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Data Mining:

Concepts and Techniques

(3rd ed.)

— Chapter 10 —

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Cluster Analysis: Basic Concepts and Methods

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

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 Statistic
  - Given a dataset D regarded as a sample of a random variable z, determine how far away z is from being uniformly distributed in the data space
  - Sample *n* points, $p_1, \ldots, p_n$, uniformly from the feature space of D. For each p_i, find its nearest neighbor in D: $y_i = min\{dist(p_i, v)\}$ where *v* in D
  - Sample *n* points, $q_1, \ldots, q_n$, uniformly from D. For each q_i, find its nearest neighbor in D – $\{q_i\}$: $x_i = min\{dist(q_i, v)\}$ where *v* in D and $v \neq q_i$
  - 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 z (and so D) is uniformly distributed, $\sum x_i$ and $\sum y_i$ are close to each other and H is close to 0.5.
  - If D is clustered, H is close to 1

Determine the Number of Clusters

- Empirical method
  - # of clusters ≈sqrt(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 (ideal clustering, e.g. built by domain experts) 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

Measuring Clustering Quality: Intrinsic Methods

- Silhouette coefficient: similarity metric between objects in the data set
  - Let C1 .. Ck be the clusters
  - For each object o in a certain cluster t
    - let a(o) be the average distance between o and the objects of Ct
    - let $b_l(o)$ be the average distance between o and the objects of cluster l; then $b(o) = \min_{l \neq t} b_l(o)$
- The silhouette coefficient is defined as follows:

$$s(o) = \frac{b(o) - a(o)}{max(a(o), b(o))}$$

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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

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