Data Mining

4. Cluster Analysis

4.4 Hierarchical Methods

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Introduction

Introduction

- A **hierarchical clustering** method works by grouping data objects into a tree of clusters.
- **Types of hierarchical clustering methods:**
  - **Agglomerative:** the hierarchical decomposition is formed in a bottom-up (merging) fashion.
  - **Divisive:** the hierarchical decomposition is formed in a top-down (splitting) fashion.

Introduction

- **Agglomerative hierarchical clustering**
  - This bottom-up strategy starts by placing each object in its own cluster and then merges these atomic clusters into larger and larger clusters, until all of the objects are in a single cluster or until certain termination conditions are satisfied.
  - Most hierarchical clustering methods belong to this category.
  - They differ only in their definition of intercluster similarity.

Introduction

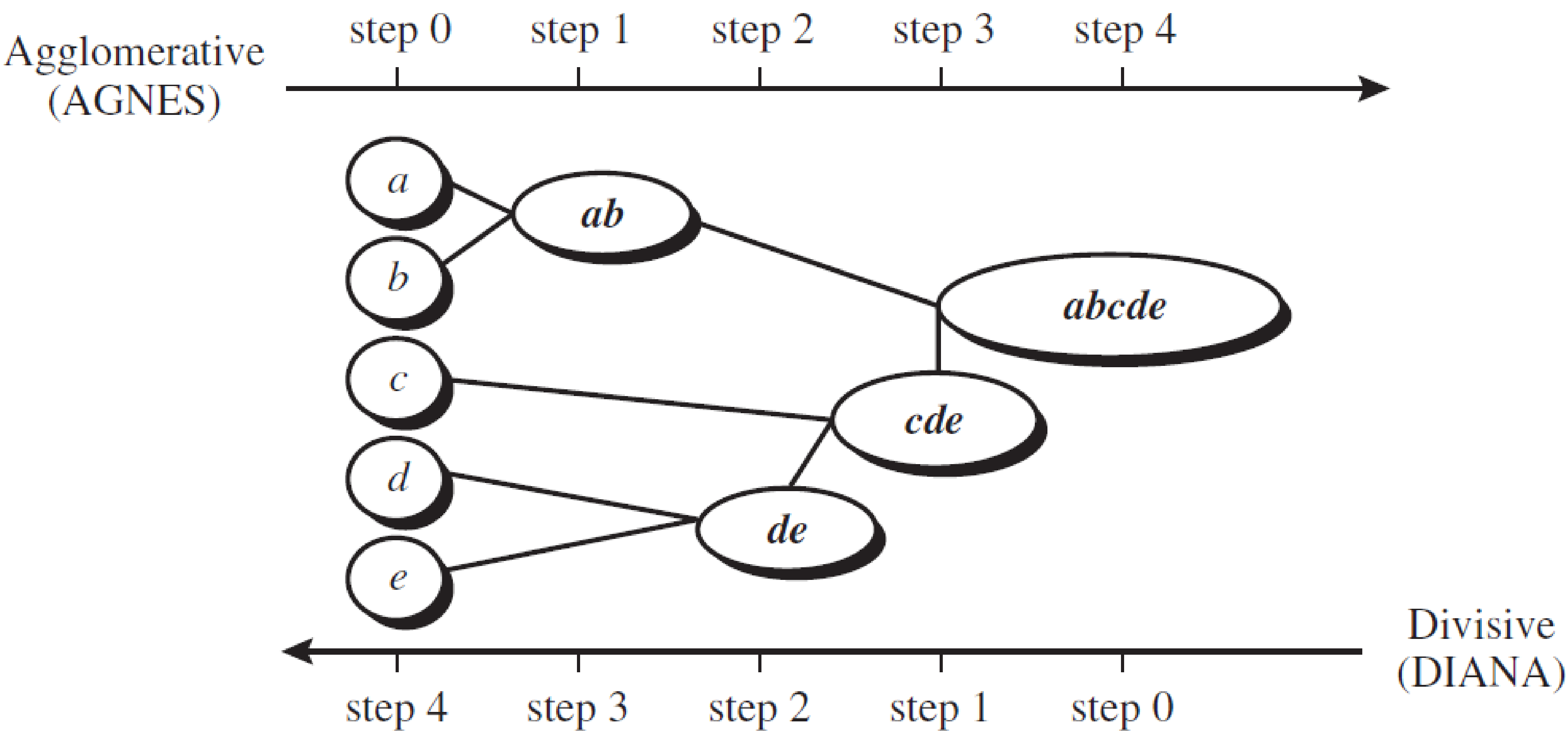
- **Divisive hierarchical clustering**
  - This top-down strategy starts with all objects in one cluster.
  - It subdivides the cluster into smaller and smaller pieces, until each object forms a cluster on its own or until it satisfies certain termination conditions,
  - Termination conditions can be
    - a desired number of clusters is obtained or
    - the diameter of each cluster is within a certain threshold.

Example

- **Example: Agglomerative versus divisive hierarchical clustering**
  - the application of AGNES (AGglomerative NESting), an agglomerative hierarchical clustering method,
  - and DIANA (DIvisive ANAlysis), a divisive hierarchical clustering method, to a data set of five objects, {***a, b, c, d, e***}**.**

Example

- Agglomerative and divisive hierarchical clustering on data objects {***a, b, c, d, e***}.

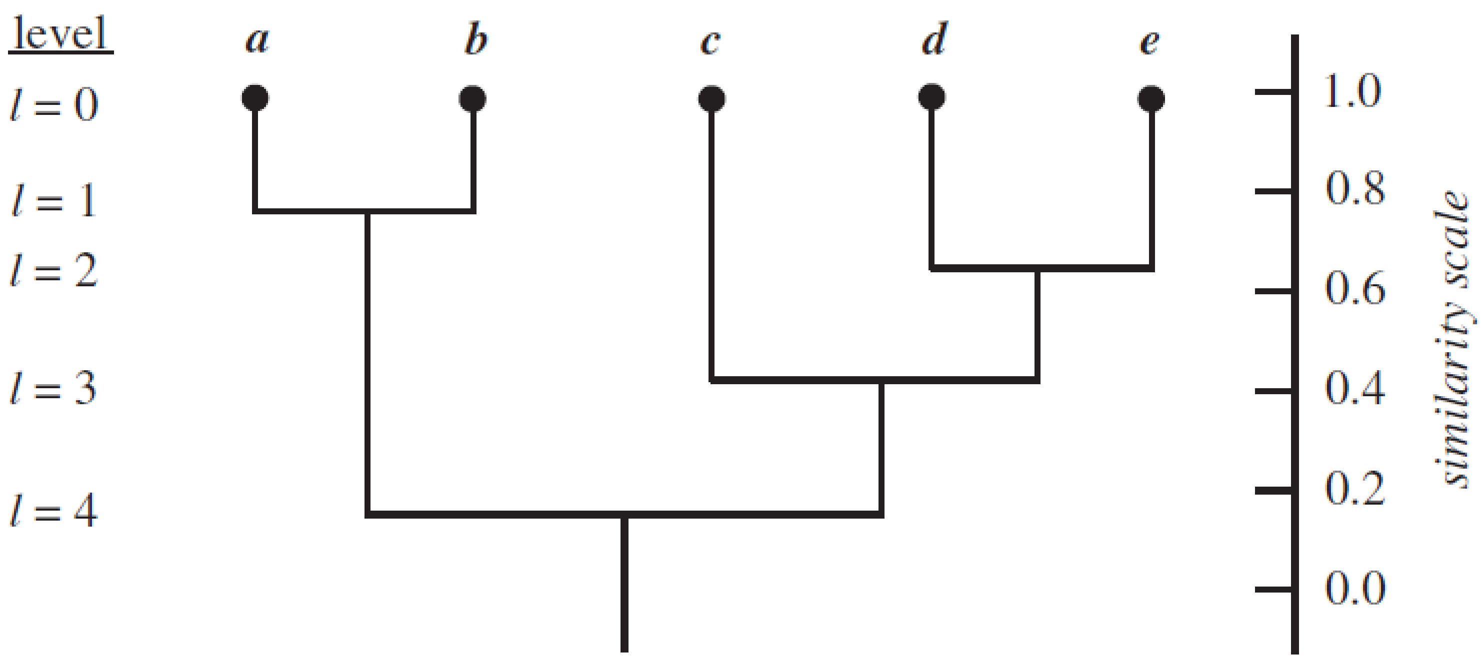


Dendrogram

- **Dendrogram**
  - A tree structure which is commonly used to represent the process of hierarchical clustering.
  - It shows how objects are grouped together step by step.

Dendrogram

- Dendrogram representation for hierarchical clustering of data objects {***a, b, c, d, e***}.



Measures for Distance Between Clusters

- Common measures for distance between clusters are as follows:
  - **Minimum distance**
  - **Maximum distance**
  - **Mean distance**
  - **Average distance**

Measures for Distance Between Clusters

- **Notation**
  - $|p - p'|$: is the distance between two objects or points, *p and p'*
  - m_i is the mean for cluster, C_i
  - n_i is the number of objects in C_i
  - m_j is the mean for cluster, C_j

Measures for Distance Between Clusters

- **Minimum distance**

$$d_{min}(C_i, C_j) = \quad min_{\mathbf{p} \in C_i, \, \mathbf{p}' \in C_j} |\mathbf{p} - \mathbf{p}'|$$

  - When an algorithm uses the **minimum distance**, it is sometimes called **a nearest-neighbor clustering algorithm.**
  - If the clustering process is terminated when the distance between nearest clusters exceeds an **arbitrary threshold**, it is called **a single-linkage algorithm**.

Measures for Distance Between Clusters

- **Maximum distance**

$$d_{max}(C_i, C_j) = \quad max_{\boldsymbol{p} \in C_i, \boldsymbol{p}' \in C_j} |\boldsymbol{p} - \boldsymbol{p}'|$$

  - When an algorithm uses the maximum distance, it is sometimes called **a farthest-neighbor clustering algorithm**.
  - If the clustering process is terminated when the maximum distance between **nearest clusters** exceeds an **arbitrary threshold**, it is called **a complete-linkage algorithm**.
  - Farthest-neighbor algorithms tend to minimize the increase in diameter of the clusters at each iteration as little as possible.

Measures for Distance Between Clusters

- **Mean distance**

$$d_{mean}(C_i, C_j) = \quad |\boldsymbol{m}_i - \boldsymbol{m}_j|$$

  - The minimum and maximum measures tend to be overly sensitive to outliers or noisy data.
  - The use of **mean or average distance** is a compromise between the minimum and maximum distances and overcomes the outlier sensitivity problem.

Measures for Distance Between Clusters

- **Average distance**

$$d_{avg}(C_i, C_j) = \frac{1}{n_i n_j} \sum_{p \in C_i} \sum_{p' \in C_j} |p - p'|$$

- Whereas the mean distance is the simplest to compute, the average distance is advantageous in that it can handle categoric as well as numeric data.
- The computation of the mean vector for categoric data can be difficult or impossible to define.

The Difficulties with Hierarchical Clustering

- The quality of a pure hierarchical clustering method suffers from its inability to perform adjustment once a merge or split decision has been executed.
- That is, if a particular merge or split decision later turns out to have been a poor choice, the method cannot backtrack and correct it.
- Recent studies have emphasized the integration of hierarchical agglomeration with iterative relocation methods.

The Difficulties with Hierarchical Clustering

- Three such methods are introduced in this chapter, including:
  - **BIRCH**,
    - begins by partitioning objects hierarchically using tree structures, where the leaf or low-level nonleaf nodes can be viewed as "microclusters" depending on the scale of resolution.
    - It then applies other clustering algorithms to perform macroclustering on the microclusters.
  - **ROCK**
    - Merges clusters based on their interconnectivity.
  - **Chameleon**,
    - Explores dynamic modeling in hierarchical clustering.

BIRCH Algorithm

BIRCH Algorithm

- **BIRCH: Balanced Iterative Reducing and Clustering Using Hierarchies**
  - BIRCH is designed for clustering a large amount of numerical data
  - It integrates the hierarchical clustering (at the initial **microclustering stage**) and other clustering methods such as **iterative partitioning** (at the later **macroclustering stage**).
  - It overcomes the two difficulties of agglomerative clustering methods:
    - (1) scalability and
    - (2) the inability to undo what was done in the previous step.

BIRCH Algorithm

- BIRCH introduces two concepts:
  - **Clustering Feature (CF)**
  - **Clustering feature tree (CF tree)**
- They are used to summarize cluster representations.
- These structures help the clustering method achieve good speed and scalability in large databases and also make it effective for incremental and dynamic clustering of incoming objects.

BIRCH Algorithm

- Given n d-dimensional data objects or points in a cluster, we can define the centroid $\boldsymbol{x_0}$, radius $\boldsymbol{R}$, and diameter $\boldsymbol{D}$ of the cluster as follows:

$$x_0 = \frac{\sum_{i=1}^{n} x_i}{n} \quad R = \sqrt{\frac{\sum_{i=1}^{n} (x_i - x_0)^2}{n}} \quad D = \sqrt{\frac{\sum_{i=1}^{n} \sum_{j=1}^{n} (x_i - x_j)^2}{n(n-1)}}$$

- Where R is the average distance from member objects to the centroid, and D is the average pairwise distance within a cluster.
- Both R and D reflect the tightness of the cluster around the centroid.

BIRCH Algorithm

- **Clustering Feature (CF)**
  - CF is a three-dimensional vector summarizing information about clusters of objects.
  - Given n d-dimensional objects or points in a cluster, $\{\boldsymbol{x}_i\}$, then the CF of the cluster is defined as:

$$\boldsymbol{CF} = \langle \boldsymbol{n}, \boldsymbol{LS}, \boldsymbol{SS} \rangle$$

  - where n is the number of points in the cluster,
  - ***LS*** is the linear sum of the n points, i.e.,

$$\sum_{i=1}^{n} x_i$$

  - ***SS*** is the square sum of the data points, i.e.,

$$\sum_{i=1}^{n} {x_i}^2$$

BIRCH Algorithm

- Clustering features are **additive**.
- For example, suppose that we have two disjoint clusters, C_1 and C_2, having the clustering features, CF_1 and CF_2, respectively.
- The clustering feature for the cluster that is formed by merging C_1 and C_2 is simply $CF_1 + CF_2$.
- Clustering features are sufficient for calculating all of the measurements that are needed for making clustering decisions in BIRCH.

BIRCH Algorithm

- **Example: Clustering feature.**
  - Suppose that there are three points, (2, 5), (3, 2), and (4, 3), in a cluster, C_1. The clustering feature of C_1 is:

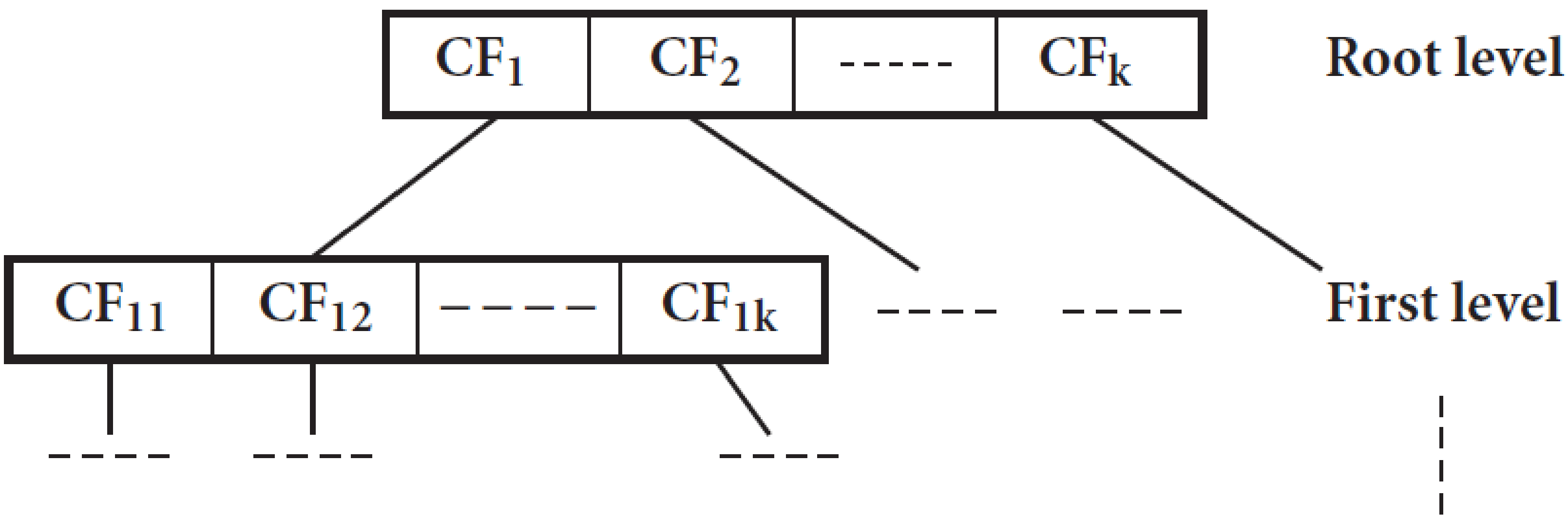
$$CF_1 = \langle 3, (2+3+4, 5+2+3), (2^2+3^2+4^2, 5^2+2^2+3^2) \rangle$$
$$= \langle 3, (9, 10), (29, 38) \rangle.$$

  - Suppose that C_1 is joint to a second cluster, C_2, where $CF_2 = \langle 3, (35, 36), (417, 440) \rangle$.
  - The clustering feature of a new cluster, C_3, that is formed by merging C_1 and C_2, is derived by adding CF_1 and CF_2. That is:

$$CF_3 = \langle 3+3, (9+35, 10+36), (29+417, 38+440) \rangle$$
$$= \langle 6, (44, 46), (446, 478) \rangle.$$

BIRCH Algorithm

- A **CF tree** is a height-balanced tree that stores the clustering features for a hierarchical clustering.



BIRCH Algorithm

- By definition, a nonleaf node in a tree has **children**.
- The nonleaf nodes store sums of the CFs of their children, and thus summarize clustering information about their children.
- **A CF tree has two parameters:**
  - **Branching factor, B**
    - specifies the maximum number of children per nonleaf node.
  - **Threshold, T**
    - specifies the maximum diameter of subclusters stored at the leaf nodes of the tree.
- These two parameters influence the size of the resulting tree.

BIRCH Algorithm Phases

- The primary phases of BIRCH are:
- **Phase 1**:
  - BIRCH scans the database to build an initial in-memory CF tree
- **Phase 2**:
  - BIRCH applies a (selected) clustering algorithm to cluster the leaf nodes of the CF tree, which removes sparse clusters as outliers and groups dense clusters into larger ones.

BIRCH Algorithm Phases

- **Phase 1:**
  - the CF tree is built dynamically as objects are inserted.
  - Thus, the method is **incremental**.
  - An object is inserted into the closest leaf entry (subcluster).
  - If the diameterc of the subcluster stored in the leaf node after insertion is larger than the threshold value, then the leaf node and possibly other nodes are split.
  - After the insertion of the new object, information about it is passed toward the root of the tree.
  - The size of the CF tree can be changed by modifying the threshold.

BIRCH Algorithm Phases

- **Phase 2**:
  - Once the CF tree is built, any clustering algorithm, such as a typical partitioning algorithm, can be used with the CF tree in Phase 2.

Computation Complexity of the Algorithm

- The computation complexity of the algorithm is $O(n)$,
  - were n is the number of objects to be clustered.
- Experiments have shown the linear scalability of the algorithm with respect to the number of objects and good quality of clustering of the data.

Weakness of BIRCH

- However, since each node in a CF tree can hold only a limited number of entries due to its size, a CF tree node does not always correspond to what a user may consider a natural cluster.
- Moreover, if the clusters are not spherical in shape, BIRCH does not perform well, because it uses the notion of radius or diameter to control the boundary of a cluster.

References

References

- J. Han, M. Kamber, **Data Mining: Concepts and Techniques**, Elsevier Inc. (2006). (Chapter 7)

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