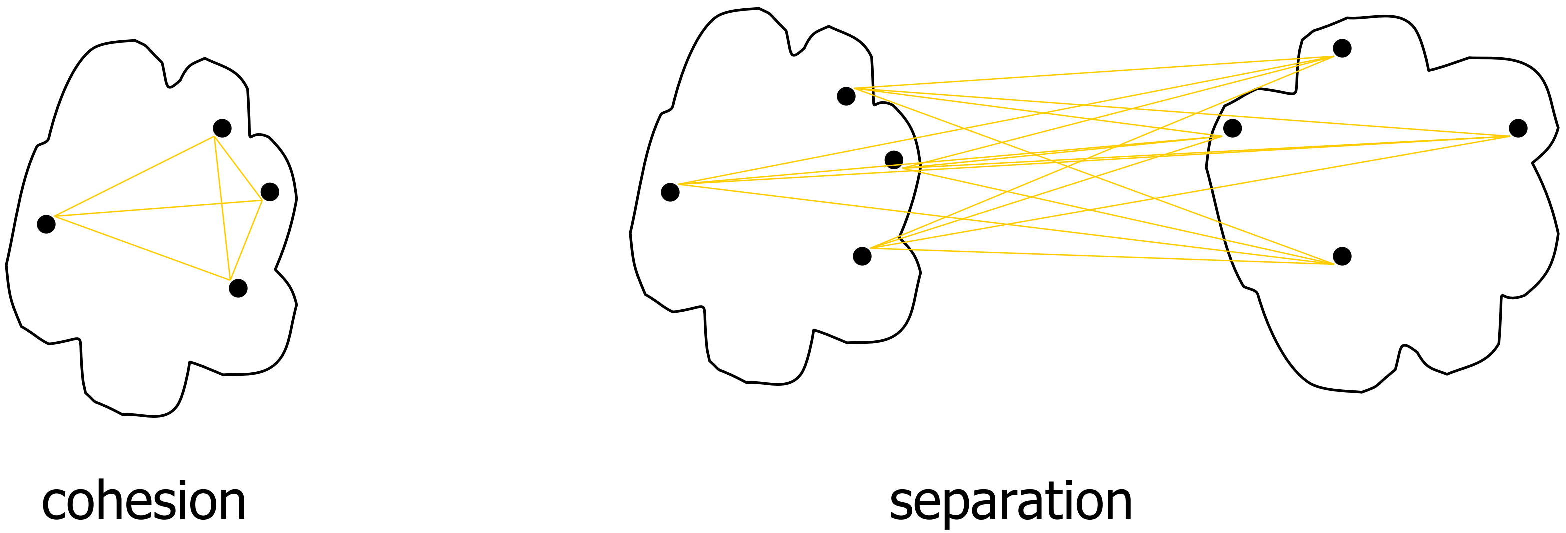
- Cluster Separation: Measure how distinct or well-separated a cluster is from other clusters
  - Separation is measured by the between cluster sum of squares

$$BSS = \sum_i |C_i| (m - m_i)^2$$

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

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.



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

Internal measures: Silhouette

- A succinct measure to evaluate how well each object lies within its cluster
- It is defined for single points
- It considers both cohesion and separation
- Can be computed for
  - Individual points
  - Individual clusters
  - Clustering result

Internal measures: Silhouette

- For each object *i*
  - *a(i):* the average dissimilarity of *i* with all other objects within the same cluster (the smaller the value, the better the assignment)
  - *b(i):* min(average dissimilarity of *i* to any other cluster, of which *i* is not a member)

$$s(i) = \frac{b(i) - a(i)}{\max\{a(i), b(i)\}}$$

- Ranges between -1 and +1
  - Typically between 0 and 1
  - The closer to 1, the better
- Silhouette for clusters and clusterings
  - The average s(i) over all data of a *cluster* measures how tightly grouped all the data in the cluster are
  - The average s(i) over all data of the *dataset* measures how appropriately the data has been clustered

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

Rand Index

- Idea
  - Any two objects that are in the same cluster should be in the same class and vice versa
- Given
  - f_{00} = number of pairs of objects having a different class and a different cluster
  - f_{01} = number of pairs of objects having a different class and the same cluster
  - f_{10} = number of pairs of objects having the same class and a different cluster
  - f_{11} = number of pairs of objects having the same class and the same cluster
- Rand Index

$$Rand\ Index = \frac{f_{00} + f_{11}}{f_{00} + f_{01} + f_{10} + f_{11}}$$

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

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