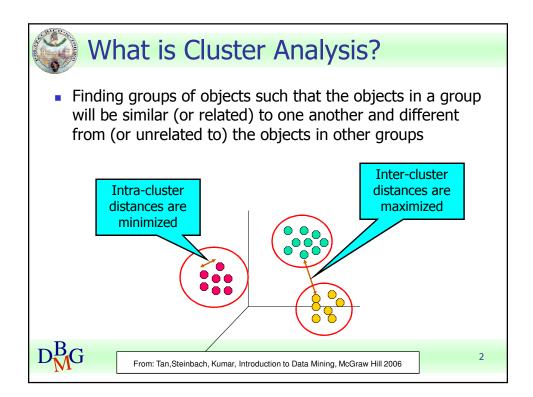


Clustering fundamentals

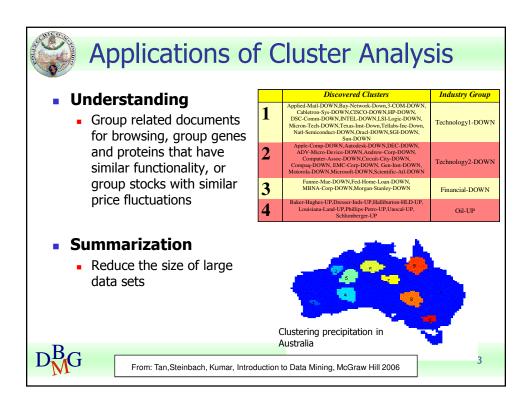


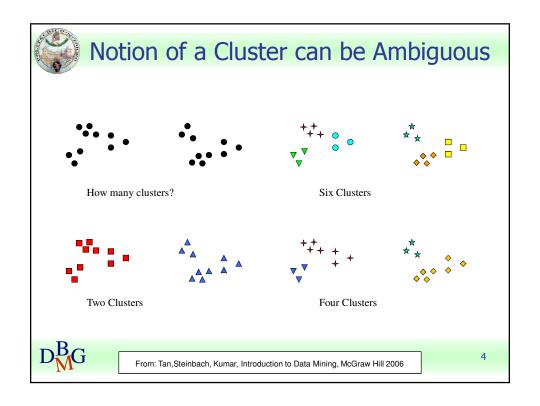
Elena Baralis, Tania Cerquitelli

Politecnico di Torino











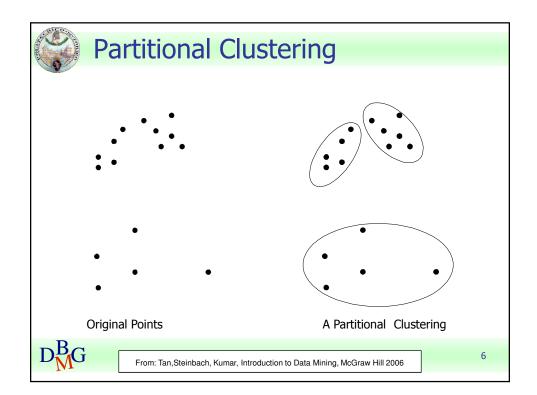


Types of Clusterings

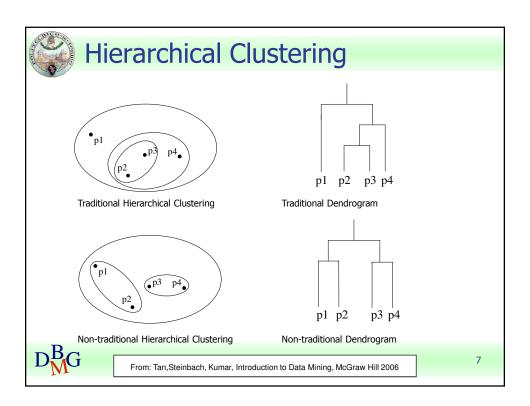
- A clustering is a set of clusters
- Important distinction between hierarchical and partitional sets of clusters
- Partitional Clustering
 - A division data objects into non-overlapping subsets (clusters) such that each data object is in exactly one subset
- Hierarchical clustering
 - A set of nested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

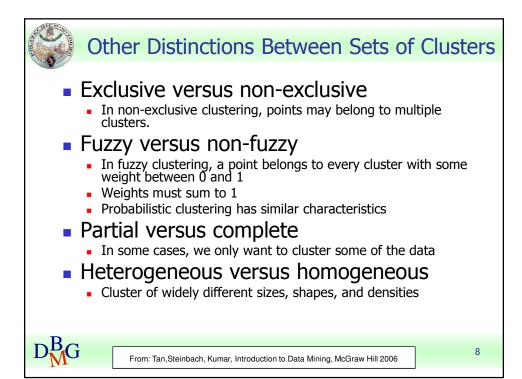


From: Tan, Steinbach, Kumar, Introduction to Data Mining, McGraw Hill 2006

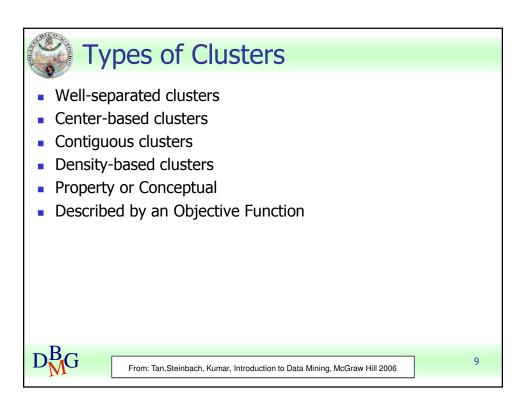


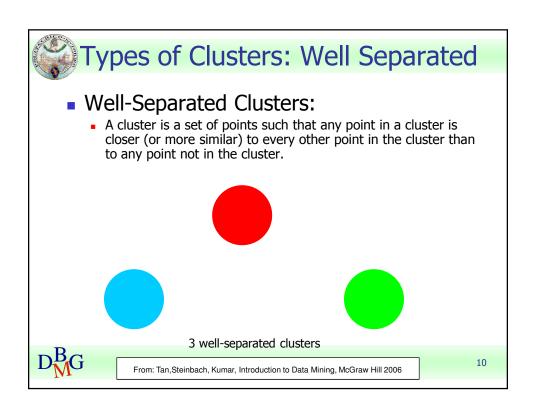




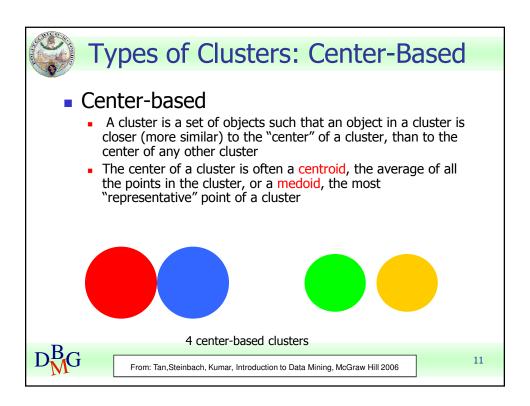


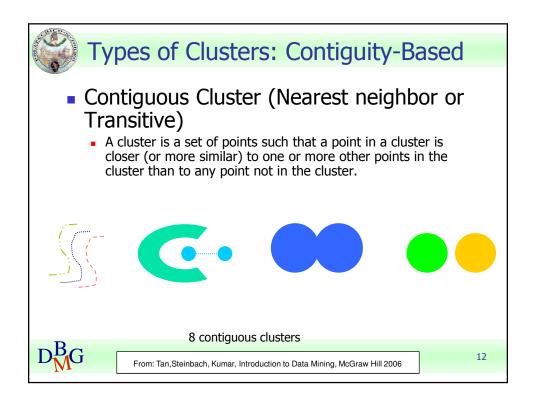




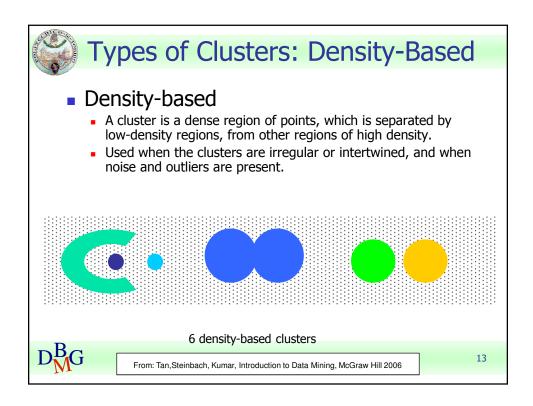


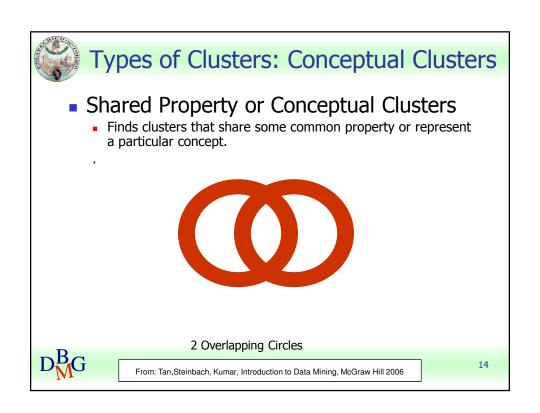
















Clustering Algorithms

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



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

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K-means Clustering

- Partitional clustering approach
- Each cluster is associated with a centroid (center point)
- Each point is assigned to the cluster with the closest centroid
- Number of clusters, K, must be specified
- The basic algorithm is very simple
- 1: Select K points as the initial centroids.
- 2: repeat
- 3: Form K clusters by assigning all points to the closest centroid.
- 4: Recompute the centroid of each cluster.
- 5: until The centroids don't change



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



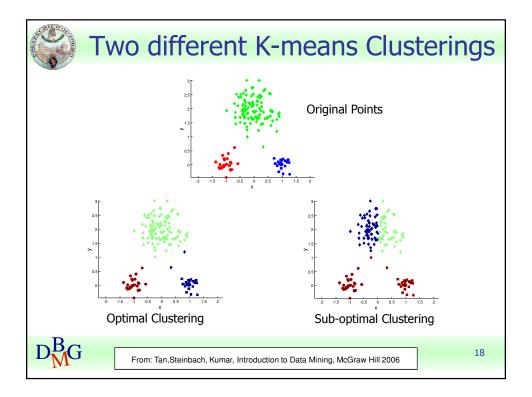


K-means Clustering – Details

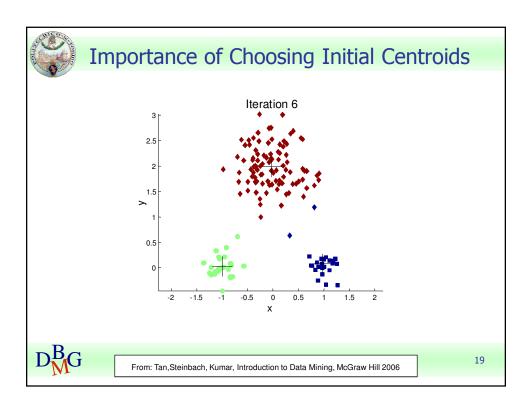
- Initial centroids are often chosen randomly.
 - Clusters produced vary from one run to another.
- The centroid is (typically) the mean of the points in the cluster.
- 'Closeness' is measured by Euclidean distance, cosine similarity, correlation, etc.
- K-means will converge for common similarity measures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

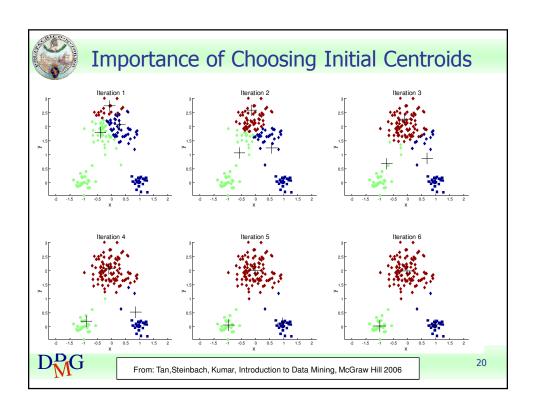


From: Tan, Steinbach, Kumar, Introduction to Data Mining, McGraw Hill 2006

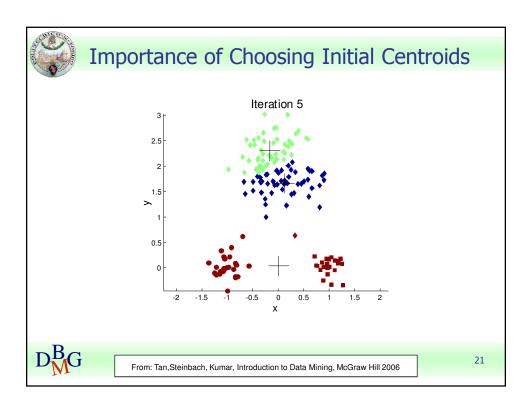


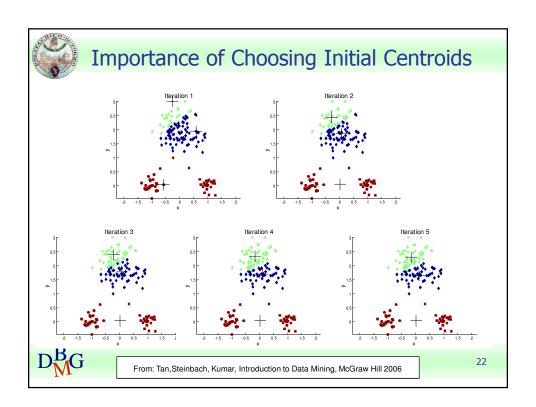
















Evaluating K-means Clusters

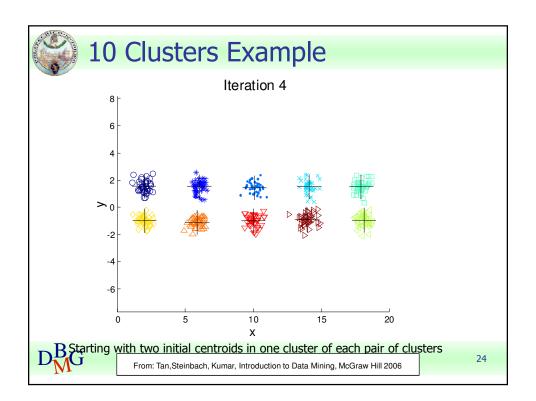
- Most common measure is Sum of Squared Error (SSE)
 - For each point, the error is the distance to the nearest cluster
 - To get SSE, we square these errors and sum them.

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

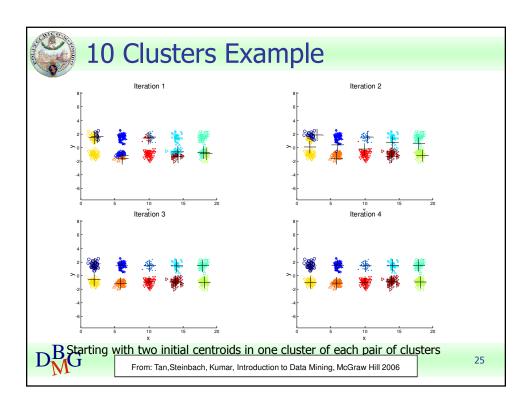
- x is a data point in cluster C_i and m_i is the representative point for cluster C_i
 - can show that m_i corresponds to the center (mean) of the cluster
- Given two clusters, we can choose the one with the smallest error
- One easy way to reduce SSE is to increase K, the number of clusters
 - A good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

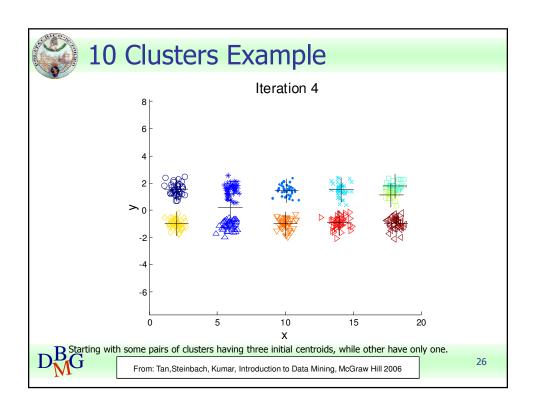


From: Tan, Steinbach, Kumar, Introduction to Data Mining, McGraw Hill 2006

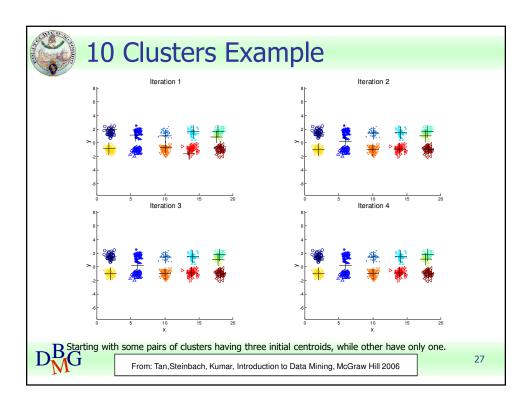














Solutions to Initial Centroids Problem

- 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

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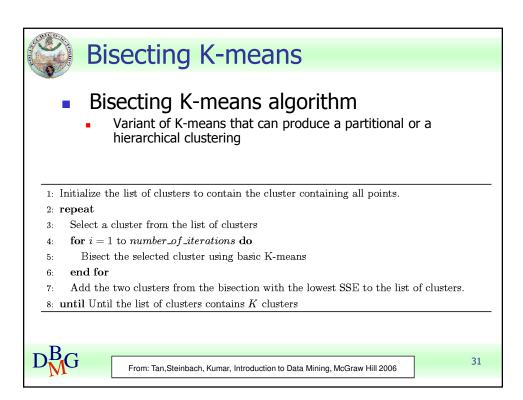
Pre-processing and Post-processing

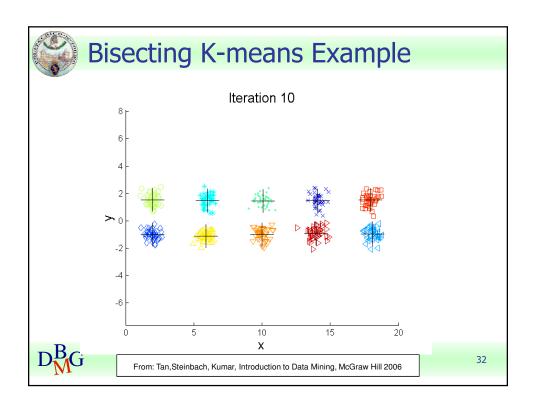
- Pre-processing
 - Normalize the data
 - Eliminate outliers
- Post-processing
 - Eliminate small clusters that may represent outliers
 - Split 'loose' clusters, i.e., clusters with relatively high SSE
 - Merge clusters that are 'close' and that have relatively low SSE
 - Can use these steps during the clustering process



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









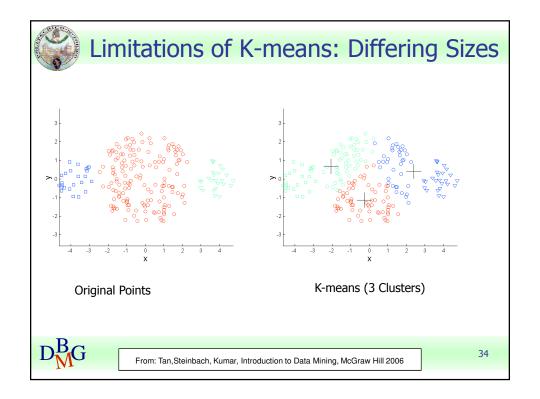


Limitations of K-means

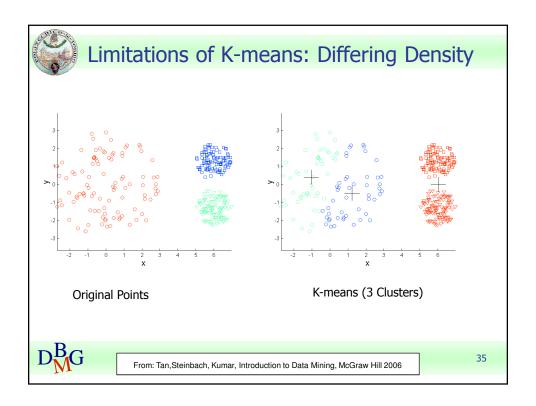
- K-means has problems when clusters are of differing
 - Sizes
 - Densities
 - Non-globular shapes
- K-means has problems when the data contains outliers.

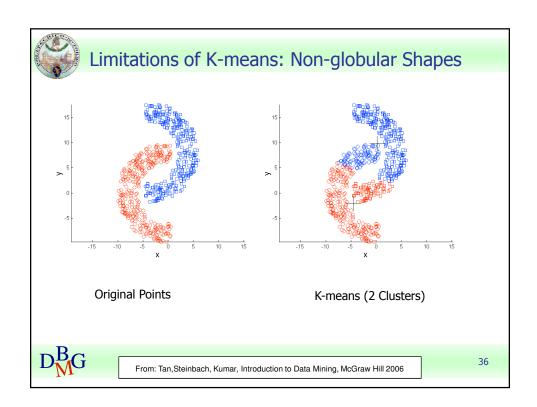


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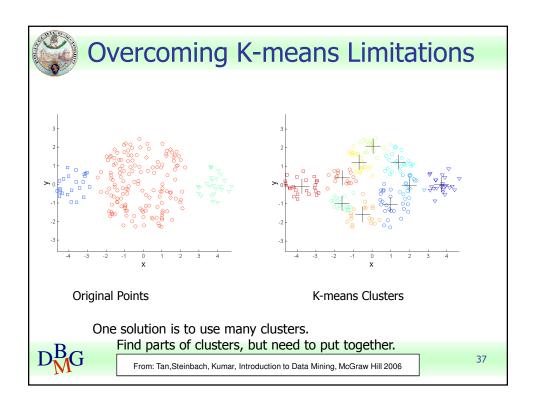


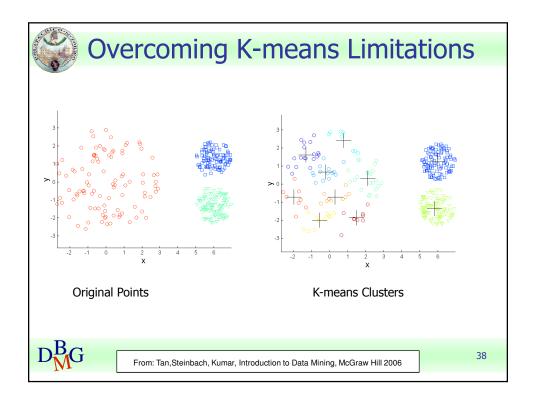




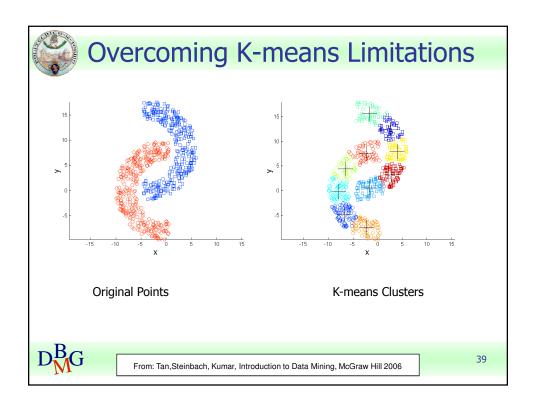


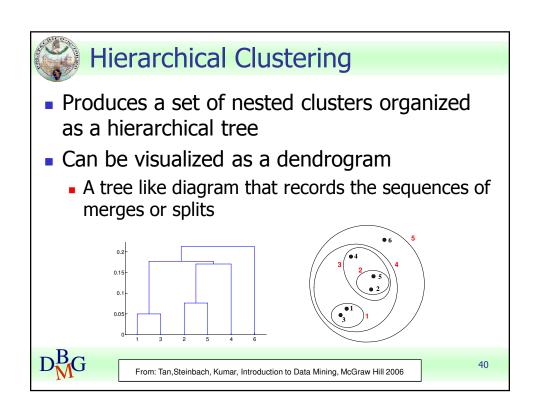
















Strengths of Hierarchical Clustering

- 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, ...)



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

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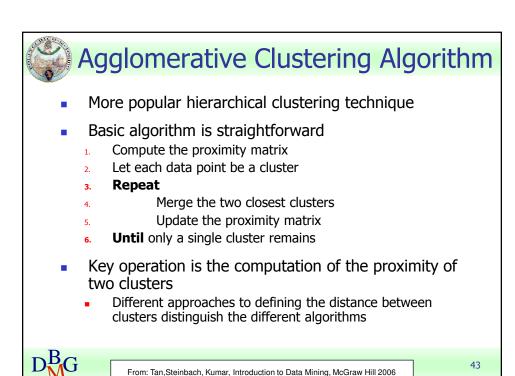
Hierarchical Clustering

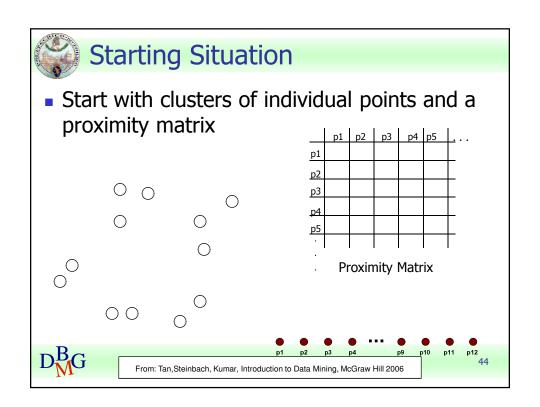
- Two main types of hierarchical clustering
 - Agglomerative:
 - Start with the points as individual clusters
 - At each step, merge the closest pair of clusters until only one cluster (or k clusters) left
 - Divisive:
 - Start with one, all-inclusive cluster
 - At each step, split a cluster until each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



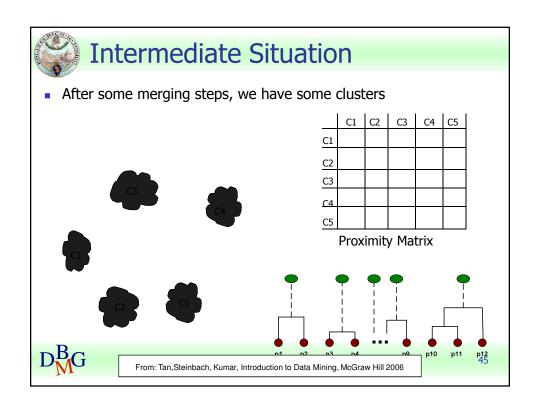
From: Tan, Steinbach, Kumar, Introduction to Data Mining, McGraw Hill 2006

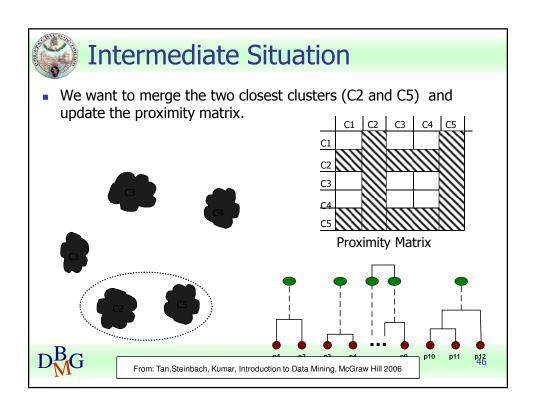




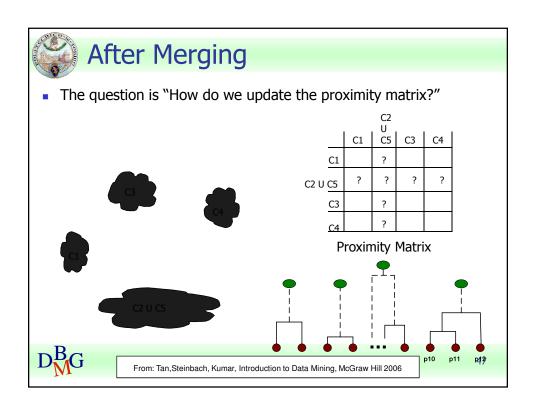


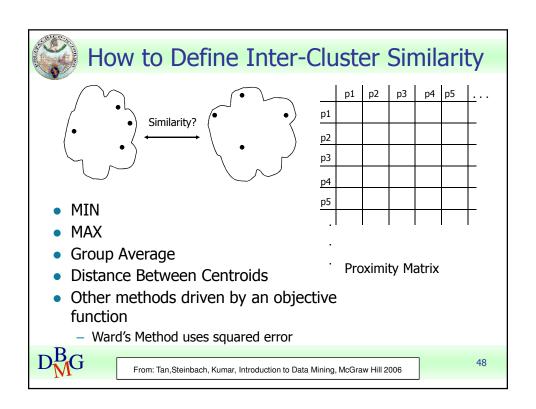




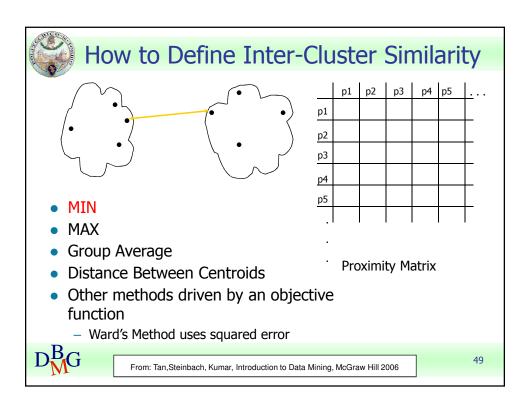


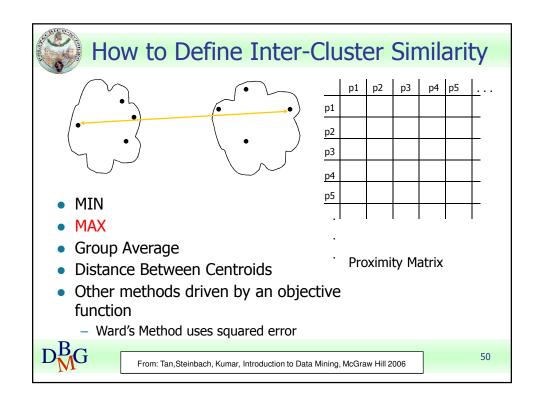




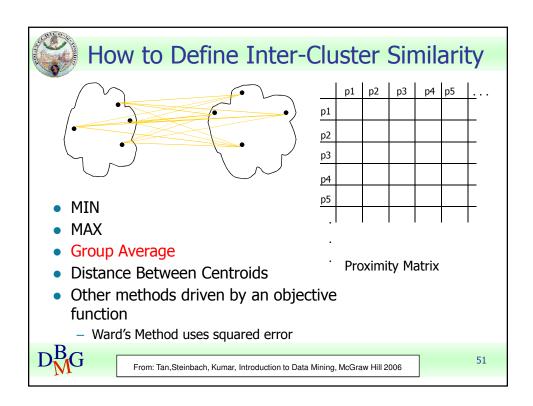


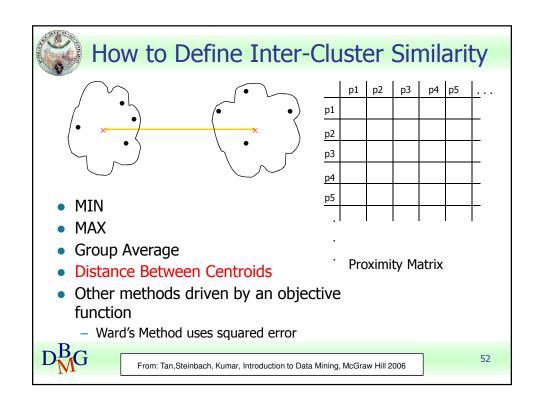




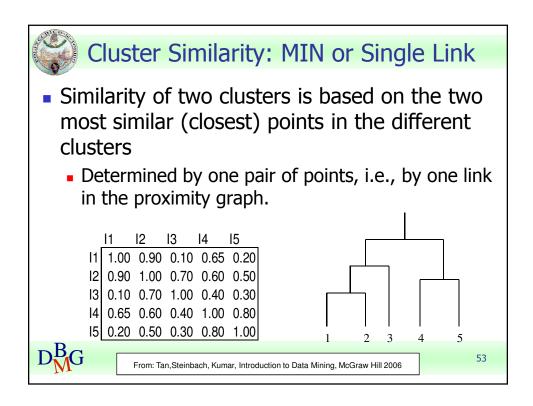


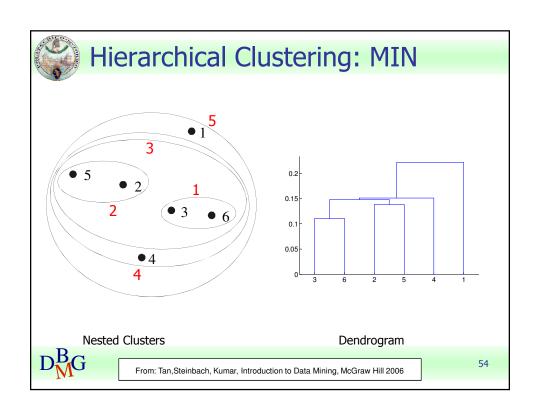




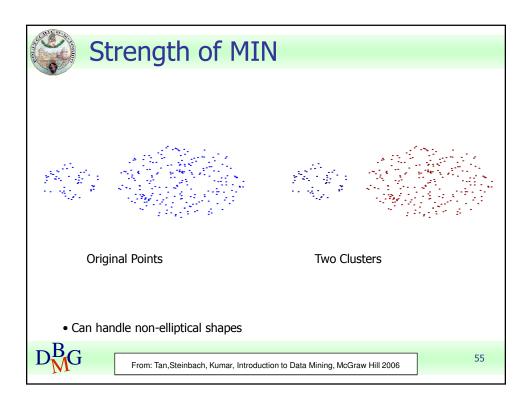


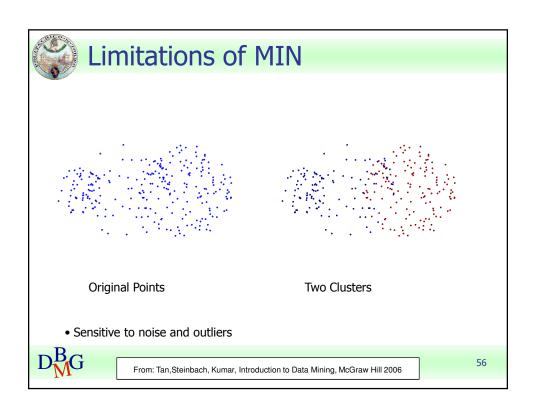




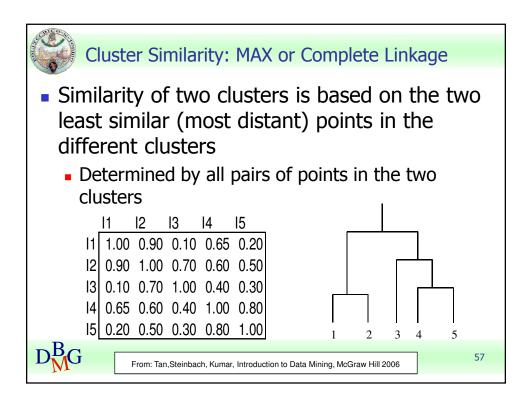


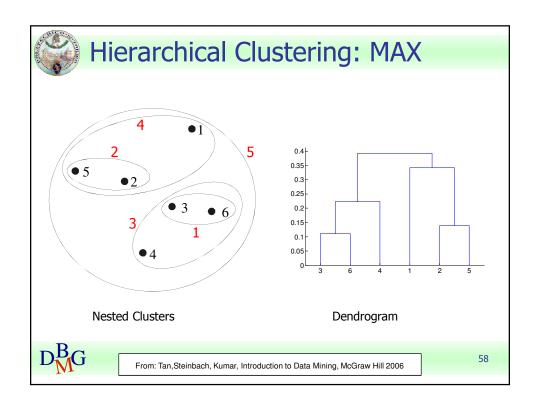




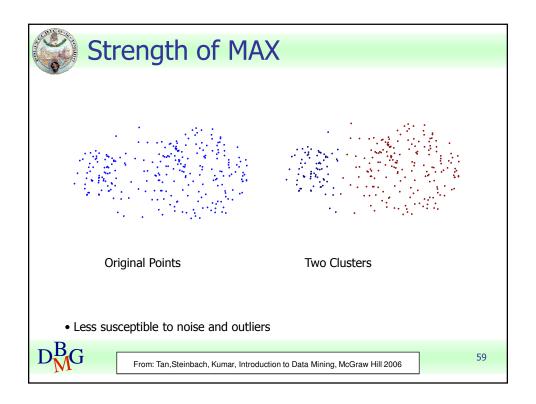


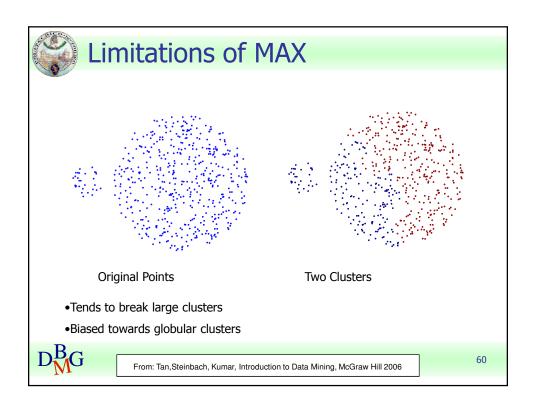




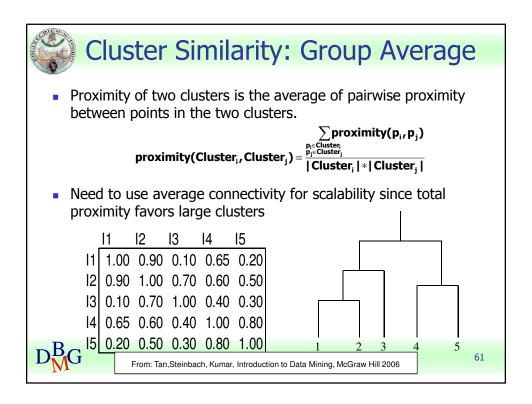


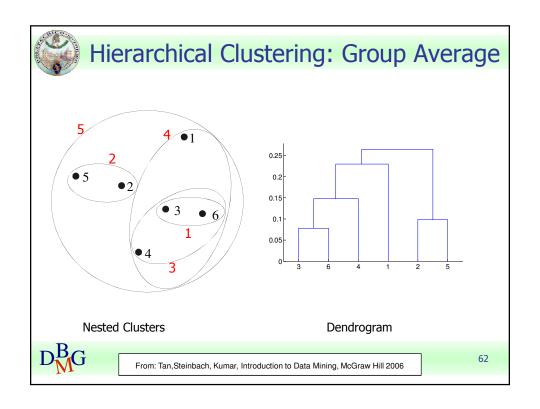
















Hierarchical Clustering: Group Average

- 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

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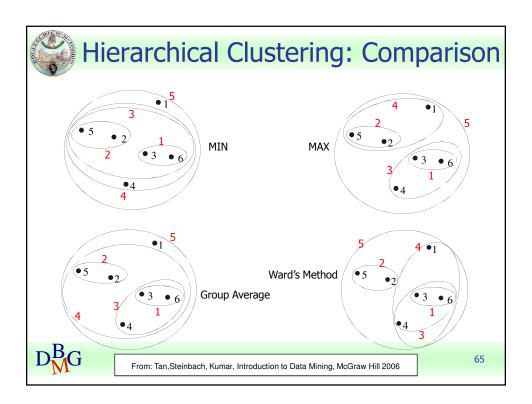
Cluster Similarity: Ward's Method

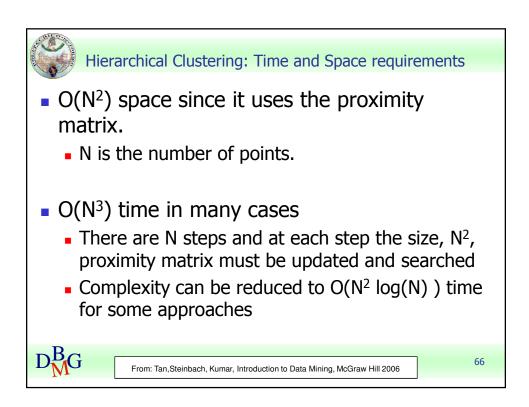
- Similarity of two clusters is based on the increase in squared error when two clusters are merged
 - Similar to group average if distance between points is distance squared
- Less susceptible to noise and outliers
- Biased towards globular clusters
- Hierarchical analogue of K-means
 - Can be used to initialize K-means



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









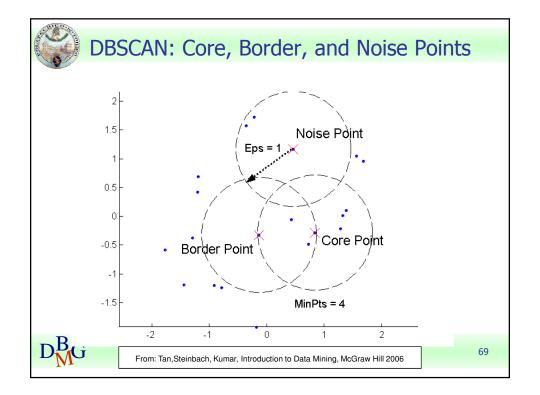


DBSCAN

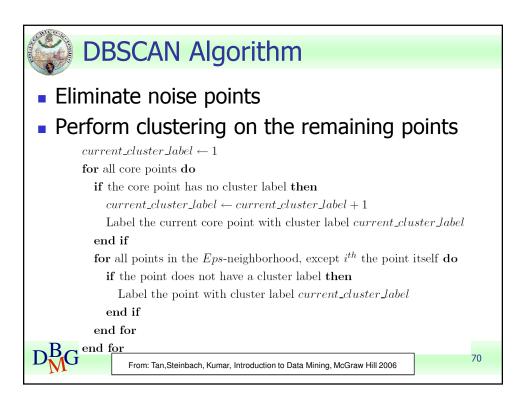
- DBSCAN is a density-based algorithm
 - Density = number of points within a specified radius (Eps)
 - A point is a core point if it has more than a specified number of points (MinPts) within Eps
 - These are points that are at the interior of a cluster
 - A border point has fewer than MinPts within 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.

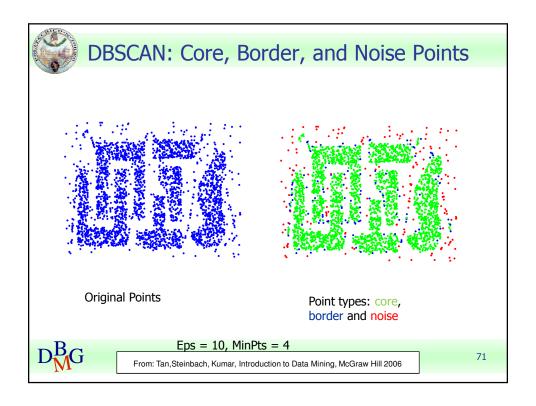


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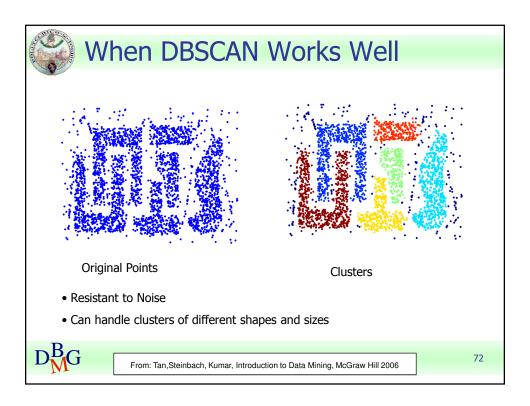


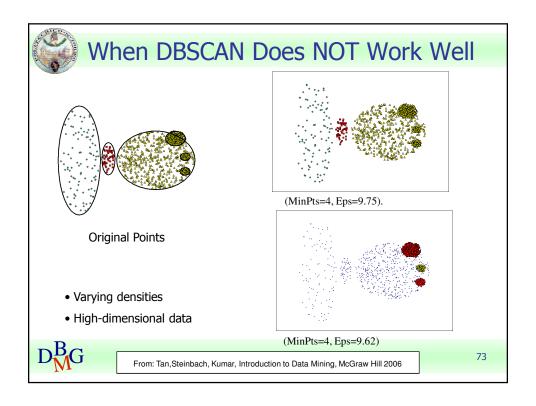










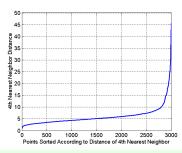






DBSCAN: Determining EPS and MinPts

- 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





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

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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



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



External Measures of Cluster Validity: Entropy and Purity

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

Table 6.6. It means clustering results for Ex Boodinent Bata Cot								
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

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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)

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

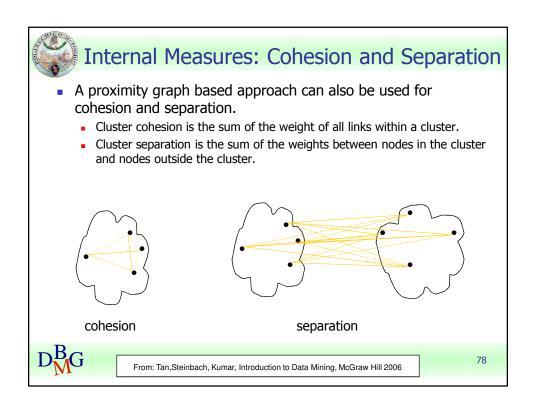
- Cluster Separation: Measure how distinct or wellseparated a cluster is from other clusters
 - Separation is measured by the between cluster sum of squares

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



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







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