

Chapter VII: Cluster analysis

Knowledge Discovery in Databases

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Chapter VII: Cluster analysis

Cluster analysis: basic concepts.

Partitioning methods.

Hierarchical methods.

Density-based methods.

Grid-based methods.

Evaluation of clustering.

Summary.



What is cluster analysis?

Cluster: A collection of data objects within a larger set that are.

Similar (or related) to one another within the same group and, dissimilar (or unrelated) to the objects outside the group.

Cluster analysis (or clustering, data segmentation, . . .).

Define similarities among data based on the characteristics found in the data (input from user!). Group similar data objects into clusters.

Unsupervised learning:

No predefined classes.

I.e., learning by observation (vs. learning by examples: supervised).

Typical applications:

As a stand-alone tool to get insight into data distribution.

As a preprocessing step for other algorithms.



Clustering for data understanding and applications

Biology:

Taxonomy of living things: kingdom, phylum, class, order, family, genus, and species.

Information retrieval:

Document clustering.

Land use:

Identification of areas of similar land use in an earth-observation database.

Marketing:

Help marketers discover distinct groups in their customer bases, and then use this knowledge to develop targeted marketing programs.

City planning:

Identifying groups of houses according to their house type, value, and geographical location.

Earthquake studies:

Observed earthquake epicenters should be clustered along continent faults.

Climate:

Understanding earth climate, find patterns of atmosphere and ocean.



Quality: what is good clustering?

A good clustering method will produce high-quality clusters.

High intra-class similarity:

Cohesive within clusters.

Low inter-class similarity:

Distinctive between clusters.

The quality of a clustering method depends on:

the similarity measure used by the method,

its implementation, and

its ability to discover some or all of the hidden patterns.



Measure the quality of clustering

Dissimilarity/similarity metric:

Similarity is expressed in terms of a distance function, typically a metric: d(x, y).

The definitions of distance functions are usually rather different for interval-scaled, Boolean, categorical, ordinal, ratio, and vector variables (see chapter 2).

Weights should be associated with different variables based on applications and data semantics.

Quality of clustering:

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.



Considerations for cluster analysis

Partitioning criteria:

Single level vs. hierarchical partitioning.

Often, multi-level hierarchical partitioning is desirable.

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., Euclidian, 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).



Requirements and challenges

Scalability:

Clustering all the data instead of only on samples.

Ability to deal with different types of attributes:

Numerical, binary, categorical, ordinal, linked, and mixture of these.

Constraint-based clustering:

User may give inputs on constraints.

Use domain knowledge to determine input parameters.

Interpretability and usability.

Others:

Discovery of clusters with arbitrary shape.

Ability to deal with noisy data.

Incremental clustering and insensitivity to input order.

High dimensionality.



Major clustering approaches

Partitioning approach:

Construct various partitions and then evaluate them by some criterion.

E.g., minimizing the sum of square errors.

Typical methods: k-means, k-medoids, CLARA, CLARANS.

Hierarchical approach:

Create a hierarchical decomposition of the set of data (or objects) using some criterion.

Typical methods: AGNES, DIANA, BIRCH, CHAMELEON.

Density-based approach:

Based on connectivity and density functions.

Typical methods: DBSCAN, OPTICS, DENCLUE.

Grid-based approach:

Based on a multiple-level granularity structure.

Typical methods: STING, WaveCluster, CLIQUE.



Major clustering approaches (II)

Model-based approach:

A model is hypothesized for each of the clusters and tries to find the best fit of that model to each other.

Typical methods: EM, SOM, COBWEB.

Frequent-pattern-based approach:

Based on the analysis of frequent patterns.

Typical methods: p-Cluster.

User-guided or constraint-based approach:

Clustering by considering user-specified or application-specific constraints.

Typical methods: COD (obstacles), constrained clustering.

Link-based clustering:

Objects are often linked together in various ways.

Massive links can be used to cluster objects: SimRank, LinkClus.



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Partitioning algorithms: basic concept

Partitioning method:

Partition a database D of n objects $o_j, j \in \{1, \ldots, n\}$ into a set of k-clusters C_i , $1 \le i \le k$ such that the sum of squared distances to c_i is minimized (where c_i is the centroid or medoid of cluster C_i):

$$\min \sum_{i=1}^{\kappa} \sum_{o \in C_i} d(o, c_i)^2. \tag{1}$$

Given k, find a partition of k clusters that optimizes the chosen partitioning criterion.

Globally optimal: exhaustively enumerate all partitions.

Heuristic methods: k-means and k-medoids algorithms.

k-means (MacQueen'67, Lloyd'57/'82):

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 method

Given k, the k-means algorithm is implemented in four steps:

- 1. Partition the database into k non-empty subsets.
 - E.g. the first $\frac{n}{k}$ objects, then the next $\frac{n}{k}$ objects, . . .
- 2. Compute the centroids of the **clusters** of the current partitioning.

The centroid is the center, i.e. mean point, of the cluster. For each attribute (or dimension), calculate the average value.

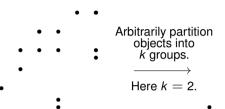
- 3. Assign each object to the cluster with the nearest centroid.
 - That is, for each object calculate distance to each of the *k* centroids and pick the one with the smallest distance.
- 4. If any object has changed its cluster, go back to step 2. Otherwise stop.

Variant:

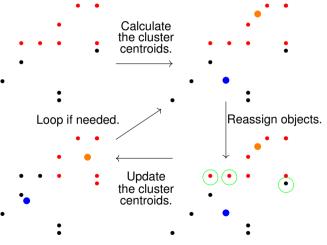
Start with arbitrarily chosen k objects as initial centroids in step 1. Continue with step 3.



An example of k-means clustering



The initial data set.





Thank you for your attention. Any questions about the seventh chapter?

Ask them now, or again, drop me a line:
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