COMP3420: Advanced Databases and Data Mining

Introduction to cluster analysis

Lecture outline

- What is cluster analysis?
- Applications and examples
- What is good clustering?
- Clustering requirements in data mining
- Measurements of cluster quality
- Similarities between data objects
- Main clustering approaches
- Partitioning algorithms
- *K-means* clustering approach

What is cluster analysis?

- A cluster is a collection of data objects
  - Similar to one another in the same cluster
  - Disimilar to the objects in other cluster
- Cluster analysis (or *clustering*) is finding similarities between data objects according to the characteristics in the data and grouping similar data objects into clusters
- Cluster analysis is unsupervised, *descriptive* data mining
  - No predefined classes
- Typical applications
  - As a stand-alone tool to get insight into data distribution
  - As a pre-processing step (data cleaning and data reduction) for other data mining algorithms

Applications of cluster analysis

- Pattern recognition
  - Image processing
- Spatial data analysis
  - Create thematic maps in geographical information systems (GIS) by clustering feature spaces
  - Detect spatial clusters for use in other spatial data mining tasks
- Economic science (especially market research)
  - Groupings of similar customers
- Internet / WWW
  - Document / Web page categorisation
  - Cluster Web log data to discover groups of similar access patterns

Examples of cluster analysis

- *Marketing:* Help marketers to discover distinct groups in their customer bases, and then use this knowledge to develop targeted marketing programs
- *Land use:* Identification of areas of similar land use in an earth observation database (satellite images, etc.)
- *Insurance:* Identify groups of (for example, motor insurance) policy holders with a high average claim cost
- *City planning:* Identifying groups of houses according to their house type, value, and geographical location

What is good clustering?

- A good clustering will produce clusters with
  - High intra-class similarity
  - Low inter-class similarity
- The quality of a clustering result depends upon both the similarity measure and the algorithm used for searching
  - Different algorithms deliver different clusterings
- The quality of a clustering is also measured by its ability to discover some or all of the hidden patterns in the data
- Clustering may not be the best way to discover interesting groups in data sets
  - Visualisation often works well, allowing human experts to identify useful groups
  - This becomes problematic with very large data sets

Clustering requirements in data mining

- Scalability to very large databases
- Ability to deal with different attribute types
- Ability to handle dynamic data
- Discovery of clusters of arbitrary shapes
- Minimal domain knowledge required to determine input parameters
- Able to deal with noise and outliers
- Insensitive to order of input records
- Handle high dimensionality
- Incorporation of user-specified constraints
- Interpretability and usability

Measurements of cluster quality

- Dissimilarity/similarity metric: Similarity is expressed in terms of a distance function, typically a metric: $d(a, b)$**,** with $s(a, b) = 1 - d(a, b)$ (if dist normalised), or $s(a, b) = 1/d(a, b)$
- There is a separate "quality" function that measures the "goodness" of a cluster
- The definitions of distance functions are usually different for interval-scaled, boolean, categorical, ordinal, ratio-scaled, and vector variables
- Weights can be associated with different variables (attributes) based on applications and data semantics
- It is hard to define "similar enough" or "good enough"
  - The answer is typically highly subjective

Similarity and dissimilarity between objects

- Distances are normally used to measure similarity and dissimilarity between two data objects
  - Two objects: $a = (a_1, a_2, \ldots a_n)$ and $b = (b_1, b_2, \ldots b_n)$
- Properties of a *distance measure d(i, j)*:
  - $d(a, a) = 0$
  - $d(a, b) >= 0$
  - $d(a, b) = d(b, a)$
  - $d(a, c) <= d(a, b) + d(b, c)$ Triangular inequality
- The larger the distance, the smaller the similarity

Minkowski distance

- Popular distance measure includes *Minkowski* distance:

$$d(a,b)=\sqrt[q]{(|a_1-b_1|^q+|a_2-b_2|^q+\ldots+|a_n-b_n|^q)}$$

where $a = (a_1, a_2, \ldots, a_n)$ and $b = (b_1, b_2, \ldots, b_n)$ are two n-dimensional data objects, and q is a positive integer

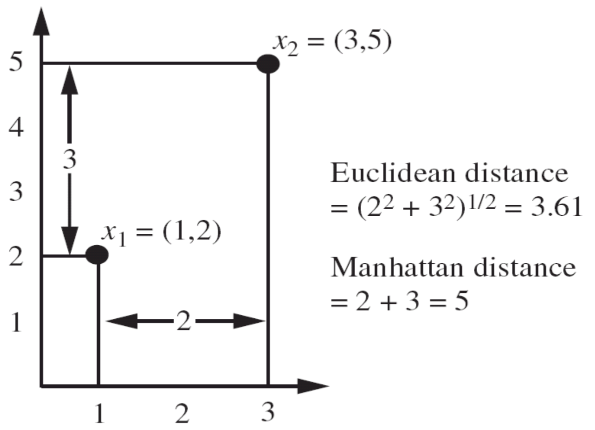
- If $q = 1$, d is the *Manhattan* distance:

$$d(a,b)=|a_1-b_1|+|a_2-b_2|+\ldots+|a_n-b_n|$$

- If $q = 2$, d is the *Euclidean* distance:

$$d(a,b)=\sqrt{(|a_1-b_1|^2+|a_2-b_2|^2+\ldots+|a_n-b_n|^2)}$$

Euclidean and *Manhattan* distance example



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Similarities for other data types

- Many different ways to measure similarities between objects
  - Binary data: contingency tables
  - Nominal variables (e.g. colors): Count number of matches (of values in different attributes) divided by total number of possible matches (i.e. attributes considered)
  - Strings: Exact or approximate string similarities (edit-distance, q-gram based, longest common sub-string, etc.)
  - Vector objects (document words, micro array gene features): cosine measure based on term-frequency/inverse document frequency (TF-IDF) *(more in the lecture on text mining later in the course)*
- A database might contain different types of attributes
- One might use a weighted sum to calculate final similarity between objects
  - For example, $d(a, b) = 0.3\, d_{name}(name_a, name_b) + 0.7\, d_{salary}(salary_a, salary_b)$

Calculate the distance between clusters

- *Single link:* Smallest distance between a data object in one cluster and a data object in the other: $d(K_i, K_j) = \min(t_{ip}, t_{jq})$
- *Complete link:* Largest distance between a data object in one cluster and a data object in the other: $d(K_i, K_j) = \max(t_{ip}, t_{jq})$
- *Average:* Average distance between a data object in one cluster and a data object in the other: $d(K_i, K_j) = \text{avg}(t_{ip}, t_{jq})$
  (same as Centroid - Distance between the centroids of two clusters)
- *Medoid:* Distance between the medoids of two clusters: $d(K_i, K_j) = d(M_i, M_j)$
  - A *medoid* is a data object centrally located in the cluster

Centroid, radius, and diameter of a cluster

- For numerical data objects t_{ip} in cluster i
- Centroid C_i: the "middle" of a cluster

$$C_i = \frac{\sum_{p=1}^{N} (t_{ip})}{N}$$

- Radius: square root of average distance from any data object of the cluster to its centroid

$$R_i = \sqrt{\frac{\sum_{p=1}^{N} (t_{ip} - c_i)^2}{N}}$$

- Diameter: square root of average mean squared distance between all pairs of data objects in the cluster

$$D_i = \sqrt{\frac{\sum_{p=1}^{N} \sum_{q=1}^{N} (t_{ip} - t_{iq})^2}{N(N-1)}}$$

Major clustering approaches (1)

- Partitioning approaches
  - Construct various partitions and then evaluate them by some criterion, for example, minimising cluster radius or diameter, or the sum of square errors
  - A fixed number, *k*, of clusters is generated
  - Typical methods: *k-means, k-medoids, CLARANS*
- Hierarchical approaches
  - Create a hierarchical decomposition of the data objects using some criterion
  - Typical methods: *Diana, Agnes, BIRCH, ROCK, CAMELEON*
- Density based approaches
  - Based on connectivity and density functions
  - Typical methods: *DBSCAN, OPTICS, DenClue*

Major clustering approaches (2)

- Grid-based approaches
  - Based on a multi-level granularity structure
  - Typical methods: *STING, WaveCluster, CLIQUE*
- Model-based approaches
  - A model is hypothesised for each of the clusters and the idea is to find the best fit of that model
  - Typical methods: *EM (Expectation-Maximisation), SOM (Self-organising maps), COBWEB*
- Frequent-pattern based approaches
  - Based on analysis of frequent patterns
  - Typical method: *pCluster*
- User-guided or constrain-based approaches
  - Clustering by considering user- or application-specific constraints
  - Typical method: *COD (obstacles), constrained clustering*

Partitioning algorithms: Basic concept

- Construct a partition of a database *D* of *n* objects into a set of *k* clusters, such that minimum sum of squared distance

$$\sum_{i=1}^{k}\sum_{t_{ip}\in Ki}(C_i - t_{ip})^2$$

- Given a *k*, find a partition of *k clusters* that optimises the chosen partitioning criterion
  - Global optimal: exhaustively enumerate all partitions
  - Heuristic methods: *k-means* and *k-medoids* algorithms
  - *k-means (MacQueen'67):* Each cluster is represented by the center of the cluster
  - *k-medoids or PAM (Partition Around Medoids) (Kaufman & Rousseeuw'87):* Each cluster is represented by one of the objects in the cluster

The *k-means* clustering algorithm

Algorithm: ***k*-means.** The *k*-means algorithm for partitioning, where each cluster's center is represented by the mean value of the objects in the cluster.

Input:

- *k*: the number of clusters,
- *D*: a data set containing *n* objects.

Output: A set of *k* clusters.

Method:

(1) arbitrarily choose *k* objects from *D* as the initial cluster centers;
(2) repeat
(3) (re)assign each object to the cluster to which the object is the most similar based on the mean value of the objects in the cluster;
(4) update the cluster means, i.e., calculate the mean value of the objects for each cluster;
(5) until no change;

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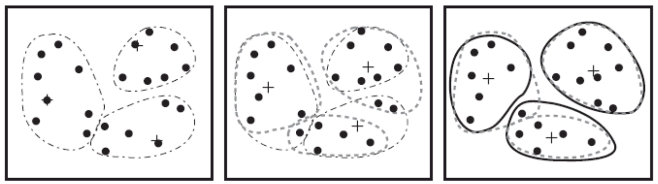
The *k-means* clustering algorithm



(a) (b) (c)

+ = centroids

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Comments on the *k-means* algorithm

- *Strength:* Relatively efficient: O(t * k * n), where *n* is the number of data objects, *k* is the number of clusters, and *t* is the number of iterations. Normally, *k* and *t* << *n*
  - In comparison: PAM: $O(k(n-k)^2)$, CLARA: $O(ks^2 + k(n-k))$ (s = sample size)
- *Comment:* Often terminates at a local optimum!
  - *K-means* will always generate *k* clusters!
  - The global optimum may be found using techniques such as deterministic annealing and genetic algorithms
  - Basic idea: running *k-means* many times with different starting configurations
- Weaknesses
  - Applicable only when *mean* is defined, then what about categorical data?
  - Need to specify *k*, the number of clusters, in advance
  - Unable to handle noisy data and outliers
  - Not suitable to discover clusters with non-convex shapes