Chapter 10. Cluster Analysis: Basic Concepts and Methods

- Cluster Analysis: Basic Concepts
- Partitioning Methods
- Hierarchical Methods
- Density-Based Methods
- Grid-Based Methods
- Evaluation of Clustering
- Summary

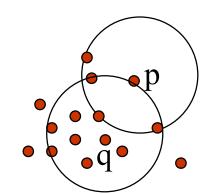
Density-Based Clustering Methods

- Clustering based on density (local cluster criterion), such as density-connected points
- Major features:
 - Discover clusters of arbitrary shape
 - Handle noise
 - One scan
 - 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) (more grid-based)

Density-Based Clustering: Basic Concepts

- Two parameters:
 - Eps: Maximum radius of the neighbourhood
 - MinPts: Minimum number of points in an Epsneighbourhood of that point
- $N_{Eps}(p)$: {q belongs to D | dist(p,q) ≤ Eps}
- Directly density-reachable: A point p is directly density-reachable from a point q w.r.t. Eps, MinPts if
 - p belongs to $N_{Eps}(q)$
 - core point condition:

$$|N_{Eps}(q)| \ge MinPts$$



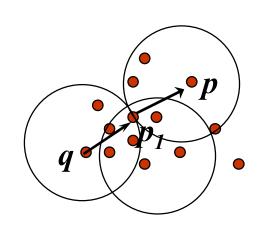
MinPts = 5

$$Eps = 1 cm$$

Density-Reachable and Density-Connected

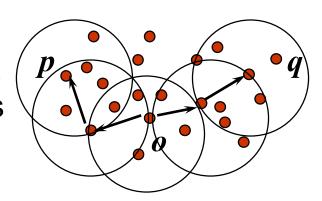
Density-reachable:

■ A point p is density-reachable from a point q w.r.t. Eps, MinPts if there is a chain of points $p_1, ..., p_n, p_1 =$ $q, p_n = p$ such that p_{i+1} is directly density-reachable from p_i



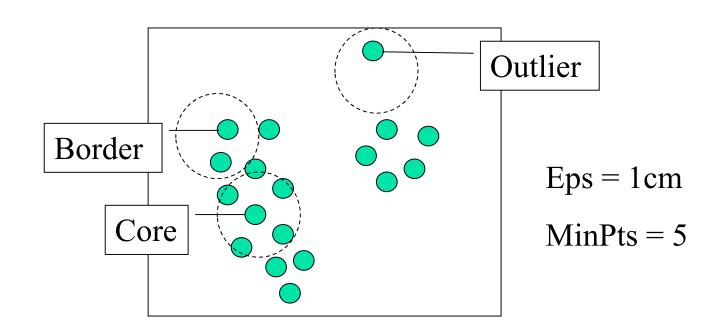
Density-connected

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



DBSCAN: Density-Based Spatial Clustering of Applications with Noise

- Relies on a density-based notion of cluster: A cluster is defined as a maximal set of density-connected points
- Discovers clusters of arbitrary shape in spatial databases with noise



DBSCAN: The Algorithm

- Arbitrary 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

DBSCAN: Sensitive to Parameters

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

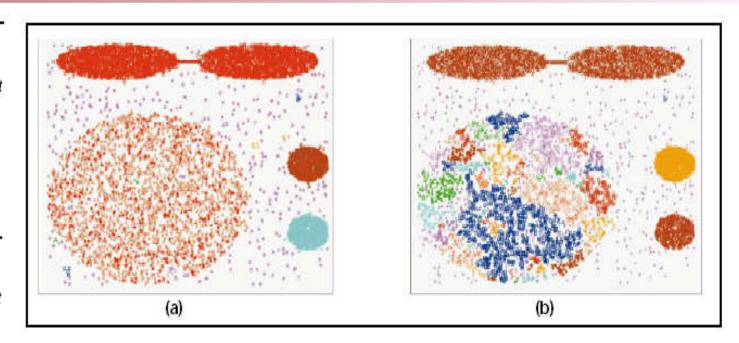
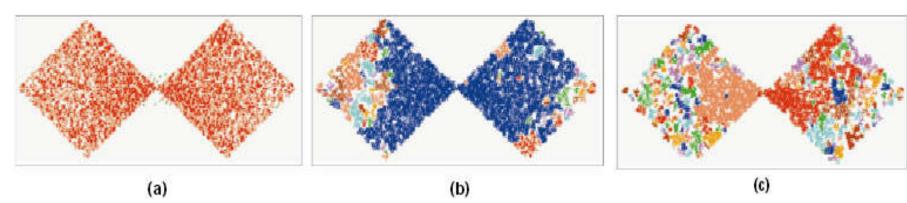


Figure 9. DBScan results for DS2 with MinPts at 4 and Eps at (a) 5.0, (b) 3.5, and (c) 3.0.



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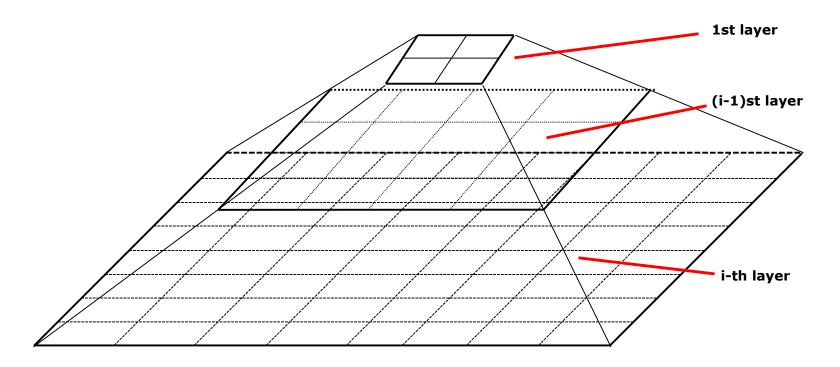
- **Evaluation of Clustering**
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Grid-Based Clustering Method

- Using multi-resolution grid data structure
- Several interesting methods
 - STING (a STatistical INformation Grid approach) by Wang, Yang and Muntz (1997)
 - WaveCluster by Sheikholeslami, Chatterjee, and Zhang (VLDB'98)
 - A multi-resolution clustering approach using wavelet method
 - CLIQUE: Agrawal, et al. (SIGMOD'98)
 - Both grid-based and subspace clustering

STING: A Statistical Information Grid Approach

- Wang, Yang and Muntz (VLDB'97)
- The spatial area is divided into rectangular cells
- There are several levels of cells corresponding to different levels of resolution



The STING Clustering Method

- Each cell at a high level is partitioned into a number of smaller cells in the next lower level
- Statistical info of each cell is calculated and stored beforehand and is used to answer queries
- Parameters of higher level cells can be easily calculated from parameters of lower level cell
 - count, mean, s, min, max
 - type of distribution—normal, uniform, etc.
- Use a top-down approach to answer spatial data queries
- Start from a pre-selected layer—typically with a small number of cells
- For each cell in the current level compute the confidence interval

STING Algorithm and Its Analysis

- Remove the irrelevant cells from further consideration
- When finish examining the current layer, proceed to the next lower level
- Repeat this process until the bottom layer is reached
- Advantages:
 - Query-independent, easy to parallelize, incremental update
 - O(K), where K is the number of grid cells at the lowest level
- Disadvantages:
 - All the cluster boundaries are either horizontal or vertical, and no diagonal boundary is detected

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Assessing Clustering Tendency

- Assess if non-random structure exists in the data by measuring the probability that the data is generated by a uniform data distribution
- Test spatial randomness by statistic test: Hopkins Static
 - Given a dataset D regarded as a sample of a random variable o, determine how far away o is from being uniformly distributed in the data space
 - Sample n points, $p_1, ..., p_n$, uniformly from D. For each p_i , find its nearest neighbor in D: $x_i = min\{dist\ (p_i, v)\}$ where v in D
 - Sample n points, q₁, ..., qn, uniformly from D. For each qi, find its nearest neighbor in D {qi}: yi = min{dist (qi, v)} where v in D and v ≠ qi
 - Calculate the Hopkins Statistic: $H = \frac{\sum_{i=1}^{n} y_i}{\sum_{i=1}^{n} x_i + \sum_{i=1}^{n} y_i}$
 - If D is uniformly distributed, $\sum x_i$ and $\sum y_i$ will be close to each other and H is close to 0.5. If D is highly skewed, H is close to 0

Determine the Number of Clusters

- Empirical method
 - # of clusters ≈√n/2 for a dataset of n points
- Elbow method
 - Use the turning point in the curve of sum of within cluster variance w.r.t 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
 - E.g., 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

Measuring Clustering Quality

- Two methods: extrinsic vs. intrinsic
- Extrinsic: supervised, i.e., the ground truth is available
 - Compare a clustering against the ground truth using certain clustering quality measure
 - Ex. BCubed precision and recall metrics
- Intrinsic: unsupervised, i.e., the ground truth is unavailable
 - Evaluate the goodness of a clustering by considering how well the clusters are separated, and how compact the clusters are
 - Ex. Silhouette coefficient

Measuring Clustering Quality: Extrinsic Methods

- Clustering quality measure: Q(C, C_g), for a clustering C given the ground truth C_g.
- Q is good if it satisfies the following 4 essential criteria
 - Cluster homogeneity: the purer, the better
 - Cluster completeness: should assign objects belong to the same category in the ground truth to the same cluster
 - Rag bag: 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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Summary

- Cluster analysis groups objects based on their similarity and has wide applications
- Measure of similarity can be computed for various types of data
- Clustering algorithms can be categorized into partitioning methods, hierarchical methods, density-based methods, grid-based methods, and model-based methods
- K-means and K-medoids algorithms are popular partitioning-based clustering algorithms
- Birch and Chameleon are interesting hierarchical clustering algorithms, and there are also probabilistic hierarchical clustering algorithms
- DBSCAN, OPTICS, and DENCLU are interesting density-based algorithms
- STING and CLIQUE are grid-based methods, where CLIQUE is also a subspace clustering algorithm
- Quality of clustering results can be evaluated in various ways

C\$512-\$pring 2011: An Introduction

Coverage

- Cluster Analysis: Chapter 11
- Outlier Detection: Chapter 12
- Mining Sequence Data: BK2: Chapter 8
- Mining Graphs Data: BK2: Chapter 9
- Social and Information Network Analysis
 - BK2: Chapter 9
 - Partial coverage: Mark Newman: "Networks: An Introduction", Oxford U., 2010
 - Scattered coverage: Easley and Kleinberg, "Networks, Crowds, and Markets: Reasoning About a Highly Connected World", Cambridge U., 2010
 - Recent research papers
- Mining Data Streams: BK2: Chapter 8
- Requirements
 - One research project
 - One class presentation (15 minutes)
 - Two homeworks (no programming assignment)
 - Two midterm exams (no final exam)

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