Clustering fundamentals



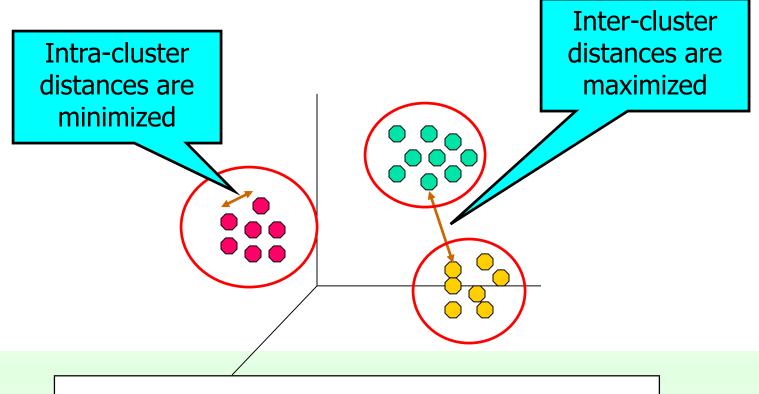
Elena Baralis, Tania Cerquitelli

Politecnico di Torino



What is Cluster Analysis?

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







Applications of Cluster Analysis

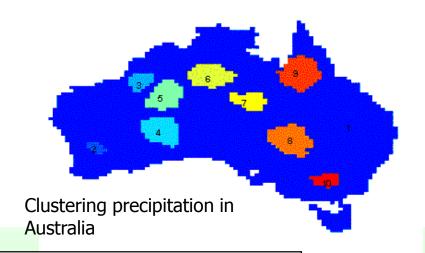
Understanding

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

	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

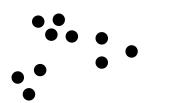
 Reduce the size of large data sets

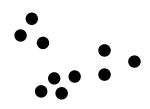


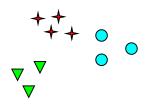




Notion of a Cluster can be Ambiguous



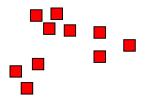


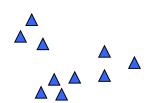


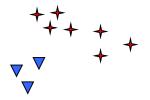


How many clusters?

Six Clusters









Two Clusters

Four Clusters





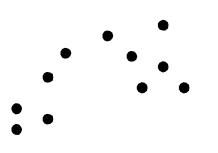
Types of Clusterings

- 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





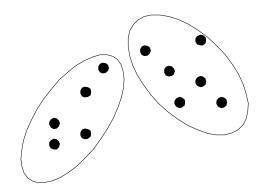
Partitional Clustering

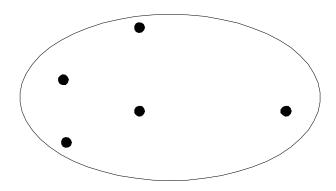




•

Original Points



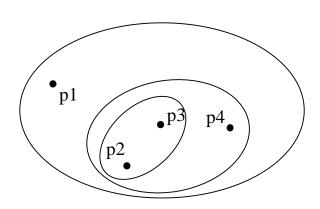


A Partitional Clustering

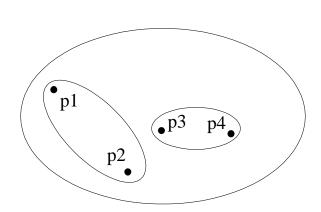




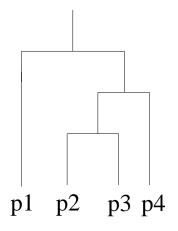
Hierarchical Clustering



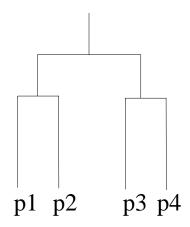
Traditional Hierarchical Clustering



Non-traditional Hierarchical Clustering



Traditional Dendrogram



Non-traditional Dendrogram





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

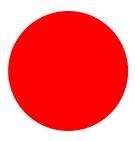




Types of Clusters: Well Separated

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.









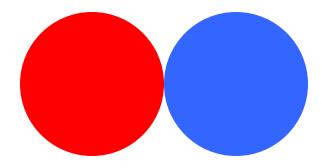
3 well-separated clusters

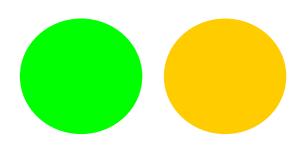


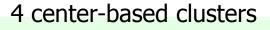
Types of Clusters: Center-Based

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









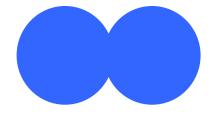


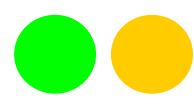
Types of Clusters: Contiguity-Based

- 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.











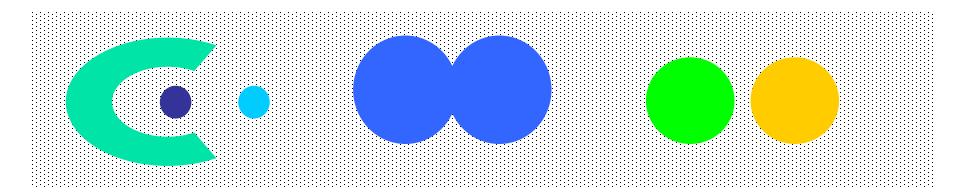
8 contiguous clusters



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

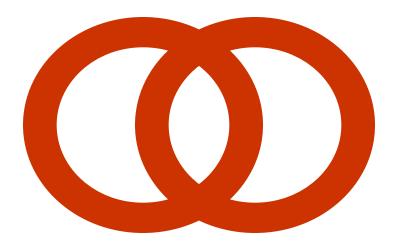


Types of Clusters: Conceptual Clusters

Shared Property or Conceptual Clusters

 Finds clusters that share some common property or represent a particular concept.







2 Overlapping Circles



Clustering Algorithms

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





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





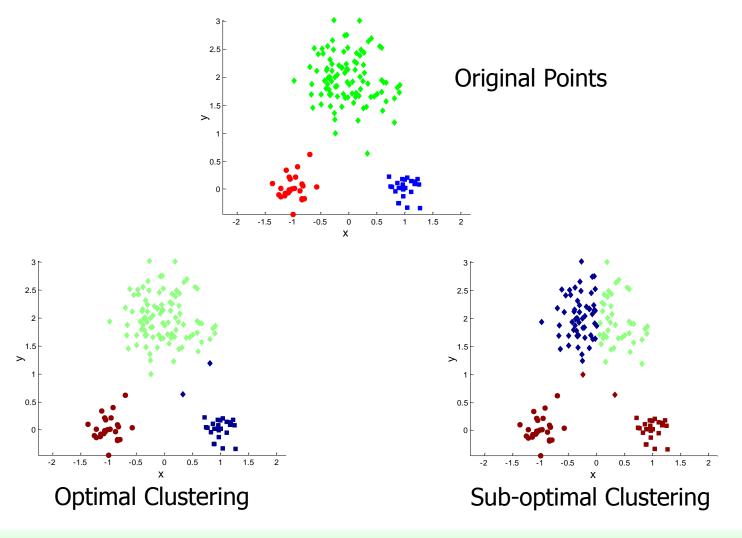
K-means Clustering – Details

- 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



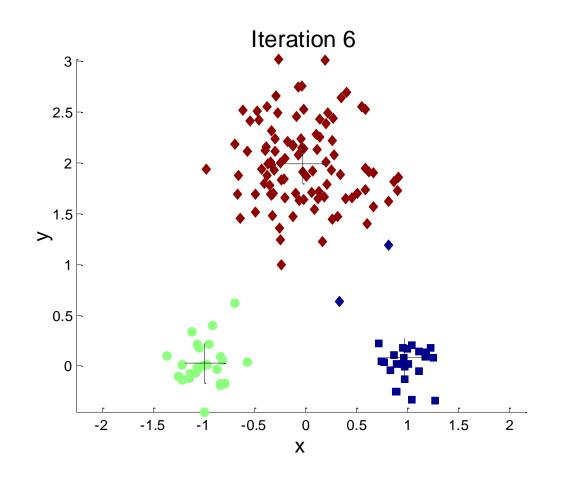


Two different K-means Clusterings



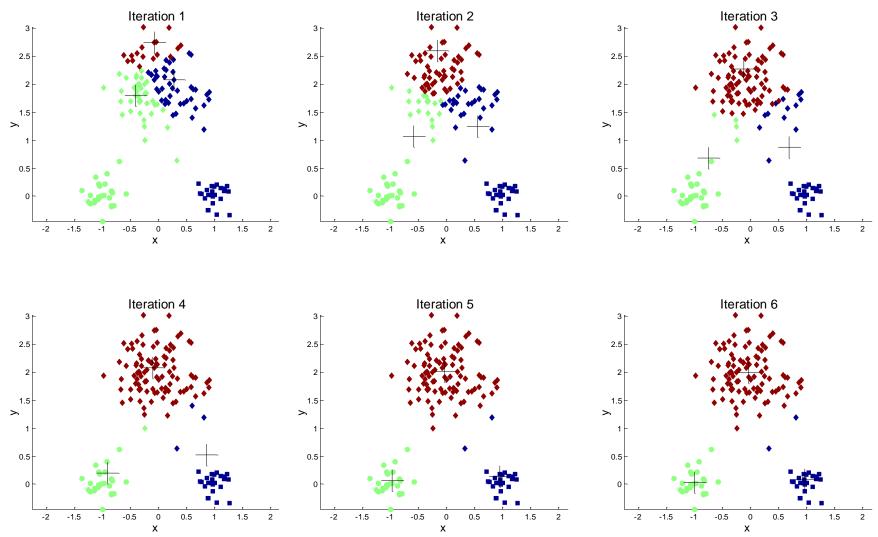






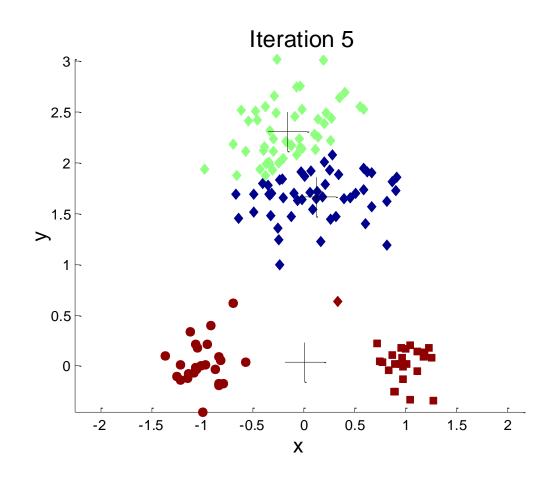






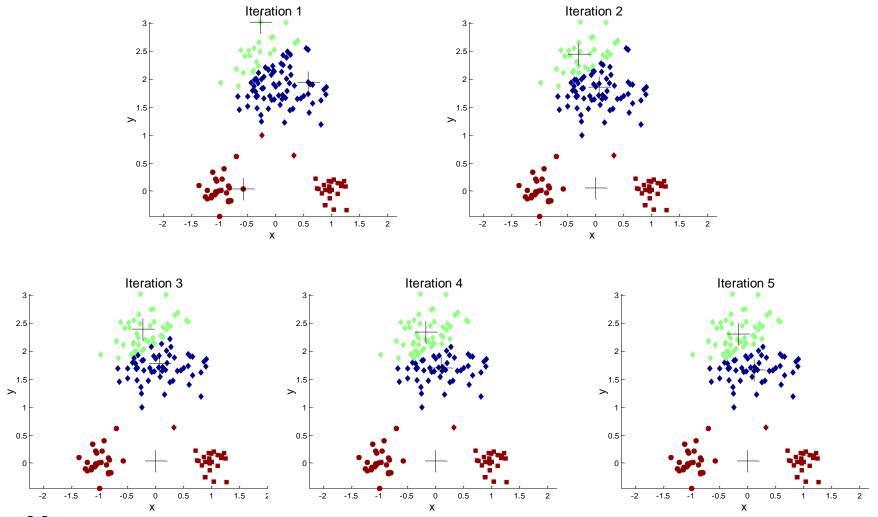
















Evaluating K-means Clusters

- 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.

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

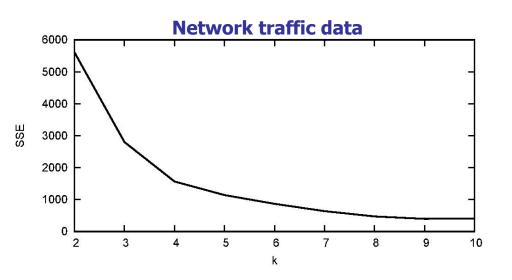
- x is a data point in cluster C_i and m_i is the representative point for cluster C_i
 - can show that m_i corresponds to the center (mean) of the cluster
- Given two clusters, we can choose the one with the smallest error
- One easy way to reduce SSE is to increase K, the number of clusters
 - A good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



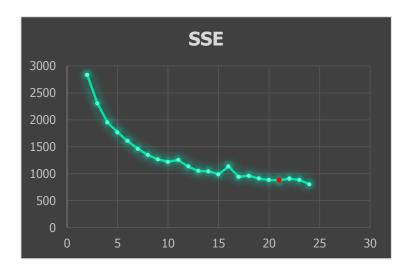


K-means parameter setting

- 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



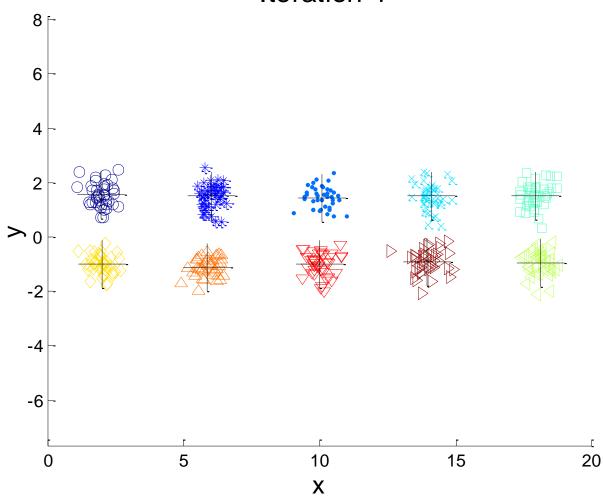
Medical records







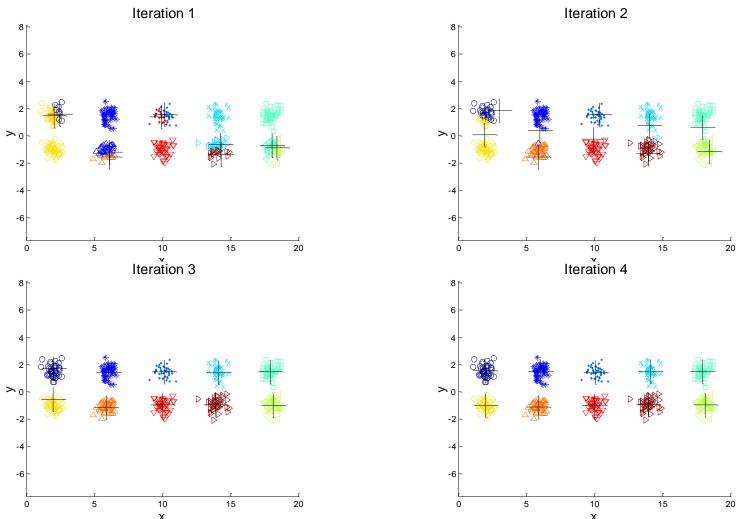




Starting with two initial centroids in one cluster of each pair of clusters

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



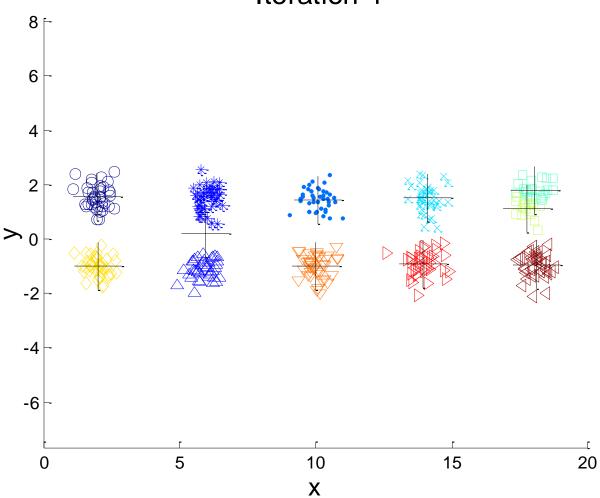


Starting with two initial centroids in one cluster of each pair of clusters

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



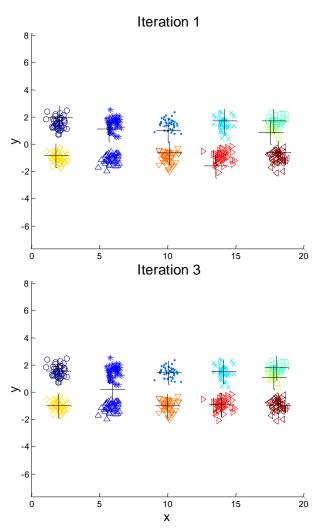


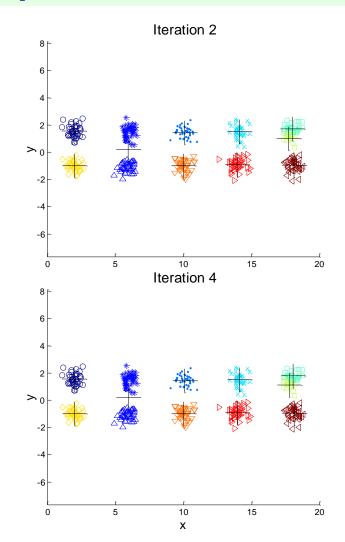


Starting with some pairs of clusters having three initial centroids, while other have only one.

27







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





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.





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





Bisecting K-means

Bisecting K-means algorithm

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

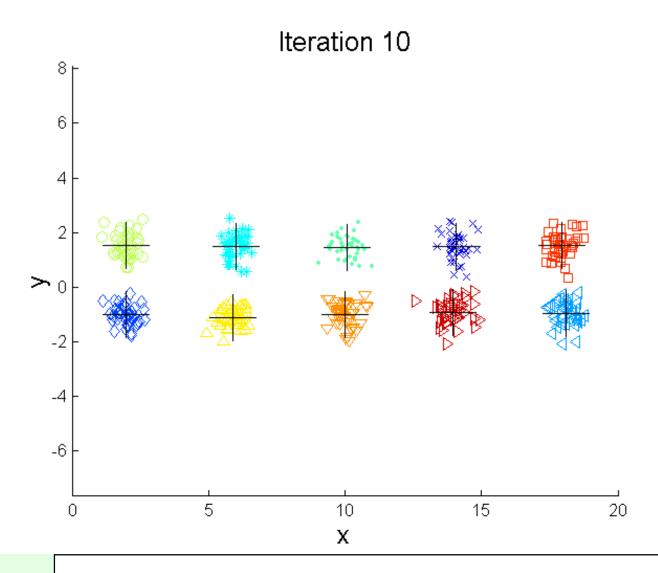
- 1: Initialize the list of clusters to contain the cluster containing all points.
- 2: repeat
- 3: Select a cluster from the list of clusters
- 4: **for** i = 1 to $number_of_iterations$ **do**
- 5: Bisect the selected cluster using basic K-means
- 6: end for
- 7: Add the two clusters from the bisection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







Bisecting K-means Example







Limitations of K-means

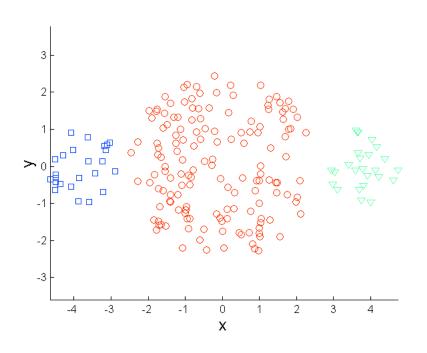
- K-means has problems when clusters are of differing
 - Sizes
 - Densities
 - Non-globular shapes

 K-means has problems when the data contains outliers.





Limitations of K-means: Differing Sizes



3 - 2 - 1 0 1 2 3 4 X

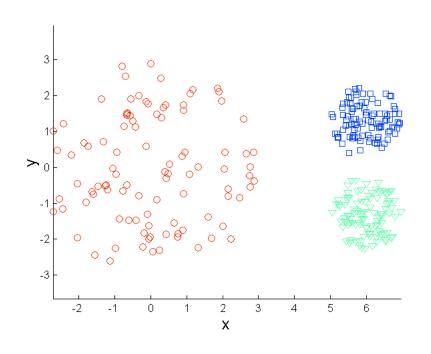
Original Points

K-means (3 Clusters)





Limitations of K-means: Differing Density



3
2
1
2
1
2
1
2
1
2
2
1
0
1
2
3
4
5
6
X

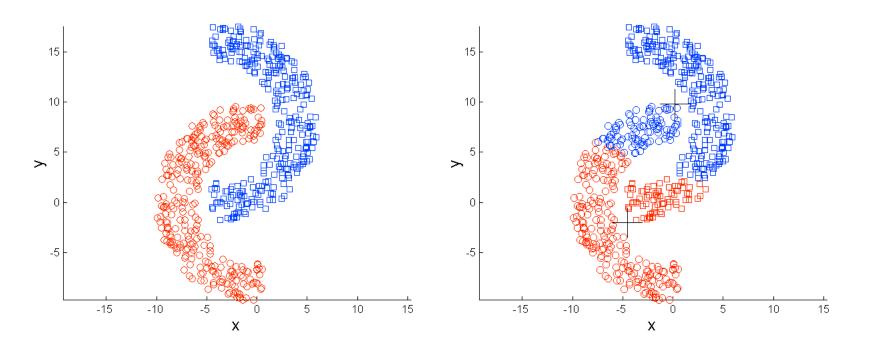
Original Points

K-means (3 Clusters)





Limitations of K-means: Non-globular Shapes



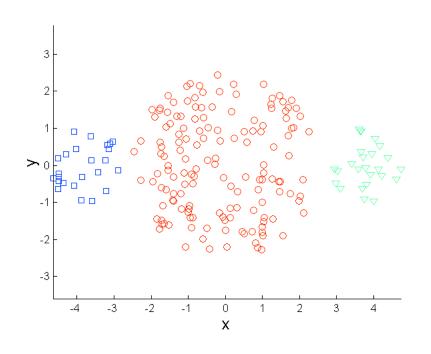
Original Points

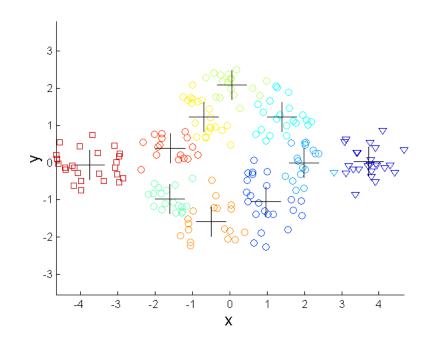
K-means (2 Clusters)





Overcoming K-means Limitations





Original Points

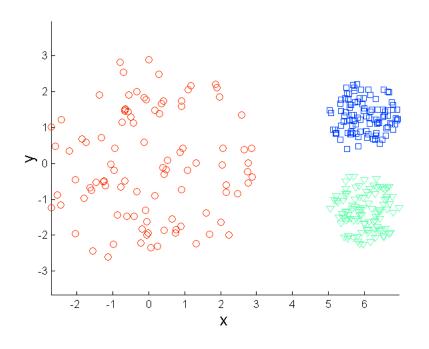
K-means Clusters

One solution is to use many clusters.

Find parts of clusters, but need to put together.



Overcoming K-means Limitations



3 - 2 - 1 0 1 2 3 4 5 6 X

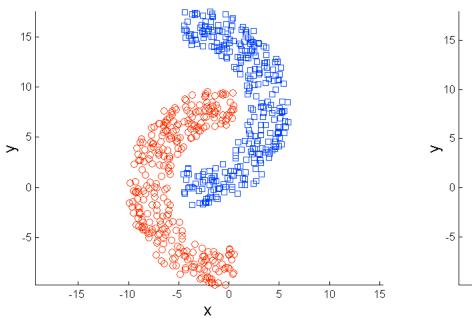
Original Points

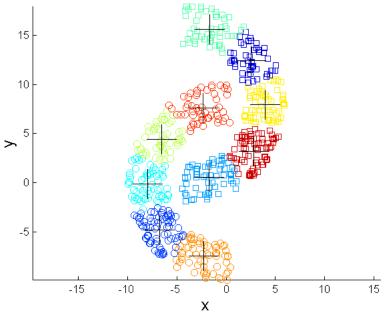
K-means Clusters





Overcoming K-means Limitations





Original Points

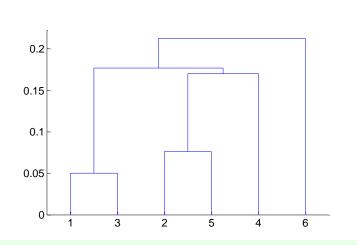
K-means Clusters

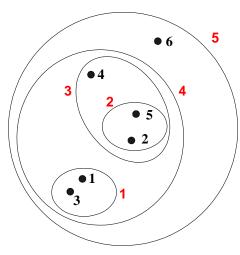




Hierarchical Clustering

- Produces a set of nested clusters organized as a hierarchical tree
- Can be visualized as a dendrogram
 - A tree like diagram that records the sequences of merges or splits









Strengths of Hierarchical Clustering

- Do not have to assume any particular number of clusters
 - Any desired number of clusters can be obtained by 'cutting' the 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

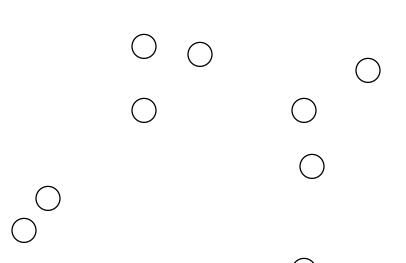
- More popular hierarchical clustering technique
- Basic algorithm is straightforward
 - 1. Compute the proximity matrix
 - Let each data point be a cluster
 - 3. Repeat
 - 4. Merge the two closest clusters
 - 5. Update the proximity matrix
 - **6. Until** only a single cluster remains
- Key operation is the computation of the proximity of two clusters
 - Different approaches to defining the distance between clusters distinguish the different algorithms

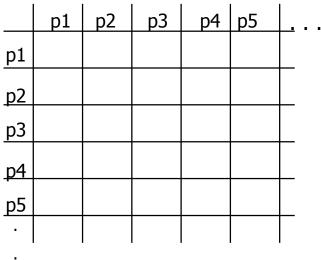




Starting Situation

Start with clusters of individual points and a proximity matrix





Proximity Matrix

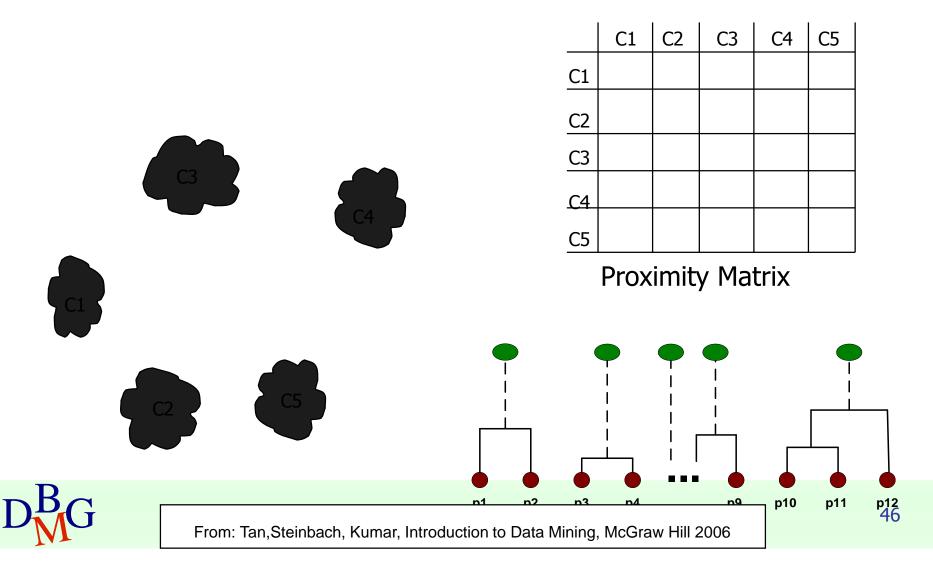


p1 p2 p3 p4 p9 p10 p11 p12



Intermediate Situation

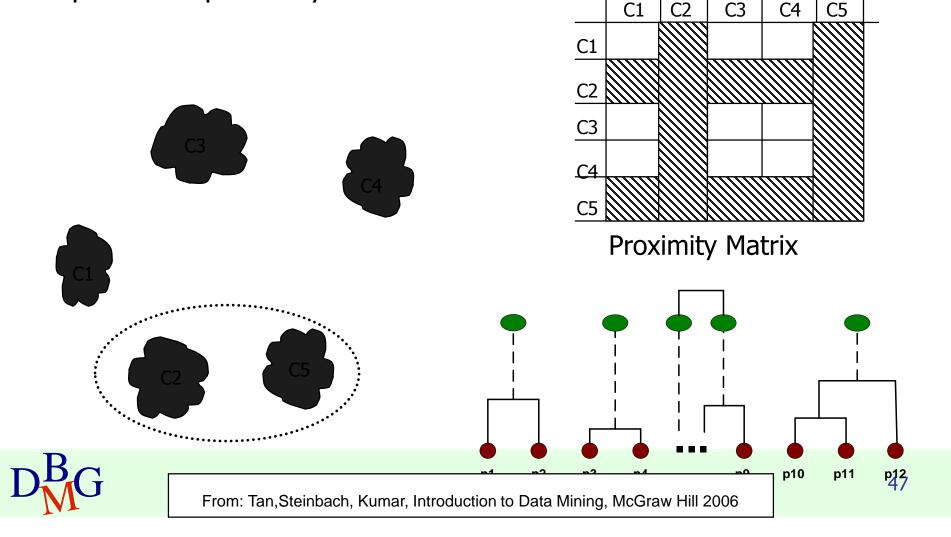
After some merging steps, we have some clusters





Intermediate Situation

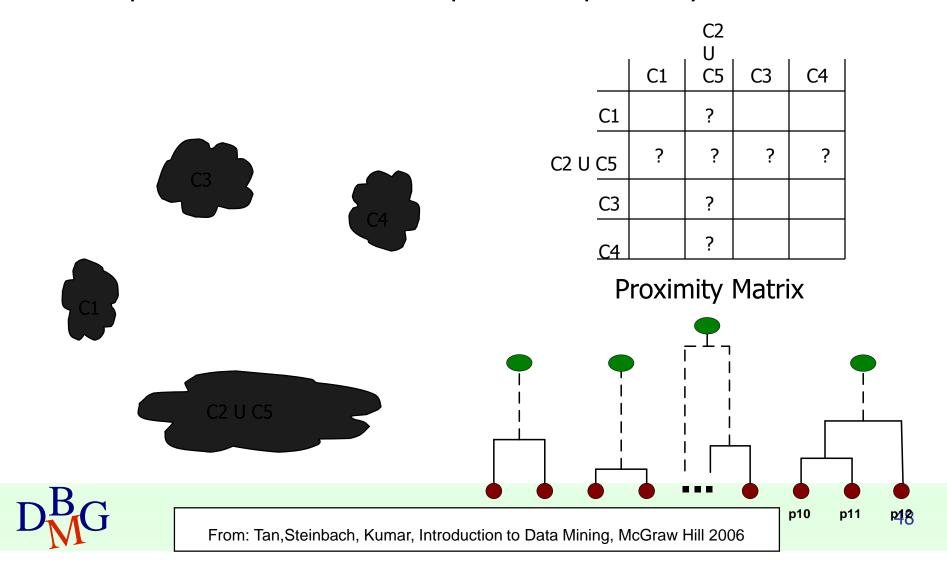
 We want to merge the two closest clusters (C2 and C5) and update the proximity matrix.



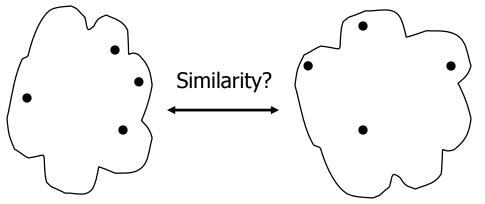


After Merging

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





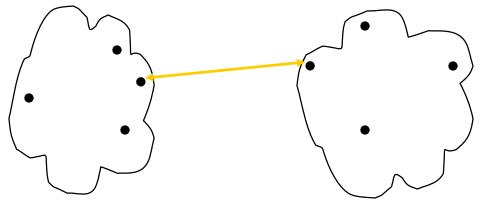


		p1	p2	рЗ	p4	p5	
p	1						_
p	2						
p	3						
p)4)5						
_							

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





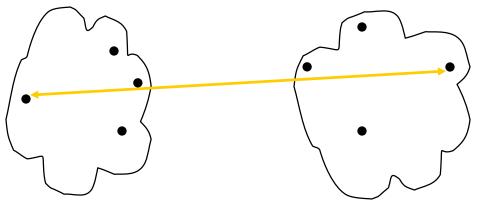


	p1	p2	рЗ	p4	p5	<u>.</u> .
p1						
p2						
p3						
p4						
<u>p4</u> p5						

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





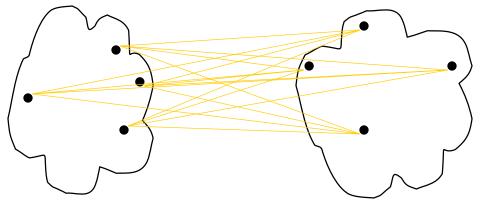


	p1	p2	рЗ	p4	p5	<u> </u>
p1						
p2						
p2 p3						
<u>p4</u> p5						

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





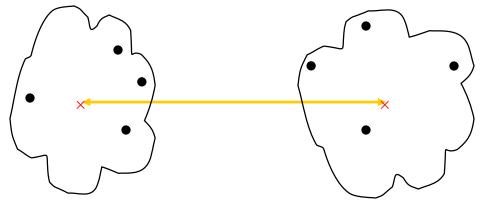


	p1	p2	рЗ	p4	p5	<u>L.</u>
p1						
<u>p2</u>						
р3						
p4						
p5						

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







	p1	p2	рЗ	p4	p5	<u>.</u> .
p1						
p2						
p3						
p4						
<u>p4</u> p5						

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

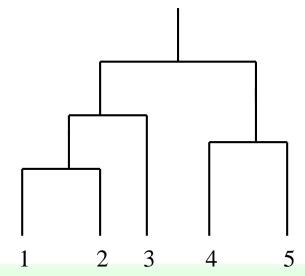




Cluster Similarity: MIN or Single Link

- 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.

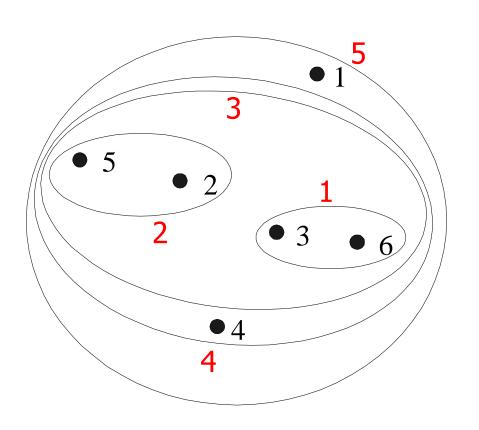
_	I 1	12	13	14	15
11	1.00	0.90	0.10	0.65	0.20
12	0.90	1.00	0.70	0.60	0.50
13	0.10	0.70	1.00	0.40	0.30
14	0.65	0.60	0.40	1.00	0.80
15	0.20	0.50	0.30	0.80	0.20 0.50 0.30 0.80 1.00

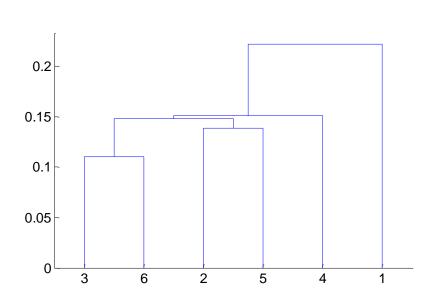






Hierarchical Clustering: MIN





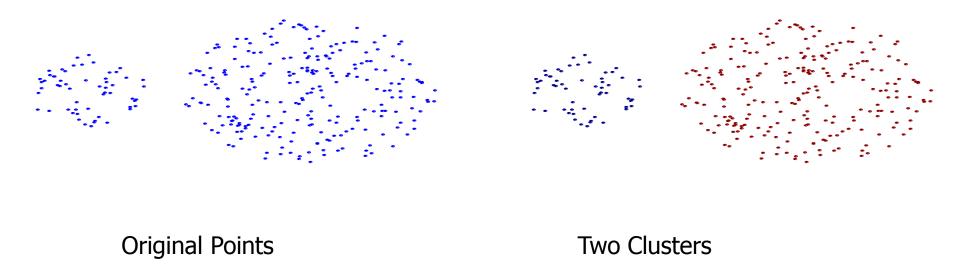
Nested Clusters

Dendrogram





Strength of MIN

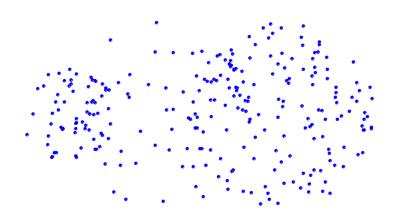


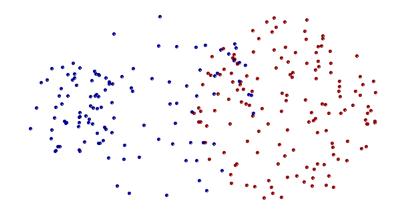
• Can handle non-elliptical shapes





Limitations of MIN





Original Points

Two Clusters

Sensitive to noise and outliers

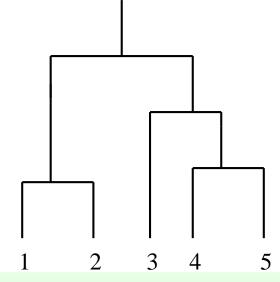




Cluster Similarity: MAX or Complete Linkage

- 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

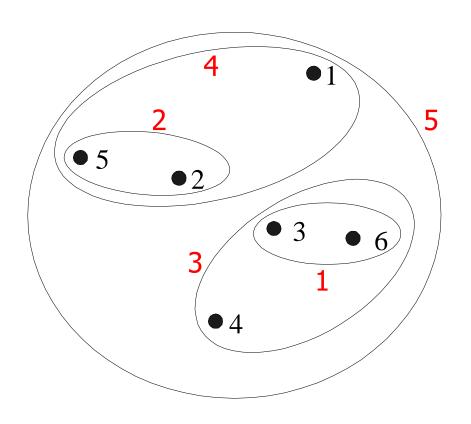
_				1 4	
I 1	1.00	0.90	0.10	0.65	0.20 0.50 0.30 0.80 1.00
12	0.90	1.00	0.70	0.60	0.50
I 3	0.10	0.70	1.00	0.40	0.30
14	0.65	0.60	0.40	1.00	0.80
15	0.20	0.50	0.30	0.80	1.00

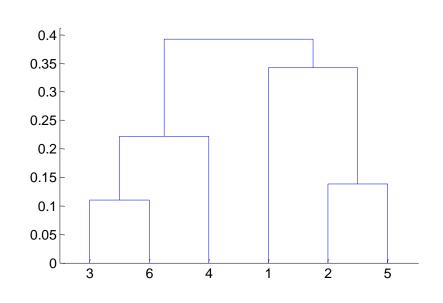






Hierarchical Clustering: MAX





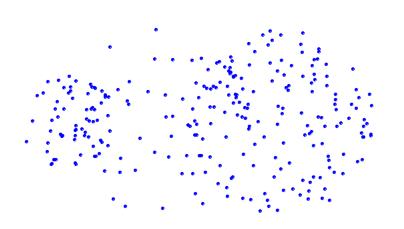
Nested Clusters

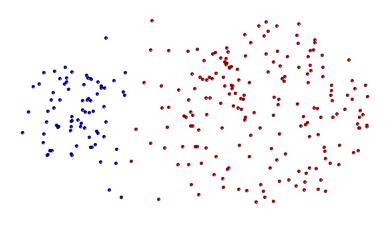
Dendrogram





Strength of MAX





Original Points

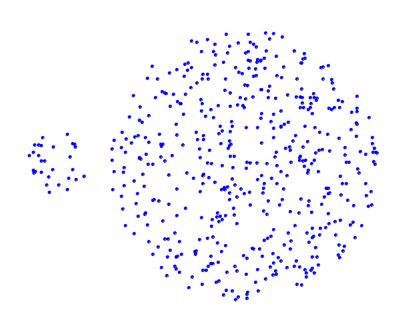
Two Clusters

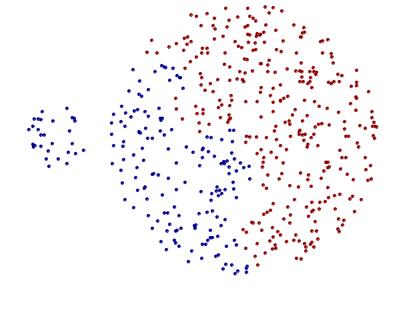
Less susceptible to noise and outliers





Limitations of MAX





Original Points

Two Clusters

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





Cluster Similarity: Group Average

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

$$proximity(Cluster_{i}, Cluster_{j}) = \frac{\sum_{\substack{p_{i} \in Cluster_{i}\\p_{j} \in Cluster_{j}}} proximity(Cluster_{i}, p_{j})}{|Cluster_{i}| * |Cluster_{i}|}$$

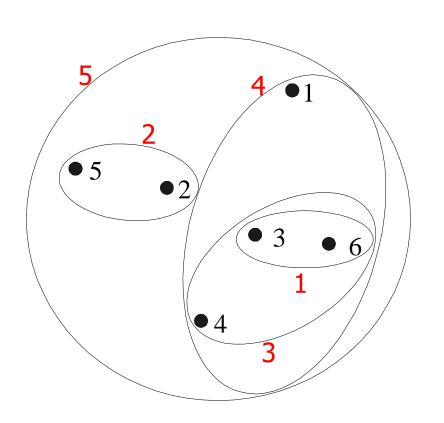
Need to use average connectivity for scalability since total proximity favors large clusters

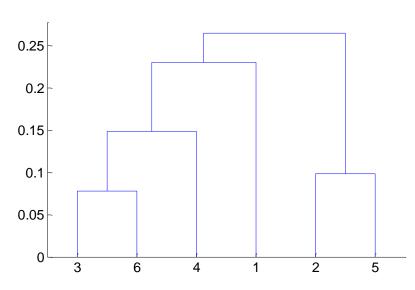
		12			
11	1.00	0.90	0.10	0.65	0.20
12	0.90	1.00	0.70	0.60	0.50
13	0.10	0.70	1.00	0.40	0.30
1 4	0.65	0.60	0.40	1.00	0.80
15	0.20	0.90 1.00 0.70 0.60 0.50	0.30	0.80	1.00

1 2 3 4 5



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





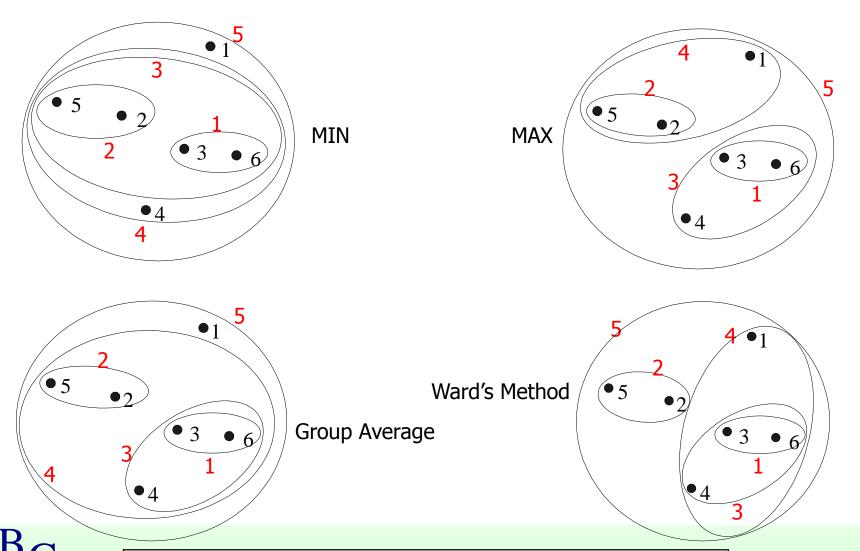
Cluster Similarity: Ward's Method

- 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





Hierarchical Clustering: Time and Space requirements

- O(N²) space since it uses the proximity matrix.
 - N is the number of points.

- O(N³) time in many cases
 - There are N steps and at each step the size, N², proximity matrix must be updated and searched
 - Complexity can be reduced to O(N² log(N)) time for some approaches





DBSCAN

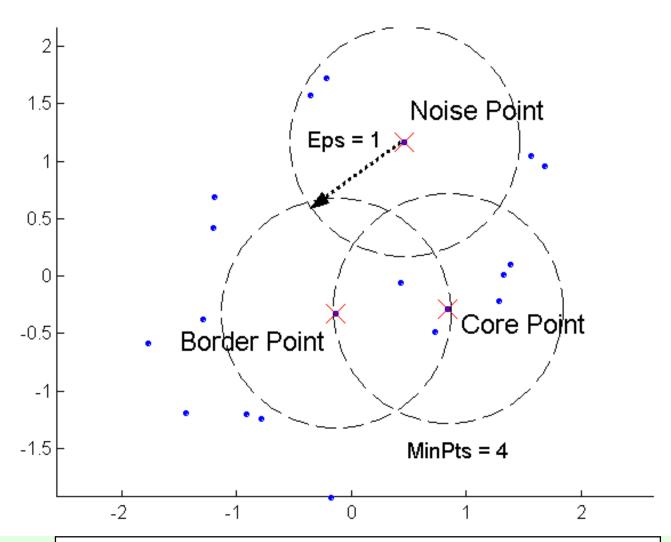
DBSCAN is a density-based algorithm

- 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.





DBSCAN: Core, Border, and Noise Points







DBSCAN Algorithm

- Eliminate noise points
- Perform clustering on the remaining points

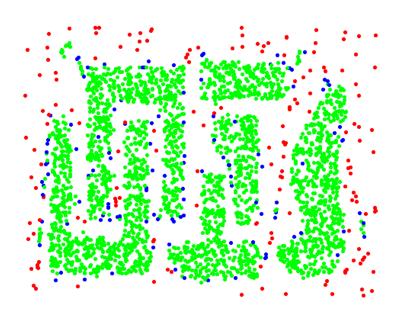
```
current\_cluster\_label \leftarrow 1
for all core points do
  if the core point has no cluster label then
    current\_cluster\_label \leftarrow current\_cluster\_label + 1
    Label the current core point with cluster label current_cluster_label
  end if
  for all points in the Eps-neighborhood,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





DBSCAN: Core, Border, and Noise Points





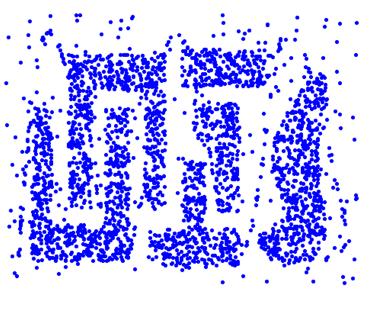
Original Points

Point types: core, border and noise





When DBSCAN Works Well



Original Points

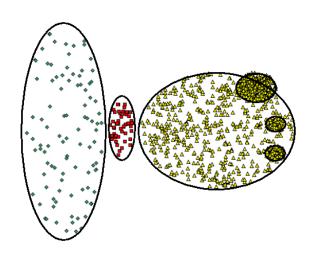
Clusters

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



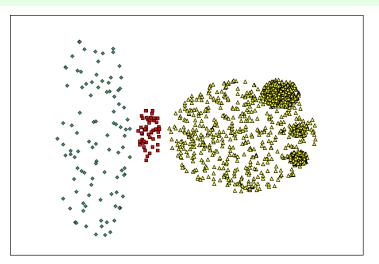


When DBSCAN Does NOT Work Well

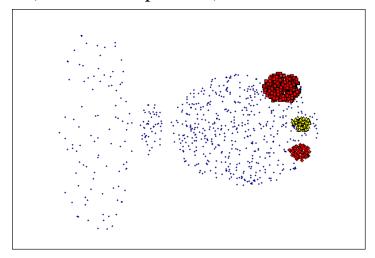


Original Points

- Varying densities
- High-dimensional data



(MinPts=4, Eps=9.75).



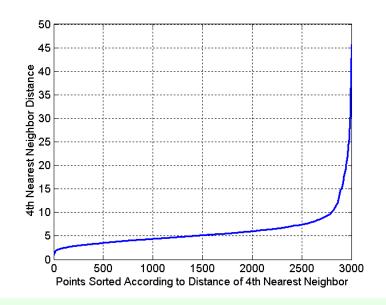
(MinPts=4, Eps=9.62)





DBSCAN: Determining EPS and MinPts

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







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





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 wellseparated a cluster is from other clusters
 - Separation is measured by the between cluster sum of squares

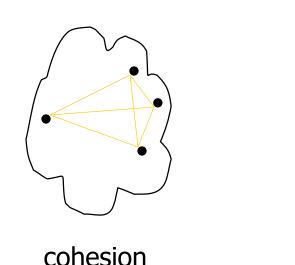
$$BSS = \sum_{i} |C_{i}| (m - m_{i})^{2}$$

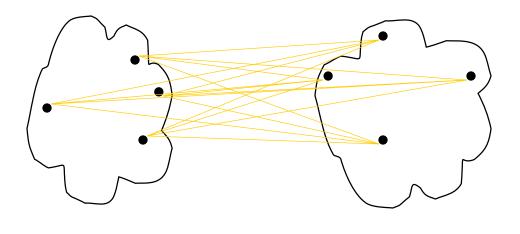




Internal Measures: Cohesion and Separation

- 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.





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

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

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

- 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

