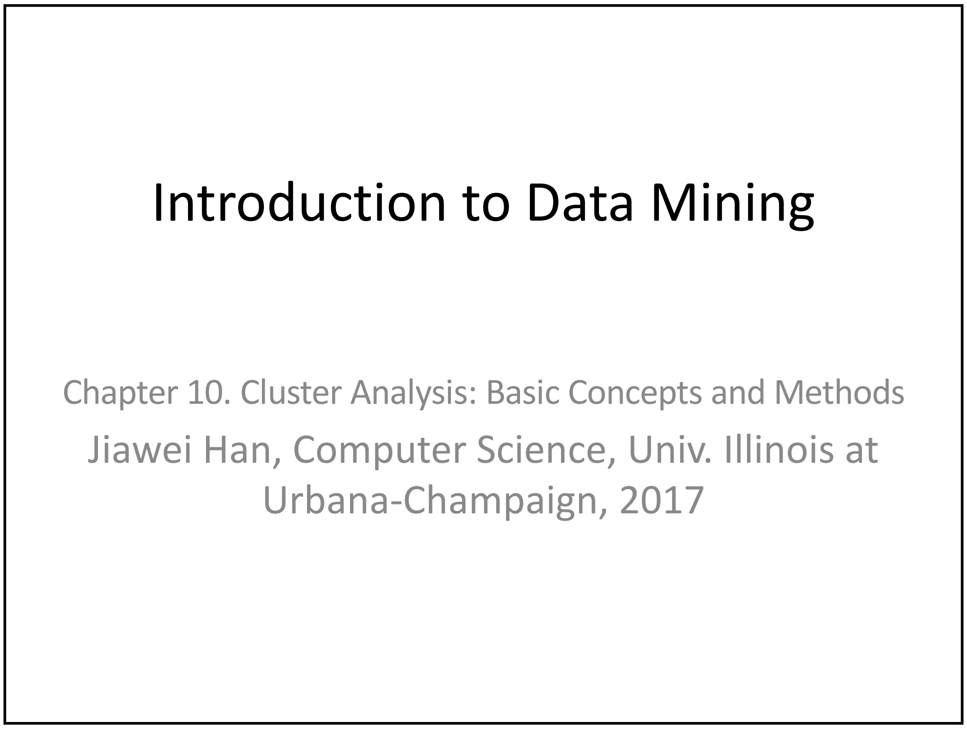

Introduction to Data Mining

Chapter 10. Cluster Analysis: Basic Concepts and Methods

Jiawei Han, Computer Science, Univ. Illinois at Urbana-Champaign, 2017

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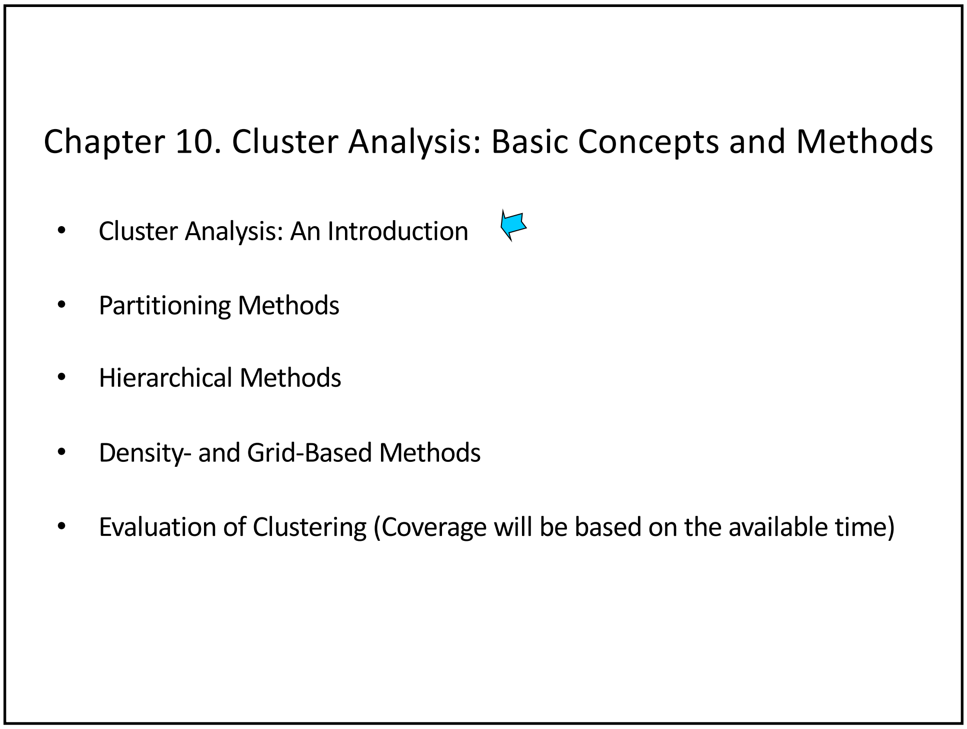
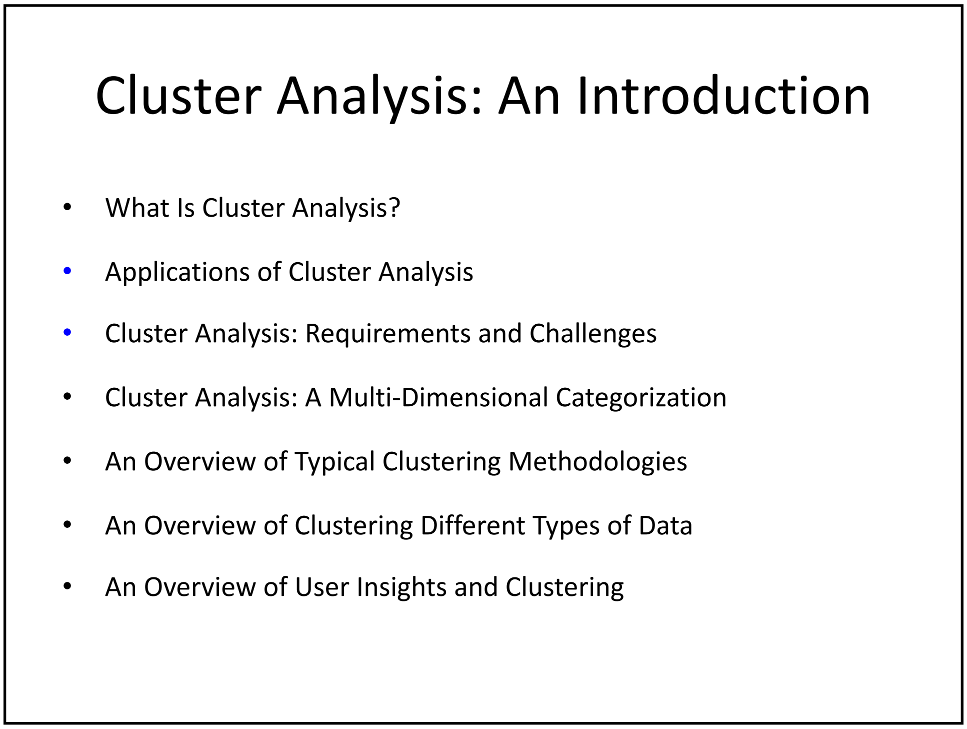


Chapter 10. Cluster Analysis: Basic Concepts and Methods

- Cluster Analysis: An Introduction
- Partitioning Methods
- Hierarchical Methods
- Density- and Grid-Based Methods
- Evaluation of Clustering (Coverage will be based on the available time)

2



Cluster Analysis: An Introduction

- What Is Cluster Analysis?
- Applications of Cluster Analysis
- Cluster Analysis: Requirements and Challenges
- Cluster Analysis: A Multi-Dimensional Categorization
- An Overview of Typical Clustering Methodologies
- An Overview of Clustering Different Types of Data
- An Overview of User Insights and Clustering

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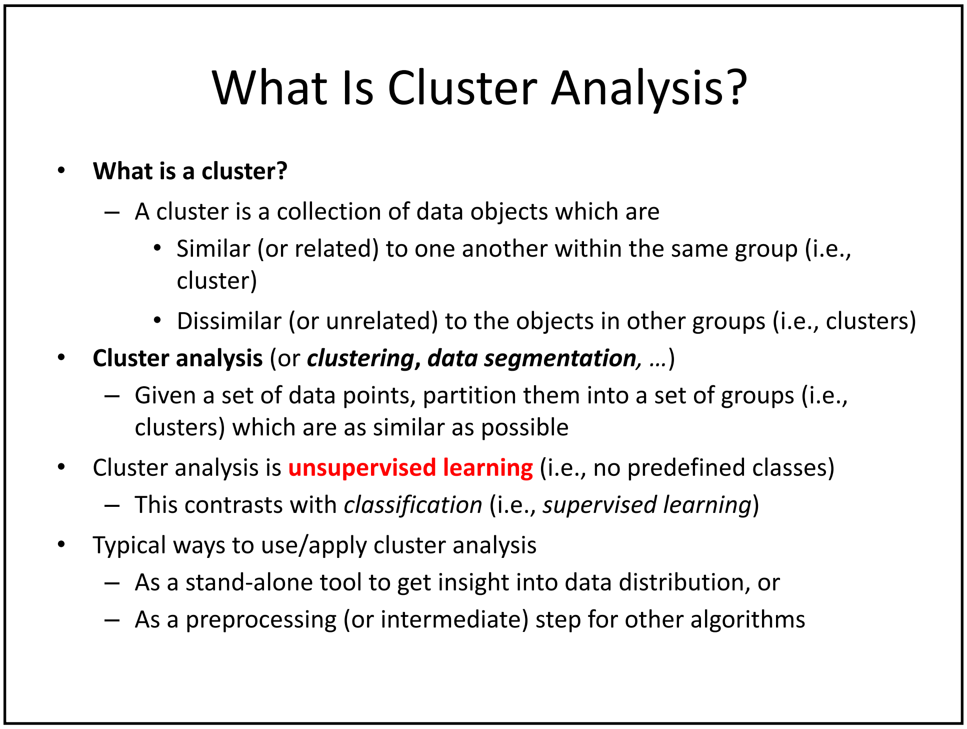

What Is Cluster Analysis?

- **What is a cluster?**
  - A cluster is a collection of data objects which are
    - Similar (or related) to one another within the same group (i.e., cluster)
    - Dissimilar (or unrelated) to the objects in other groups (i.e., clusters)
- **Cluster analysis** (or ***clustering*, *data segmentation***, *…*)
  - Given a set of data points, partition them into a set of groups (i.e., clusters) which are as similar as possible
- Cluster analysis is **unsupervised learning** (i.e., no predefined classes)
  - This contrasts with *classification* (i.e., *supervised learning*)
- Typical ways to use/apply cluster analysis
  - As a stand-alone tool to get insight into data distribution, or
  - As a preprocessing (or intermediate) step for other algorithms

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What Is Good Clustering?

- A good clustering method will produce high quality clusters which should have
  - **High intra-class similarity:** Cohesive within clusters
  - **Low inter-class similarity:** Distinctive between clusters
- **Quality function**
  - There is usually a separate “quality” function that measures the “goodness” of a cluster
  - It is hard to define “similar enough” or “good enough”
    - The answer is typically highly subjective
- There exist many similarity measures and/or functions for different applications
- Similarity measure is critical for cluster analysis

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Cluster Analysis: Applications

- A key intermediate step for other data mining tasks
  - Generating a compact summary of data for classification, pattern discovery, hypothesis generation and testing, etc.
  - Outlier detection: Outliers—those “far away” from any cluster
- Data summarization, compression, and reduction
  - Ex. Image processing: Vector quantization
- Collaborative filtering, recommendation systems, or customer segmentation
  - Find like-minded users or similar products
- Dynamic trend detection
  - Clustering stream data and detecting trends and patterns
- Multimedia data analysis, biological data analysis and social network analysis
  - Ex. Clustering images or video/audio clips, gene/protein sequences, etc.

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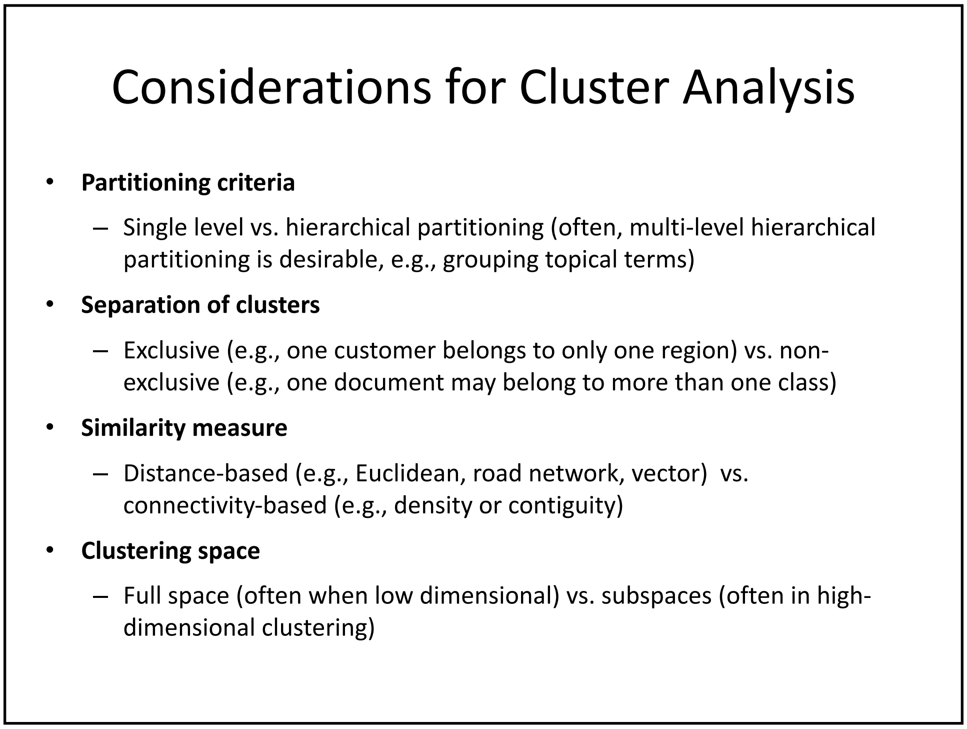

Considerations for Cluster Analysis

- **Partitioning criteria**
  - Single level vs. hierarchical partitioning (often, multi-level hierarchical partitioning is desirable, e.g., grouping topical terms)
- **Separation of clusters**
  - Exclusive (e.g., one customer belongs to only one region) vs. non-exclusive (e.g., one document may belong to more than one class)
- **Similarity measure**
  - Distance-based (e.g., Euclidean, road network, vector) vs. connectivity-based (e.g., density or contiguity)
- **Clustering space**
  - Full space (often when low dimensional) vs. subspaces (often in high-dimensional clustering)

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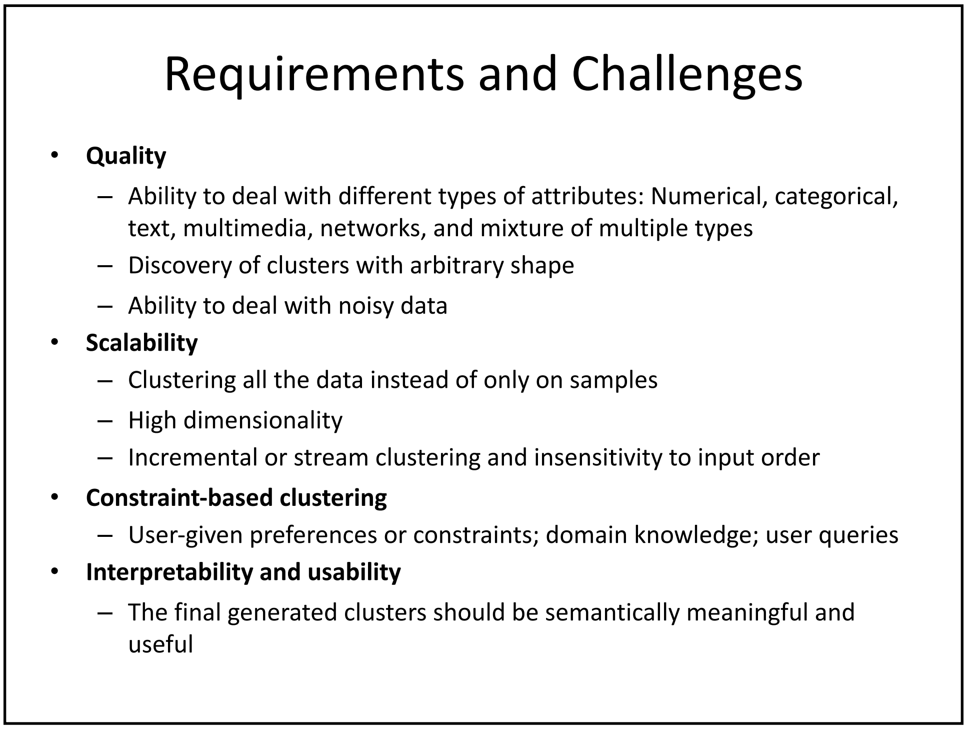

Requirements and Challenges

- **Quality**
  - Ability to deal with different types of attributes: Numerical, categorical, text, multimedia, networks, and mixture of multiple types
  - Discovery of clusters with arbitrary shape
  - Ability to deal with noisy data
- **Scalability**
  - Clustering all the data instead of only on samples
  - High dimensionality
  - Incremental or stream clustering and insensitivity to input order
- **Constraint-based clustering**
  - User-given preferences or constraints; domain knowledge; user queries
- **Interpretability and usability**
  - The final generated clusters should be semantically meaningful and useful

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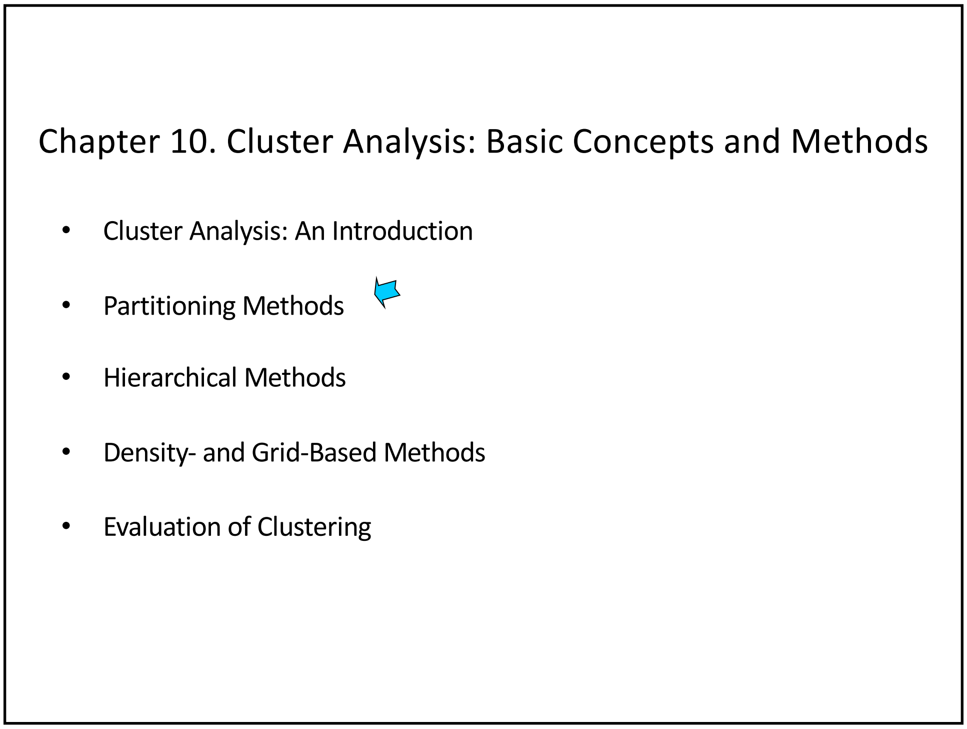

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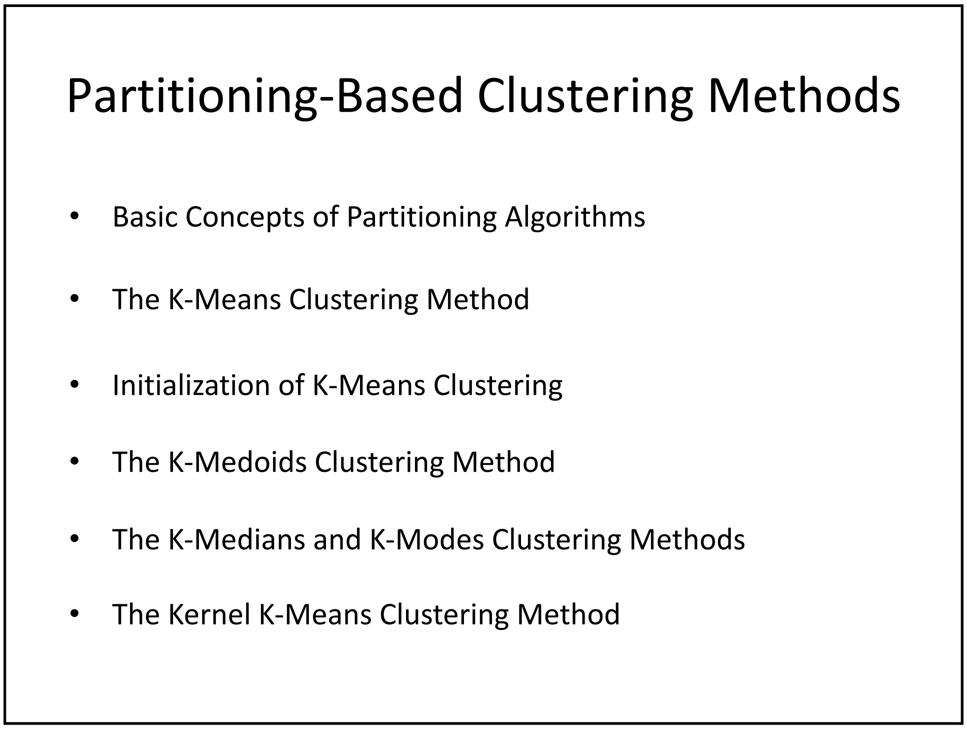

Partitioning-Based Clustering Methods

- Basic Concepts of Partitioning Algorithms
- The K-Means Clustering Method
- Initialization of K-Means Clustering
- The K-Medoids Clustering Method
- The K-Medians and K-Modes Clustering Methods
- The Kernel K-Means Clustering Method

Partitioning Algorithms: Basic Concepts

- Partitioning method: Discovering the groupings in the data by optimizing a specific objective function and iteratively improving the quality of partitions
- *K*-partitioning method: Partitioning a dataset ***D*** of ***n*** objects into a set of ***K*** clusters so that an objective function is optimized (e.g., the sum of squared distances is minimized, where c_k is the centroid or medoid of cluster C_k)
  - A typical objective function: **Sum of Squared Errors** (**SSE**)

$$SSE(C) = \sum_{k=1}^{K} \sum_{x_i \in C_k} || x_i - c_k ||^2$$

- Problem definition: Given *K*, find a partition of *K clusters* that optimizes the chosen partitioning criterion
  - Global optimal: Needs to exhaustively enumerate all partitions
  - Heuristic methods (i.e., greedy algorithms): *K-Means*, *K-Medians*, *K-Medoids*, etc.

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The *K-Means* Clustering Method

- *K-Means* (MacQueen'67, Lloyd'57/'82)
  - Each cluster is represented by the center of the cluster
- Given K, the number of clusters, the *K-Means* clustering algorithm is outlined as follows
  - Select *K* points as initial centroids
  - **Repeat**
    - Form *K* clusters by assigning each point to its closest centroid
    - Re-compute the centroids (i.e., *mean point*) of each cluster
  - **Until** convergence criterion is satisfied
- Different kinds of measures can be used
  - Manhattan distance (L_1 norm), Euclidean distance (L_2 norm), Cosine similarity

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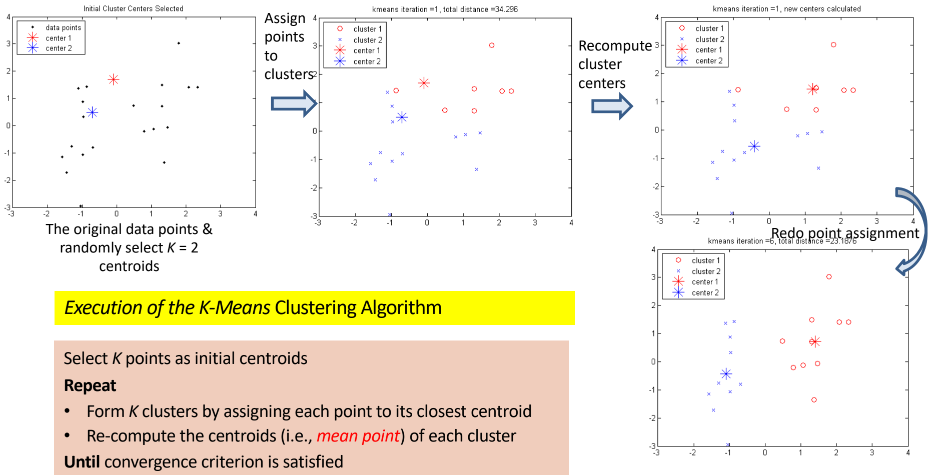
Example: *K-Means* Clustering



The original data points & randomly select *K* = 2 centroids

Execution of the K-Means Clustering Algorithm

```
Select K points as initial centroids
Repeat
  • Form K clusters by assigning each point to its closest centroid
  • Re-compute the centroids (i.e., mean point) of each cluster
Until convergence criterion is satisfied
```

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Discussion on the *K-Means* Method

- **Efficiency**: *O*(*tKn*) where *n*: # of objects, *K*: # of clusters, and *t:* # of iterations
  - Normally, *K*, *t* << *n*; thus, an efficient method
- K-means clustering often ***terminates at*** **a** ***local optimal***
  - Initialization can be important to find high-quality clusters
- **Need to specify *K,*** the *number* of clusters, in advance
  - There are ways to automatically determine the "*best*" *K*
  - In practice, one often runs a range of values and selected the "*best*" *K* value
- **Sensitive to noisy data and *outliers***
  - Variations: Using K-medians, K-medoids, etc.
- K-means is applicable only to objects in a continuous n-dimensional space
  - Using the K-modes for ***categorical data***
- Not suitable to discover clusters with ***non-convex shapes***
  - Using density-based clustering, kernel *K*-means, etc.

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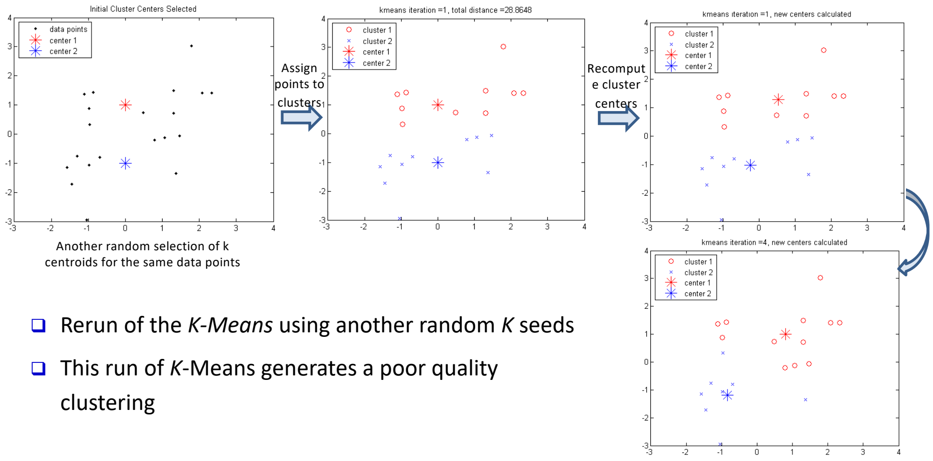
Variations of *K-Means*

- There are many variants of the *K-Means* method, varying in different aspects
  - Choosing better initial centroid estimates
    - *K-means++, Intelligent K-Means, Genetic K-Means*
  - Choosing different representative prototypes for the clusters
    - *K-Medoids, K-Medians, K-Modes*
  - Applying feature transformation techniques
    - *Weighted K-Means, Kernel K-Means*

Poor Initialization in K-Means May Lead to Poor Clustering

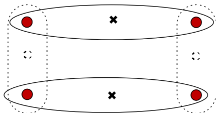


Another random selection of k centroids for the same data points

- ❑ Rerun of the *K-Means* using another random *K* seeds
- ❑ This run of *K*-Means generates a poor quality clustering

Initialization of K-Means: Problem and Solution

- Different initializations may generate rather different clustering results (some could be far from optimal)
- Original proposal (MacQueen'67): Select *K* seeds randomly
  - – Need to run the algorithm multiple times using different seeds



- ❑ There are many methods proposed for better initialization of *k* seeds
  - ❑ ***K-Means++*** (Arthur & Vassilvitskii'07):
    - ❑ The first centroid is selected at random
    - ❑ The next centroid selected is the one that is farthest from the currently selected (selection is based on a weighted probability score)
    - ❑ The selection continues until *K* centroids are obtained

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Handling Outliers: From *K-Means* to *K-Medoids*

- The *K-Means* algorithm is sensitive to outliers!—since an object with an extremely large value may substantially distort the distribution of the data
- *K-Medoids*: Instead of taking the **mean** value of the object in a cluster as a reference point, **medoids** can be used, which is the **most centrally located** object in a cluster
- The *K-Medoids* clustering algorithm:
  - Select *K* points as the initial representative objects (i.e., as initial *K medoids*)
  - **Repeat**
    - – Assigning each point to the cluster with the closest medoid
    - – Randomly select a non-representative object o_i
    - – Compute the total cost *S* of swapping the medoid *m* with o_i
    - – If $S < 0$, then swap *m* with o_i to form the new set of medoids
  - **Until** convergence criterion is satisfied

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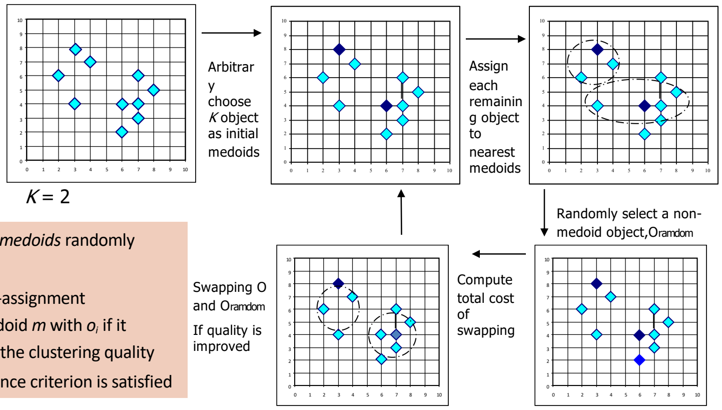
PAM: A Typical *K-Medoids* Algorithm



Arbitrary choose *K* object as initial medoids

Assign each remaining object to nearest medoids

Randomly select a non-medoid object,Oramdom

Compute total cost of swapping

Swapping O and Oramdom

If quality is improved

K = 2

```
Select initial K medoids randomly
Repeat
    Object re-assignment
    Swap medoid m with $o_i$ if it improves the clustering quality
Until convergence criterion is satisfied
```

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Discussion on *K-Medoids* Clustering

- *K-Medoids* Clustering: Find *representative* objects (medoids) in clusters
- *PAM* (Partitioning Around Medoids: Kaufmann & Rousseeuw 1987)
  - Starts from an initial set of medoids, and
  - Iteratively replaces one of the medoids by one of the non-medoids if it improves the total sum of the squared errors (SSE) of the resulting clustering
  - *PAM* works effectively for small data sets but does not scale well for large data sets (due to the computational complexity)
  - Computational complexity: PAM: $O(K(n - K)^2)$ (quite expensive!)
- Efficiency improvements on PAM
  - *CLARA* (Kaufmann & Rousseeuw, 1990):
    - PAM on samples; $O(Ks^2 + K(n - K))$, s is the sample size
  - *CLARANS* (Ng & Han, 1994): Randomized re-sampling, ensuring efficiency + quality

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K-Medians: Handling Outliers by Computing Medians

- Medians are less sensitive to outliers than means
  - Think of the median salary vs. mean salary of a large firm when adding a few top executives!
- ***K-Medians***: Instead of taking the **mean** value of the object in a cluster as a reference point, **medians** are used (L_1-norm as the distance measure)
- The criterion function for the *K-Medians* algorithm:
- The *K-Medians* clustering algorithm:

$$S = \sum_{k=1}^{K} \sum_{x_{i} \in C_k} | x_{ij} - med_{kj} |$$

  - Select *K* points as the initial representative objects (i.e., as initial *K medians*)
  - **Repeat**
    - Assign every point to its nearest median
    - Re-compute the median using the median of each individual feature
  - **Until** convergence criterion is satisfied

K-Modes: Clustering Categorical Data

- *K-Means* cannot handle non-numerical (categorical) data
  - Mapping categorical value to 1/0 cannot generate quality clusters
- ***K-Modes*: An extension to *K-Means* by replacing means of clusters with *modes***
  - Mode: The value that appears most often in a **set** of data values
- Dissimilarity measure between object X and the center of a cluster Z
  - $\Phi(x_j, z_j) = 1 - n_j^r/n_l$ when $x_j = z_j$; 1 when x_j ǂ z_j
    - where z_j is the categorical value of attribute j in Z_l, n_l is the number of objects in cluster *l*, and n_j^r is the number of objects whose attribute value is r
- This dissimilarity measure (distance function) is **frequency-based**
- Algorithm is still based on iterative *object cluster assignment* and *centroid update*
- A ***fuzzy K-Modes*** method is proposed to calculate a ***fuzzy cluster membership value*** for each object to each cluster
- A mixture of categorical and numerical data: Using a ***K-Prototype*** method

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Hierarchical Clustering Methods

- Basic Concepts of Hierarchical Algorithms
- Agglomerative Clustering Algorithms
- Divisive Clustering Algorithms
- Extensions to Hierarchical Clustering
- BIRCH: A Micro-Clustering-Based Approach
- CURE: Exploring Well-Scattered Representative Points
- CHAMELEON: Graph Partitioning on the KNN Graph of the Data
- Probabilistic Hierarchical Clustering

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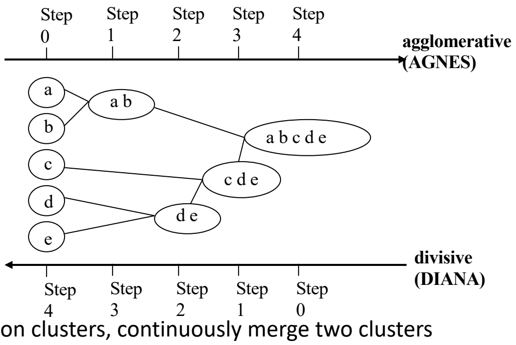
Hierarchical Clustering: Basic Concepts



- Hierarchical clustering
  - Generate a clustering hierarchy (drawn as a **dendrogram**)
  - Not required to specify ***K,*** the number of clusters
  - More deterministic
  - No iterative refinement
- Two categories of algorithms:
  - ❑ **Agglomerative**: Start with singleton clusters, continuously merge two clusters at a time to build a **bottom-up** hierarchy of clusters
  - ❑ **Divisive:** Start with a huge macro-cluster, split it continuously into two groups, generating a **top-down** hierarchy of clusters

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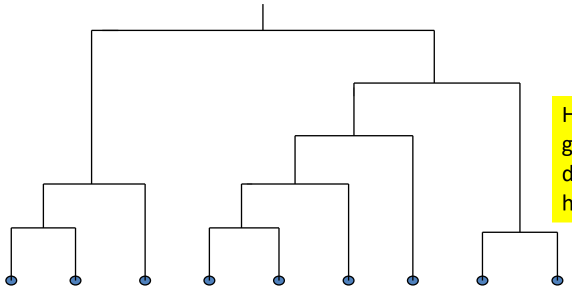
Dendrogram: Shows How Clusters are Merged

- Dendrogram: Decompose a set of data objects into a tree of clusters by multi-level nested partitioning
- A clustering of the data objects is obtained by cutting the dendrogram at the desired level, then each connected component forms a cluster



Hierarchical clustering generates a dendrogram (a hierarchy of clusters)

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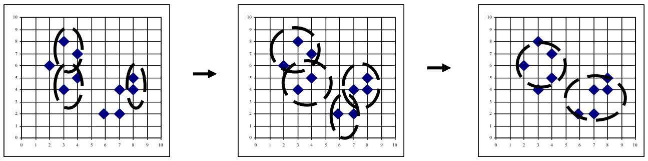
Agglomerative Clustering Algorithm

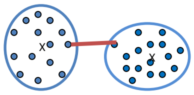
- AGNES (AGglomerative NESting) (Kaufmann and Rousseeuw, 1990)
  - Use the **single-link** method and the dissimilarity matrix
  - Continuously merge nodes that have the least dissimilarity
  - Eventually all nodes belong to the same cluster



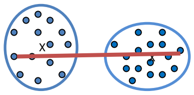
- ❑ Agglomerative clustering varies on different similarity measures among clusters
  - ❑ Single link (nearest neighbor)
  - ❑ Complete link (diameter)
  - ❑ Average link (group average)
  - ❑ Centroid link (centroid similarity)

Single Link vs. Complete Link in Hierarchical Clustering

- Single link (nearest neighbor)
  - The similarity between two clusters is the similarity between their most similar (nearest neighbor) members
  - Local similarity-based: Emphasizing more on close regions, ignoring the overall structure of the cluster
  - Capable of clustering non-elliptical shaped group of objects
  - Sensitive to noise and outliers

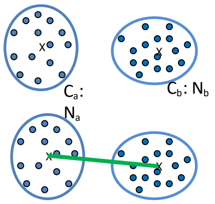


- Complete link (diameter)
  - The similarity between two clusters is the similarity between their most dissimilar members
  - Merge two clusters to form one with the smallest diameter
  - Nonlocal in behavior, obtaining compact shaped clusters
  - Sensitive to outliers



Agglomerative Clustering: Average vs. Centroid Links

- Agglomerative clustering with **average link**
  - **Average link**: The average distance between an element in one cluster and an element in the other (i.e., all pairs in two clusters)
    - Expensive to compute
- Agglomerative clustering with **centroid link**
  - **Centroid link**: The distance between the centroids of two clusters
- **Group Averaged Agglomerative Clustering (GAAC)**
  - Let two clusters C_a and C_b be merged into C_{aUb}. The new centroid is:
    - N_a is the cardinality of cluster C_a, and c_a is the centroid of C_a
  - The similarity measure for GAAC is the average of their distances

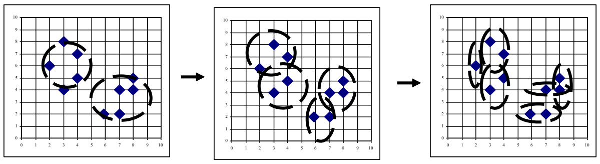


$$c_{a\cup b} = \frac{N_a c_a + N_b c_b}{N_a + N_b}$$

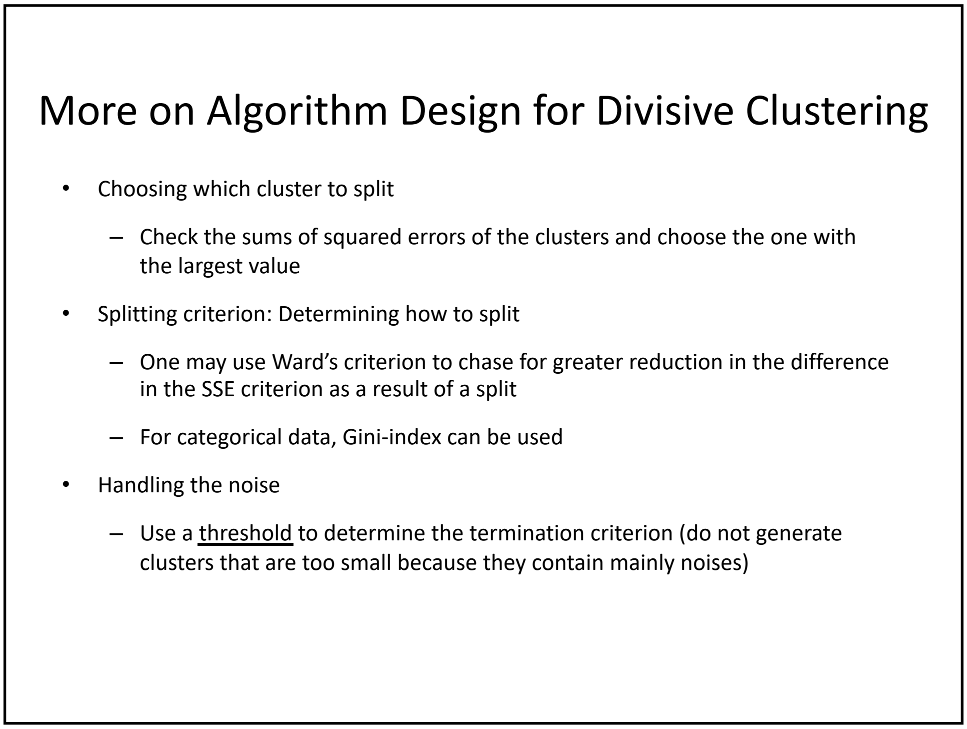
- ❑ Agglomerative clustering with **Ward's criterion**
  - ❑ **Ward's criterion:** The increase in the value of the SSE criterion for the clustering obtained by merging them into C_a U C_b: $W(C_{a\cup b}, c_{a\cup b}) - W(C,c) = \frac{N_a N_b}{N_a + N_b} d(c_a, c_b)$

Divisive Clustering

- DIANA (Divisive Analysis) (Kaufmann and Rousseeuw,1990)
  - Implemented in some statistical analysis packages, e.g., Splus
- Inverse order of AGNES: Eventually each node forms a cluster on its own



- ❑ Divisive clustering is a top-down approach
  - ❑ The process starts at the root with all the points as one cluster
  - ❑ It recursively splits the higher level clusters to build the dendrogram
  - ❑ Can be considered as a global approach
  - ❑ More efficient when compared with agglomerative clustering



More on Algorithm Design for Divisive Clustering

- Choosing which cluster to split
  - Check the sums of squared errors of the clusters and choose the one with the largest value
- Splitting criterion: Determining how to split
  - One may use Ward's criterion to chase for greater reduction in the difference in the SSE criterion as a result of a split
  - For categorical data, Gini-index can be used
- Handling the noise
  - Use a threshold to determine the termination criterion (do not generate clusters that are too small because they contain mainly noises)

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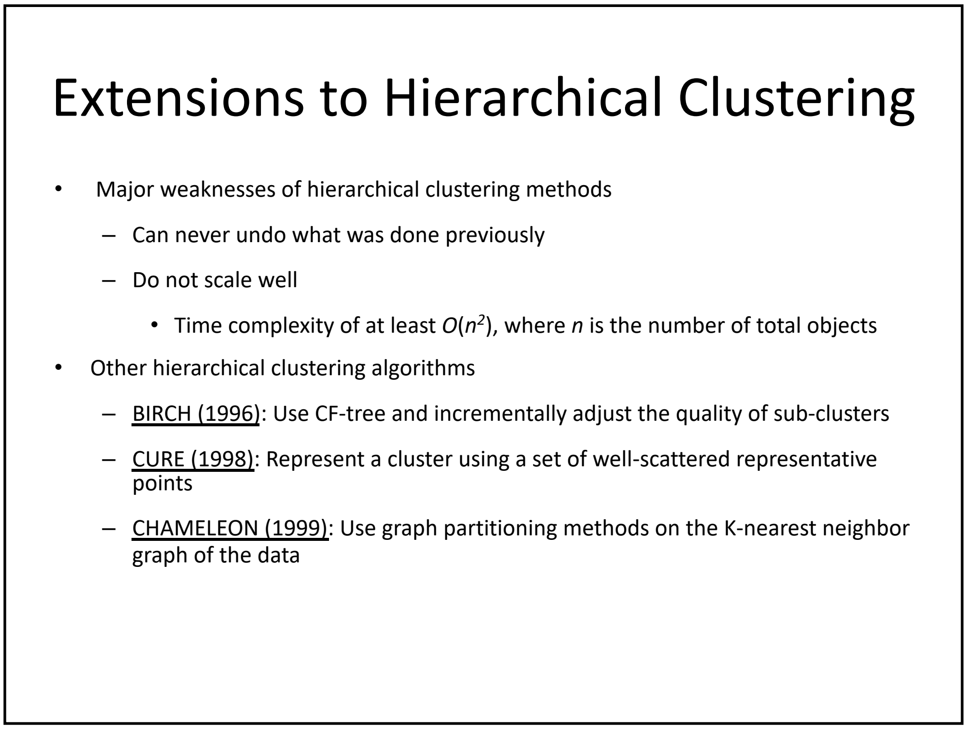

Extensions to Hierarchical Clustering

- Major weaknesses of hierarchical clustering methods
  - Can never undo what was done previously
  - Do not scale well
    - Time complexity of at least $O(n^2)$, where n is the number of total objects
- Other hierarchical clustering algorithms
  - BIRCH (1996): Use CF-tree and incrementally adjust the quality of sub-clusters
  - CURE (1998): Represent a cluster using a set of well-scattered representative points
  - CHAMELEON (1999): Use graph partitioning methods on the K-nearest neighbor graph of the data

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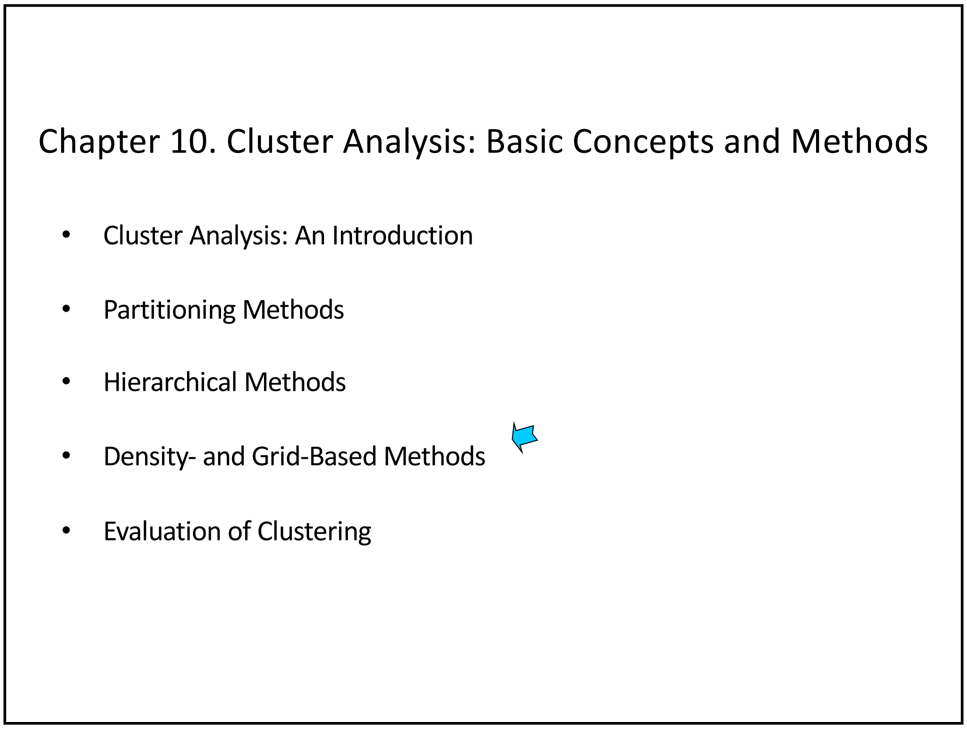

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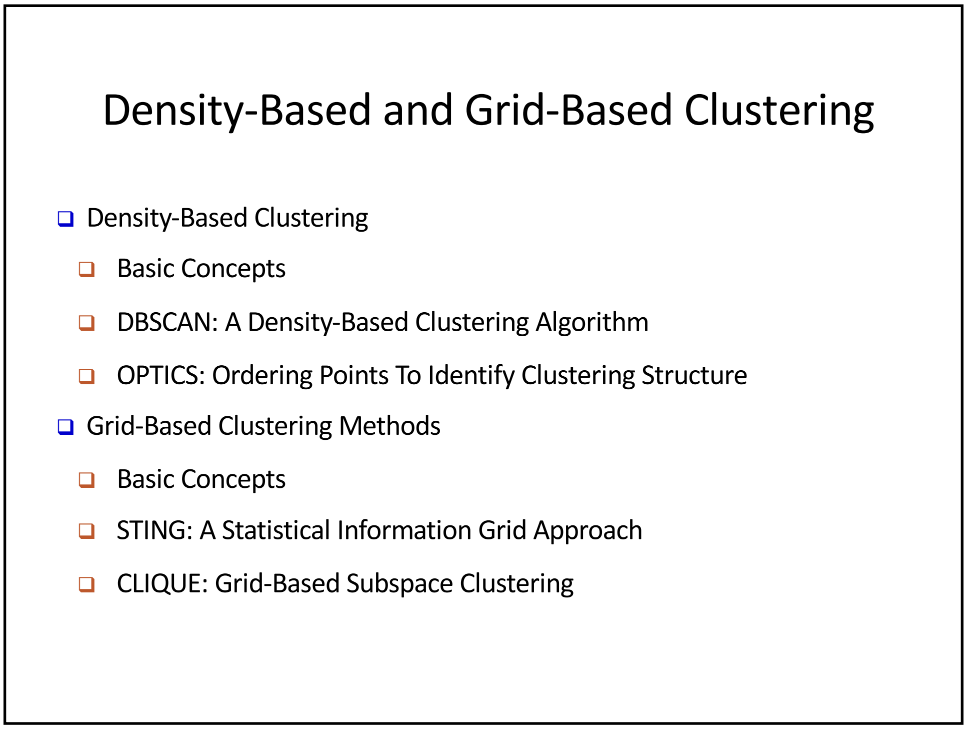

Density-Based and Grid-Based Clustering

- Density-Based Clustering
  - Basic Concepts
  - DBSCAN: A Density-Based Clustering Algorithm
  - OPTICS: Ordering Points To Identify Clustering Structure
- Grid-Based Clustering Methods
  - Basic Concepts
  - STING: A Statistical Information Grid Approach
  - CLIQUE: Grid-Based Subspace Clustering

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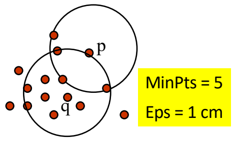
Density-Based Clustering Methods

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

DBSCAN: A Density-Based Spatial Clustering Algorithm

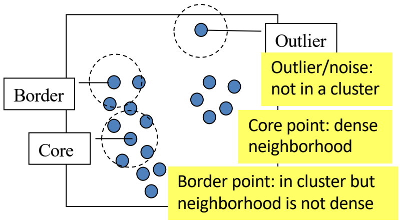
- DBSCAN (M. Ester, H.-P. Kriegel, J. Sander, and X. Xu, KDD'96)
  - Discovers clusters of arbitrary shape: Density-Based Spatial Clustering of Applications with Noise
- A *density-based* notion of cluster
  - A *cluster* is defined as a maximal set of density-connected points
- Two parameters*:*
  - *Eps* (*ε*): Maximum radius of the neighborhood
  - *MinPts*: Minimum number of points in the

  Eps-neighborhood of a point
- The Eps(*ε*)-neighborhood of a point *q*:
  - $N_{Eps}(q)$: {p belongs to D | dist(p, q) ≤ Eps}



MinPts = 5

Eps = 1 cm



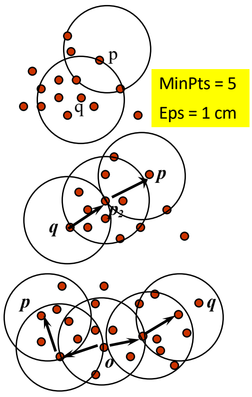
Outlier/noise: not in a cluster

Core point: dense neighborhood

Border point: in cluster but neighborhood is not dense

DBSCAN: Density-Reachable and Density-Connected

- **Directly density-reachable**:
  - A point *p* is directly density-reachable from a point *q* w.r.t. *Eps* (*ε*), *MinPts* if
    - *p* belongs to $N_{Eps}(q)$
    - **core point** condition: $|N_{Eps}(q)| \geq MinPts$
- **Density-reachable**:
  - A point *p* is density-reachable from a point *q* w.r.t. *Eps*, *MinPts* if there is a chain of points $p_1, \ldots, p_n$, $p_1 = q$, $p_n = p$ such that p_{i+1} is directly density-reachable from p_i
- **Density-connected:**
  - A point *p* is density-connected to a point *q* w.r.t. *Eps*, *MinPts* if there is a point *o* such that both *p* and *q* are density-reachable from *o* w.r.t. *Eps* and *MinPts*



MinPts = 5

Eps = 1 cm

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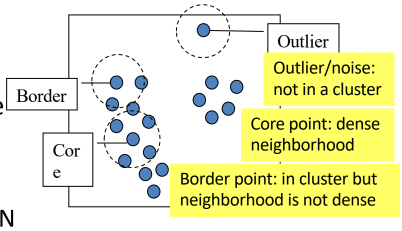
DBSCAN: The Algorithm

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



Outlier/noise: not in a cluster

Core point: dense neighborhood

Border point: in cluster but neighborhood is not dense

- ❑ **Computational complexity**
  - ❑ If a spatial index is used, the computational complexity of DBSCAN is O(nlogn), where n is the number of database objects
  - ❑ Otherwise, the complexity is O(n^2)

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DBSCAN is sensitive to the setting of parameters

Figure 8. DBScan results for DS1 with MinPts at 4 and Eps at (a) 0.5 and (b) 0.4.

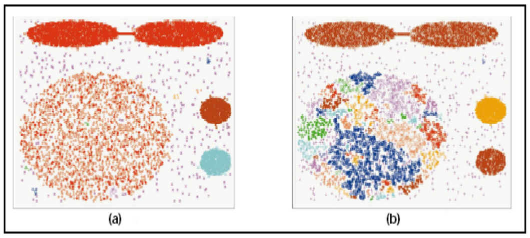
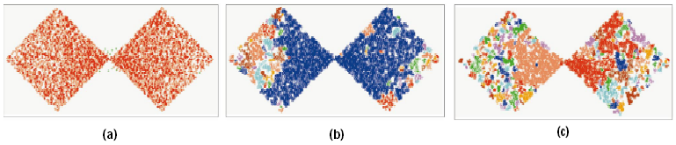


Figure 9. DBScan results for DS2 with MinPts at 4 and Eps at (a) 5.0, (b) 3.5, and (c) 3.0.



Ack. Figures from G. Karypis, E.-H. Han, and V. Kumar, *COMPUTER*, 32(8), 1999

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Grid-Based Clustering Methods

- Grid-Based Clustering: Explore multi-resolution grid data structure in clustering
  - Partition the data space into a finite number of cells to form a grid structure
  - Find clusters (dense regions) from the cells in the grid structure
- Features and challenges of a typical grid-based algorithm
  - Efficiency and scalability: # of cells << # of data points
  - Uniformity: *Uniform, hard to handle highly irregular data distributions*
  - Locality: Limited by *predefined cell sizes, borders, and the density* threshold
  - Curse of dimensionality: *Hard to cluster high-dimensional data*
- Example of grid-based method:
  - **STING** (a STatistical INformation Grid approach) (Wang, Yang and Muntz, VLDB'97)
  - **CLIQUE** (Agrawal, Gehrke, Gunopulos, and Raghavan, SIGMOD'98)
    - Both grid-based and subspace clustering

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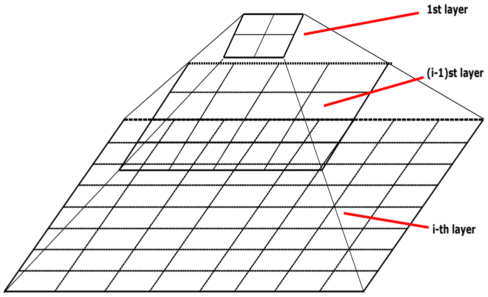
STING: A Statistical Information Grid Approach

- STING (Statistical Information Grid) (Wang, Yang and Muntz, VLDB’97)
- The spatial area is divided into rectangular cells at different levels of resolution, and these cells form a tree structure
- *A cell at a high level contains a number of smaller cells of the next lower level*

- ❑ *Statistical information* of each cell is calculated and stored beforehand and is used to answer queries
- ❑ Parameters of higher level cells can be easily calculated from that of lower level cell, including
  - ❑ *count*, *mean*, *s*(standard deviation), *min*, *max*
  - ❑ type of distribution—*normal*, *uniform*, etc.



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Query Processing in STING and Its Analysis

- To process a *region query*
  - Start at the *root* and proceed to the next lower level, using the STING index
  - Calculate the *likelihood that a cell is relevant to the query* at some confidence level using the statistical information of the cell
  - Only *children of likely relevant cells are recursively explored*
  - Repeat this process until the bottom layer is reached
- Advantages
  - Query-independent, easy to parallelize, incremental update
  - Efficiency: Complexity is O(K)
    - K: # of grid cells at the lowest level, and K << N (i.e., # of data points)
- Disadvantages
  - Its *probabilistic* nature may imply a loss of accuracy in query processing

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Chapter 10. Cluster Analysis: Basic Concepts and Methods

- Cluster Analysis: An Introduction
- Partitioning Methods
- Hierarchical Methods
- Density- and Grid-Based Methods
- Evaluation of Clustering

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Clustering Validation

- Clustering Validation: Basic Concepts
- Clustering Evaluation: Measuring Clustering Quality
- External Measures for Clustering Validation
  - I: Matching-Based Measures
  - II: Entropy-Based Measures
  - III: Pairwise Measures
- Internal Measures for Clustering Validation
- Relative Measures
- Cluster Stability
- Clustering Tendency

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Clustering Validation and Assessment

- Major issues on clustering validation and assessment
  - **Clustering evaluation**
    - Evaluating the goodness of the clustering
  - **Clustering stability**
    - To understand the sensitivity of the clustering result to various algorithm parameters, e.g., # of clusters
  - **Clustering tendency**
    - Assess the suitability of clustering, i.e., whether the data has any inherent grouping structure

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Measuring Clustering Quality

- **Clustering Evaluation**: Evaluating the goodness of clustering results
  - No commonly recognized best suitable measure in practice

- **Three categorization of measures**: External, internal, and relative
  - **External**: Supervised, employ criteria not inherent to the dataset
    - Compare a clustering against *prior or expert-specified knowledge* (i.e., the *ground truth*) using certain clustering quality measure
  - **Internal**: Unsupervised, criteria derived from data itself
    - Evaluate the goodness of a clustering by considering how well the clusters are *separated* and how *compact* the clusters are, e.g., silhouette coefficient
  - **Relative**: Compare different clustering results, usually those obtained via *different parameter settings* for the same algorithm

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Measuring Clustering Quality: External Methods

- Given the **ground truth** *T, Q*(*C, T*) is the **quality measure** for a clustering *C*
- *Q*(*C, T*) is good if it satisfies the following **four** essential criteria
  - **Cluster homogeneity**
    - The purer (data points are members of a single class), the better
  - **Cluster completeness**
    - Assign objects belonging to the same category in the ground truth to the same cluster
  - **Rag bag better than alien**
    - Putting a heterogeneous object into a pure cluster should be penalized more than putting it into a *rag bag* (i.e., "*miscellaneous*" or "*other*" category)
  - **Small cluster preservation**
    - Splitting a small category into pieces is more harmful than splitting a large category into pieces

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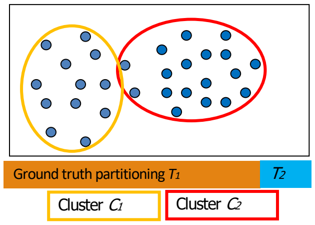
Commonly Used External Measures



- **Matching-based measures**
  - Purity, maximum matching, F-measure
- **Entropy-Based Measures**
  - Conditional entropy
  - Normalized mutual information (NMI)
  - Variation of information
- **Pairwise measures**
  - Four possibilities: True positive (TP), FN, FP, TN
  - Jaccard coefficient, Rand statistic, Fowlkes-Mallow measure
- **Correlation measures**
  - Discretized Huber static, normalized discretized Huber static

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Matching-Based Measures (I): Purity vs. Maximum Matching

n_{ij}: # of points that are common to cluster C_i and ground-truth partition T_j

- **Purity**: Quantifies the extent that cluster C_i contains points only from one (ground truth) partition:
  - Total purity of clustering C:

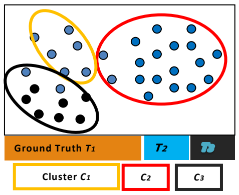
$$purity_i = \frac{1}{n_i} \max_{j=1}^{k} \{n_{ij}\}$$

$$purity = \sum_{i=1}^{r} \frac{n_i}{n} purity_i = \frac{1}{n} \sum_{i=1}^{r} \max_{j=1}^{k} \{n_{ij}\}$$

  - Perfect clustering if purity = 1 and $r = k$ (the number of clusters obtained is the same as that in the ground truth)
  - Ex. 1 (green): $purity_1$ = 30/50; $purity_2$ = 20/25; $purity_3$ = 25/25; *purity* = (30 + 20 + 25)/100 = 0.75
  - Two clusters may share the same majority partition

❑ **Maximum matching**: Only one cluster can match one partition

- ❑ Match: Pairwise matching, weight $w(e_{ij}) = n_{ij}$ $\quad \mathrm{w}(M) = \sum_{e \in M} w(e)$
- ❑ Maximum weight matching: $match = \arg\max_{M} \{\frac{w(M)}{n}\}$
- ❑ Ex2. (green) *match* = *purity* = 0.75



C\T	T_1	T_2	T_3	Sum
C_1	0	20	**30**	**50**
C_2	0	**20**	5	**25**
C_3	**25**	0	0	**25**
m_j	25	40	35	100

C\T	T_1	T_2	T_3	Sum
C_1	0	30	20	50
C_2	0	20	5	25
C_3	25	0	0	25
m_j	25	50	25	100

Matching-Based Measures (II): F-Measure

❑ **Precision**: The fraction of points in C_i from the majority partition T_{j_i} (i.e., the same as purity), where j_i is the partition that contains the maximum # of points from C_i

$$prec_i = \frac{1}{n_i} \max_{j=1}^{k} \{n_{ij}\} = \frac{n_{ij_i}}{n_i}$$

- ❑ Ex. For the green table
  - ❑ $prec_1$ = 30/50; $prec_2$ = 20/25; $prec_3$ = 25/25

❑ **Recall**: The fraction of point in partition T_{j_i} shared in common with cluster C_i, where $m_{j_i} = |T_{j_i}|$

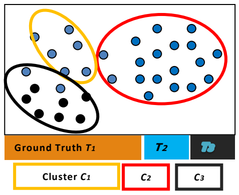
$$recall_i = \frac{n_{ij_i}}{|T_{j_i}|} = \frac{n_{ij_i}}{m_{j_i}}$$

- ❑ Ex. For the green table
  - ❑ $recall_1$ = 30/35; $recall_2$ = 20/40; $recall_3$ = 25/25

❑ **F-measure** for C_i: The harmonic means of $prec_i$ and $recall_i$: $F_i = \frac{2n_{ij_i}}{n_i + m_{j_i}}$

❑ F-measure for clustering C: average of all clusters: $F = \frac{1}{r} \sum_{i=1}^{r} F_i$

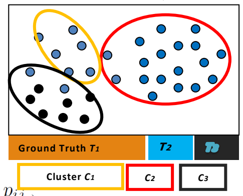
- ❑ Ex. For the green table
  - ❑ F_1 = 60/85; F_2 = 40/65; F_3 = 1; F = 0.774



C\T	T_1	T_2	T_3	Sum
C_1	0	20	**30**	50
C_2	0	**20**	5	25
C_3	**25**	0	0	25
m_j	25	40	35	100

Entropy-Based Measures (I): Conditional Entropy

- **Entropy of clustering** ***C***: $H(\mathcal{C}) = -\sum_{i=1}^{r} p_{C_i} \log p_{C_i}$ $p_{C_i} = \frac{n_i}{n}$ (i.e., the probability of cluster C_i)



- **Entropy of partitioning** ***T***: $H(\mathcal{T}) = -\sum_{j=1}^{k} p_{T_j} \log p_{T_j}$

$$H(\mathcal{T}|C_i) = -\sum_{j=1}^{k} (\frac{n_{ij}}{n_i}) \log(\frac{n_{ij}}{n_i})$$

- **Entropy of** ***T*** **with respect to cluster** ***C**$_i$*:

$$H(\mathcal{T}|\mathcal{C}) = -\sum_{i=1}^{r} (\frac{n_i}{n}) H(\mathcal{T}|C_i) = -\sum_{i=1}^{r}\sum_{j=1}^{k} p_{ij} \log(\frac{p_{ij}}{p_{C_i}})$$

- **Conditional entropy of** ***T*** **with respect to clustering** ***C***: $H(\mathcal{T}|\mathcal{C}) = -\sum_{i=1}^{r}\sum_{j=1}^{k} p_{ij}(\log p_{ij} - \log p_{C_i}) = -\sum_{i=1}^{r}\sum_{j=1}^{k} p_{ij} \log p_{ij} + \sum_{i=1}^{r} (\log p_{C_i} \sum_{j=1}^{k} p_{ij})$
  - The more a cluster's members are split into different partitions, the higher the conditional entropy
  - For a *perfect clustering*, the *conditional entropy value is 0*, where the worst possible conditional entropy value is *log k*

$$= -\sum_{i=1}^{r}\sum_{j=1}^{k} p_{ij} \log p_{ij} + \sum_{i=1}^{r} (p_{C_i} \log p_{C_i}) = H(\mathcal{C}, \mathcal{T}) - H(\mathcal{C})$$

Entropy-Based Measures (II): Normalized Mutual Information (NMI)

- **Mutual information**: $I(C,T) = \sum_{i=1}^{r}\sum_{j=1}^{k} p_{ij} \log(\frac{p_{ij}}{p_{C_i} \cdot p_{T_j}})$
  - Quantifies the **amount of shared info** between the clustering *C* and partitioning *T*
  - Measures the dependency between the observed joint probability p_{ij} of *C* and *T*, and the expected joint probability p_{Ci} . p_{Tj} under the independence assumption
  - *When C and T are independent*, $p_{ij} = p_{Ci}$. p_{Tj}, *I*(*C*, *T*) = 0. However, there is no upper bound on the mutual information
- **Normalized mutual information** (NMI)

$$NMI(\mathcal{C}, \mathcal{T}) = \sqrt{\frac{I(\mathcal{C}, \mathcal{T})}{H(\mathcal{C})} \cdot \frac{I(\mathcal{C}, \mathcal{T})}{H(\mathcal{T})}} = \frac{I(\mathcal{C}, \mathcal{T})}{\sqrt{H(\mathcal{C}) \cdot H(\mathcal{T})}}$$

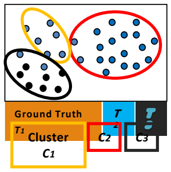
  - Value range of NMI: [0,1]. **Value close to 1 indicates a good clustering**

Pairwise Measures: Four Possibilities for Truth Assignment

- **Four possibilities** based on the agreement between cluster label and partition label
  - *TP*: true positive—Two points ***x****ᵢ* and ***x****ⱼ* belong to the same partition *T* , and they also in the same cluster *C*

$$TP = \ |\{(\mathbf{x}_i, \mathbf{x}_j) : y_i = y_j \text{ and } \hat{y}_i = \hat{y}_j\}|$$

where y_i: the true partition label , and $\hat{y}_i$: the cluster label for point $\boldsymbol{x}_i$



  - *FN*: false negative: $FN = \ |\{(\mathbf{x}_i, \mathbf{x}_j) : y_i = y_j \text{ and } \hat{y}_i \neq \hat{y}_j\}|$
  - *FP: false positive* $FP = \ |\{(\mathbf{x}_i, \mathbf{x}_j) : y_i \neq y_j \text{ and } \hat{y}_i = \hat{y}_j\}|$
  - *TN*: true negative $TN = \ |\{(\mathbf{x}_i, \mathbf{x}_j) : y_i \neq y_j \text{ and } \hat{y}_i \neq \hat{y}_j\}|$
- Calculate the four measures: $N = \binom{n}{2}$

Total # of pairs of points

$$TP = \sum_{i=1}^{r}\sum_{j=1}^{k}\binom{n_{ij}}{2} = \frac{1}{2}((\sum_{i=1}^{r}\sum_{j=1}^{k} n_{ij}^{2}) - n) \quad FN = \sum_{j=1}^{k}\binom{m_j}{2} - TP$$

$$FP = \sum_{i=1}^{r}\binom{n_i}{2} - TP \quad TN = N - (TP + FN + FP) = \frac{1}{2}(n^2 - \sum_{i=1}^{r} n_i^2 - \sum_{j=1}^{k} m_j^2 + \sum_{i=1}^{r}\sum_{j=1}^{k} n_{ij}^2)$$

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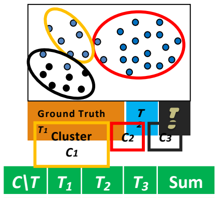
Pairwise Measures: Jaccard Coefficient and Rand Statistic

- **Jaccard coefficient:** Fraction of true positive point pairs, but after ignoring the true negatives (thus asymmetric)
  - *Jaccard* = *TP*/(*TP* + *FN* + *FP*) [i.e., denominator ignores *TN*]
  - *Perfect clustering*: *Jaccard* = 1
- **Rand Statistic**:
  - *Rand* = (*TP* + *TN*)/*N*
  - Symmetric; perfect clustering: *Rand* = 1
- **Fowlkes-Mallow Measure**:
  - Geometric mean of precision and recall

$$FM = \sqrt{prec \times recall} = \frac{TP}{\sqrt{(TP + FN)(TP + FP)}}$$

- Using the above formulas, one can calculate all the measures for the green table



$C\backslash T$	T_1	T_2	T_3	Sum
C_1	0	20	30	50
C_2	0	20	5	25
C_3	25	0	0	25
m_j	25	40	35	100

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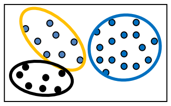
Internal Measures (I): BetaCV Measure

- A trade-off in maximizing *intra-cluster compactness* and *inter-cluster separation*
- Given a clustering *C* = {*C*$_1$, . . ., *C*$_k$} with *k* clusters, cluster *C*$_i$ containing *n*$_i$ = |*C*$_i$| points
  - Let *W*(*S*, *R*) be sum of weights on all edges with one vertex in *S* and the other in *R*
  - The sum of all the intra-cluster weights over all clusters: $W_{in} = \frac{1}{2}\sum_{i=1}^{k} W(C_i, C_i)$
  - The sum of all the inter-cluster weights: $W_{out} = \frac{1}{2}\sum_{i=1}^{k} W(C_i, \overline{C_i}) = \sum_{i=1}^{k-1}\sum_{j>i} W(C_i, C_j)$
  - The number of distinct intra-cluster edges: $N_{in} = \sum_{i=1}^{k}\binom{n_i}{2}$
  - The number of distinct inter-cluster edges: $N_{out} = \sum_{i=1}^{k-1}\sum_{j=i+1}^{k} n_i n_j$



- **Beta-CV measure**: $BetaCV = \frac{W_{in} / N_{in}}{W_{out} / N_{out}}$
  - The **ratio of the mean intra-cluster distance to the mean inter-cluster distance**
  - The **smaller**, the **better** the clustering

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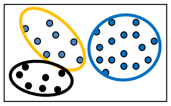
Internal Measures (II): Normalized Cut and Modularity

- **Normalized cut:** $NC = \sum_{i=1}^{k}\frac{W(C_i, \overline{C_i})}{vol(C_i)} = \sum_{i=1}^{k}\frac{W(C_i, \overline{C_i})}{W(C_i, \mathrm{V})} = \sum_{i=1}^{k}\frac{W(C_i, \overline{C_i})}{W(C_i, C_i) + W(C_i, \overline{C_i})} = \sum_{i=1}^{k}\frac{1}{\frac{W(C_i, C_i)}{W(C_i, \overline{C_i})} + 1}$

  where *vol*(*C*$_i$) = *W*(*C*$_i$, *V*) is the volume of cluster *C*$_i$
  - The **higher** normalized cut value, the **better** the clustering



- **Modularity** (for graph clustering)
  - Modularity *Q* is defined as $Q = \sum_{i=1}^{k}\left(\frac{W(C_i, C_i)}{W(V, V)} - \left(\frac{W(C_i, V)}{W(V, V)}\right)^2\right)$

  where
  - Modularity measures the **difference between the observed and expected fraction** of weights on edges within the clusters.
  - The **smaller** the value, the **better** the clustering—the intra-cluster distances are lower than expected

$$W(V, V) = \sum_{i=1}^{k} W(C_i, V) = \sum_{i=1}^{k} W(C_i, C_i) + \sum_{i=1}^{k} W(C_i, \overline{C_i}) = 2(W_{in} + W_{out})$$

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Relative Measure

- Relative measure: Directly compare different clusterings, usually those obtained via different parameter settings for the same algorithm

- **Silhouette coefficient** as an **internal measure**: *Check cluster cohesion and separation*
  - For each point ***x***$_i$, its silhouette coefficient s_i is: $s_i = \frac{\mu_{out}^{\min}(\mathbf{x}_i) - \mu_{in}(\mathbf{x}_i)}{\max\{\mu_{out}^{\min}(\mathbf{x}_i), \mu_{in}(\mathbf{x}_i)\}}$

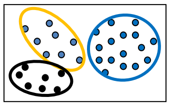
    where $\mu_{in}(\mathbf{x}_i)$ is the mean distance from $\mathbf{x}_i$ to points in its own cluster

    $\mu_{out}^{\min}(\mathbf{x}_i)$ is the mean distance from $\mathbf{x}_i$ to points in its closest cluster
  - Silhouette coefficient (*SC*) is the mean values of s_i across all the points: $SC = \frac{1}{n}\sum_{i=1}^{n} s_i$
  - *SC* close to +1 implies good clustering
    - Points are close to their own clusters but far from other clusters

- **Silhouette coefficient** as a **relative measure**: Estimate the # of clusters in the data $SC_i = \frac{1}{n_i}\sum_{x_j \in C_i} s_j$

  Pick the *k* value that yields the best clustering, i.e., yielding high values for *SC* and SC_i ($1 \le i \le k$)

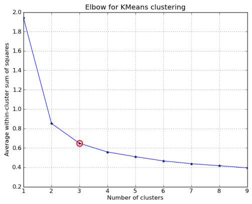
Cluster Stability



- Clusterings obtained from several datasets sampled from the same underlying distribution as ***D*** should be similar or “stable”
- Typical approach:
  - Find good parameter values for a given clustering algorithm
- Example: Find a good value of *k*, the correct number of clusters
- A **bootstrapping approach** to find the best value of *k* (judged on stability)
  - Generate *t* samples of size *n* by sampling from ***D*** with replacement
  - For each sample $\boldsymbol{D}_i$, run the same clustering algorithm with *k* values from 2 to k_{max}
  - Compare the distance between all pairs of clusterings $C_k(\boldsymbol{D}_i)$ and $C_k(\boldsymbol{D}_j)$ via some distance function
    - Compute the expected pairwise distance for each value of *k*
  - The value *k** that exhibits the least deviation between the clusterings obtained from the resampled datasets is the best choice for *k* since it exhibits the most stability

Other Methods for Finding K, the Number of Clusters

- **Empirical method**
  - # of clusters: $k \approx \sqrt{n/2}$ for a dataset of n points (e.g., *n* = 200, *k* = 10)
- **Elbow method**: Use the turning point in the curve of the sum of within cluster variance with respect to the # of clusters



- **Cross validation method**
  - Divide a given data set into *m* parts
  - Use *m* – 1 parts to obtain a clustering model
  - Use the remaining part to test the quality of the clustering
    - For example, for each point in the test set, find the closest centroid, and use the sum of squared distance between all points in the test set and the closest centroids to measure how well the model fits the test set
  - For any *k* > 0, repeat it *m* times, compare the overall quality measure w.r.t. different *k's*, and find # of clusters that fits the data the best

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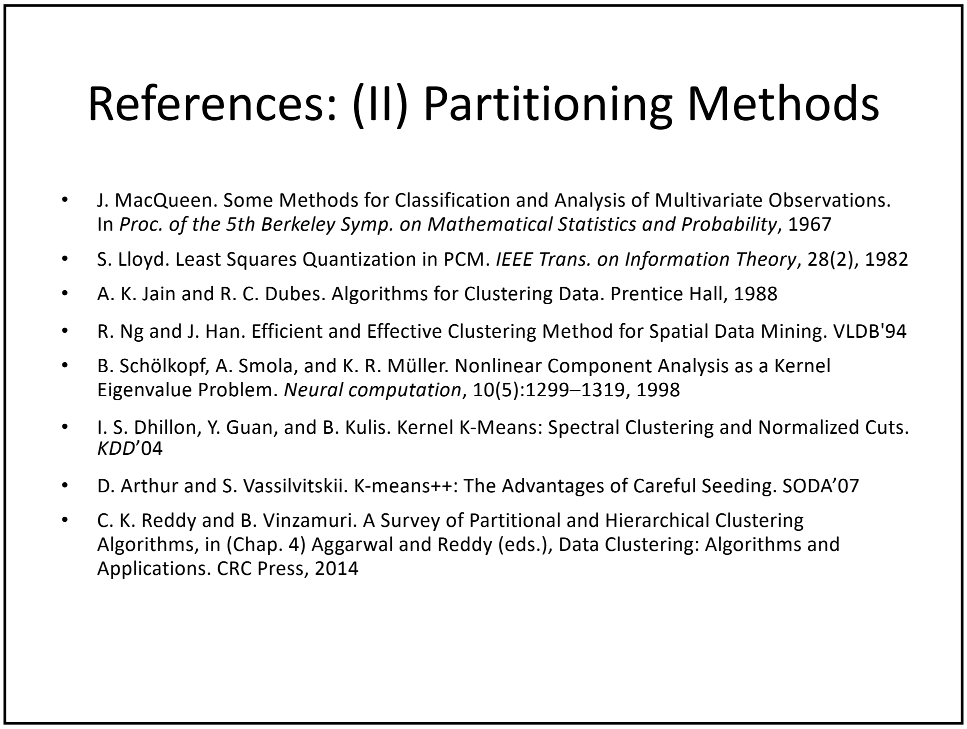

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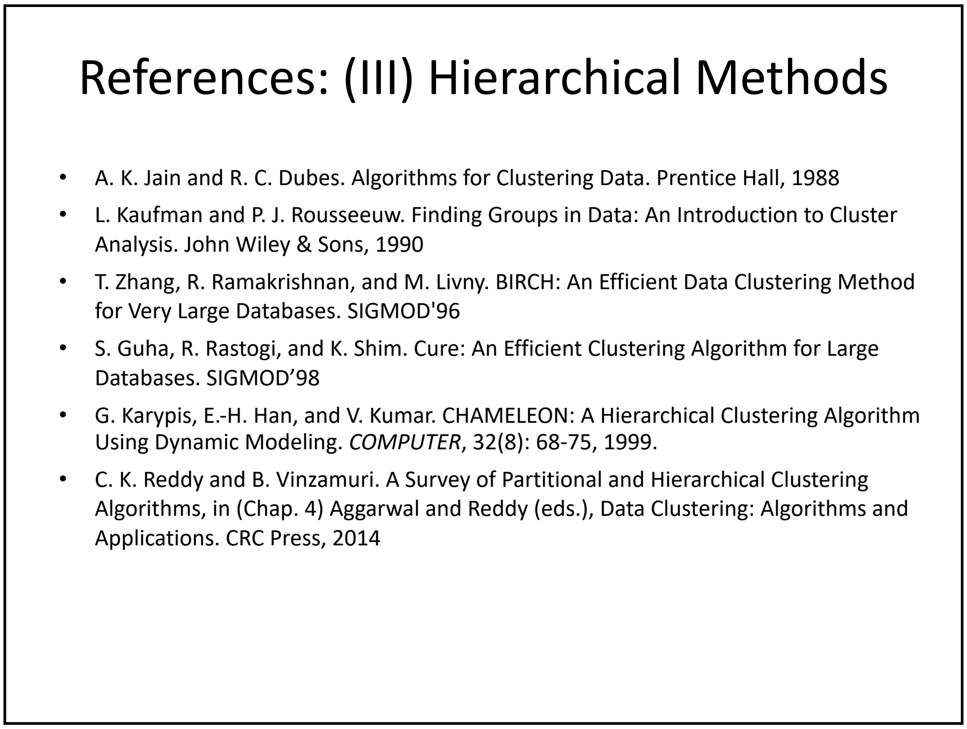

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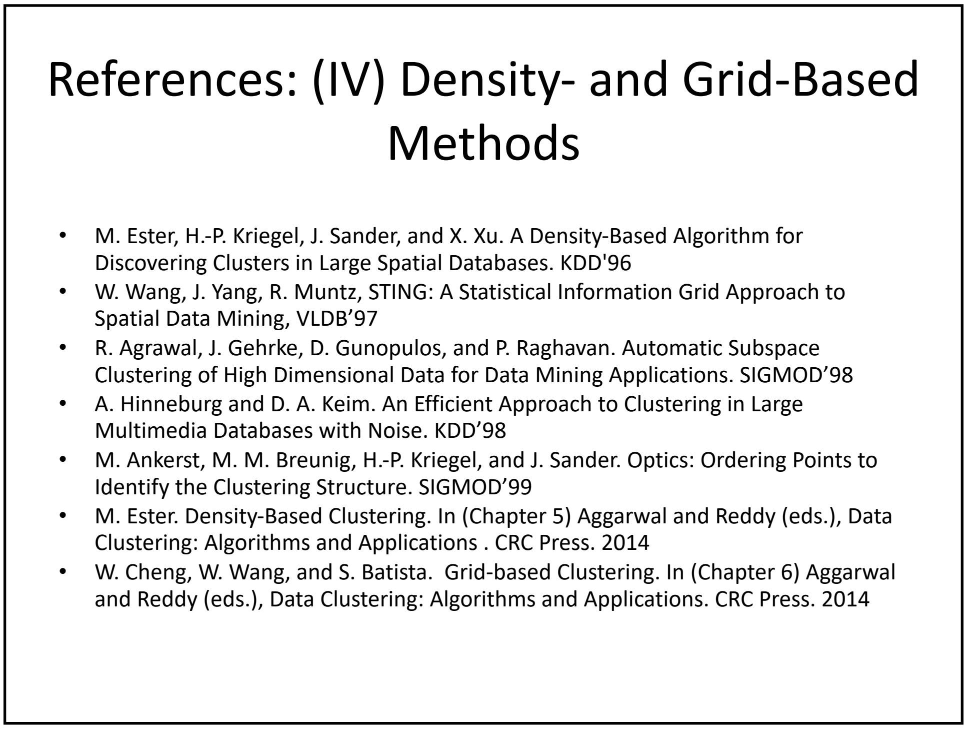

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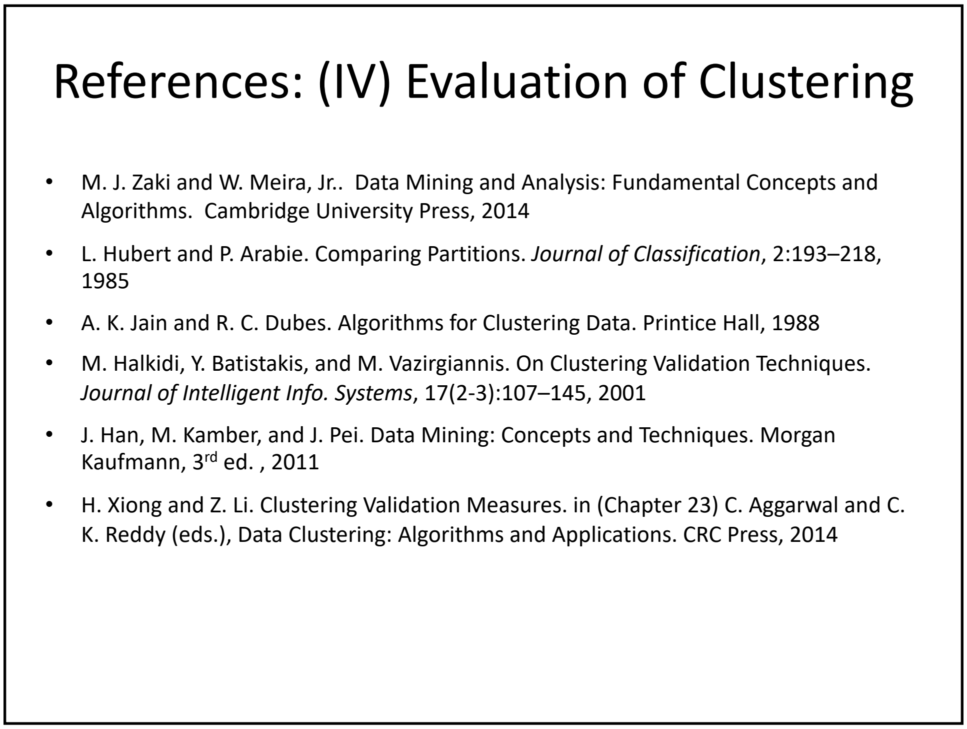

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