Pattern Recognition Lecture
"Clustering: Hierarchical Algorithms"

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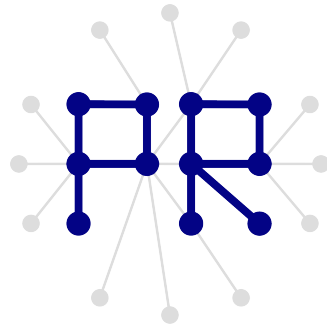

Overview

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General Idea and Applications

- Instead of producing a single clustering (like sequential algorithms), hierarchical algorithms produce a hierarchy of clusterings.
- This kind of algorithms is usually found in the social sciences and biological taxonomy.
- Further fields of application are: medicine, archaeology, computer science, and engineering.

Initial Definitions

- Let us recall that $X = \{\mathbf{x}_i, i = 1, \ldots, N\}$ is a set of l-dimensional vectors that are to be clustered.
- Also recall the definition of clustering $\mathbb{R} = \{C_j, j = 1, \ldots, m\}$ where $C_j \subset X$.
- A clustering $\mathbb{R}_1$ containing k clusters is said to be nested in the clustering $\mathbb{R}_2$ which contains $r < k$ clusters, if each cluster in $\mathbb{R}_1$ is a subset of a set in $\mathbb{R}_2$. Note that at least one cluster of $\mathbb{R}_1$ is a proper subset of a set in $\mathbb{R}_2$ $(\mathbb{R}_1 \neq \mathbb{R}_2)$.
- If $\mathbb{R}_1$ is nested in $\mathbb{R}_2$ we denote it by $\mathbb{R}_1 \sqsubset \mathbb{R}_2$.

Examples for the Term "Nested Clusterings"

- For example, $\mathbb{R}_1 = \{\{\mathbf{x}_1, \mathbf{x}_3\}; \{\mathbf{x}_4\}; \{\mathbf{x}_2, \mathbf{x}_5\}\}$ is nested in $\mathbb{R}_2 = \{\{\mathbf{x}_1, \mathbf{x}_3, \mathbf{x}_4\}; \{\mathbf{x}_2, \mathbf{x}_5\}\}$
- But, $\mathbb{R}_1$ is not nested in $\mathbb{R}_3 = \{\{\mathbf{x}_1, \mathbf{x}_4\}; \{\mathbf{x}_3\}; \{\mathbf{x}_2, \mathbf{x}_5\}\}$.
- It is clear that a clustering is not nested to itself.

Two Main Categories of Hierarchical Algorithms

- Hierarchical algorithms produce a hierarchy of nested clusterings.
- More specifically, these algorithms involve N steps, as many as the number of data vectors.
- At each step t, a new clustering is obtained based on the clustering produced at the previous step $t-1$.
- There are two main categories of these algorithms, the agglomerative and the divisive hierarchical algorithms.

Agglomerative Algorithms - General Idea

- The initial clustering $\mathbb{R}_0$ for the agglomerative algorithms consists of N clusters, each containing a single element of X.
- A the first step, the clustering $\mathbb{R}_1$ is produced. It contains $N-1$ sets, such that $\mathbb{R}_0 \sqsubset \mathbb{R}_1$.
- This procedure continues until the final clustering, $\mathbb{R}_{N-1}$, is obtained. It contains a single set, that is, the set of data, X. Notice that for the hierarchy of the resulting clusterings, we have:

$$\mathbb{R}_0 \sqsubset \mathbb{R}_1 \sqsubset \cdots \sqsubset \mathbb{R}_{N-1}$$

Divisive Algorithms - General Idea

- The divisive algorithms follow the inverse path. The initial clustering $\mathbb{R}_0$ consists of a single set, X.
- At the first step, the clustering $\mathbb{R}_1$ is produced. It consists of two sets, such that $\mathbb{R}_1 \sqsubset \mathbb{R}_0$.
- This procedure continues until the final clustering $\mathbb{R}_{N-1}$ is obtained. It contains N sets, each consisting of a single element of X. In this case we have

$$\mathbb{R}_{N-1} \sqsubset \mathbb{R}_{N-2} \sqsubset \cdots \sqsubset \mathbb{R}_0$$

Overview

Generalised Agglomerative Scheme (GAS)

Let $g(C_i, C_j)$ be a function defined for all possible pairs of clusters of X. This function measures the proximity between C_i and C_j. Let t denote the current level of hierarchy. Then, the general agglomerative scheme may be stated as follows:

- Initialisation
  - Choose $\mathbb{R}_0 = \{C_i = \{\mathbf{x}_i\}, i = 1, \ldots, N\}$
  - $t = 0$
- Repeat:
  - $t = t + 1$
  - Among all possible pairs of clusters (C_r, C_s) in $\mathbb{R}_{t-1}$ find the one, say, (C_i, C_j), such that

$$g(C_i, C_j) = \begin{cases} \min\limits_{r,s} g(C_r, C_s) & \text{if } g \text{ is a dissimilarity function} \\ \max\limits_{r,s} g(C_r, C_s) & \text{if } g \text{ is a similarity function} \end{cases}$$

  - Define $C_q = C_i \cup C_j$ and produce the new clustering $\mathbb{R}_t = \{\mathbb{R}_{t-1} \setminus \{C_i, C_j\}\} \cup \{C_q\}$
- Until all vectors lie in a single cluster.

GAS - the Nesting Property

- GAS creates a hierarchy of N clusterings, so that each one is nested in all successive clusterings, that is, $\mathbb{R}_{t_1} \sqsubset \mathbb{R}_{t_2}$, for $t_1 < t_2$, $t_2 = 1, \ldots, N-1$.

- If two vectors come together into a single cluster at level t of the hierarchy, they will remain in the same cluster for all subsequent clusterings.

- A disadvantage of the nesting property is that there is no way to recover from a "poor" clustering that may have occurred in an earlier level of the hierarchy.

GAS - Algorithm Complexity

- At each level t, there are $N - t$ clusters. Thus, in order to determine a the pair of clusters that is going to be merged at the $t + 1$ level,

$$\left(\begin{array}{c} N-t \\ 2 \end{array} \right) \equiv \frac{(N-t)(N-t-1)}{2}$$

pairs of clusters have to be considered.

- Thus, the total number of pairs that have to be examined throughout the whole clustering process is

$$\sum_{t=0}^{N-1} \left(\begin{array}{c} N-t \\ 2 \end{array} \right) = \sum_{k=1}^{N} \left(\begin{array}{c} k \\ 2 \end{array} \right) = \frac{(N-1)N(N+1)}{6}$$

that is, the total number of operations required by an agglomerative scheme is proportional to N^3. However, the exact complexity of the algorithm depends on the definition of g.

Pattern and Similarity Matrix

- The pattern matrix $D(X)$ is the $N \times l$ matrix, whose i-th row is the transposed i-th vector of X.

- The similarity (dissimilarity) matrix $P(X)$ is an $N \times N$ matrix whose (i, j) element equals the similarity $s(\mathbf{x}_i, \mathbf{x}_j)$ (dissimilarity $d(\mathbf{x}_i, \mathbf{x}_j)$) between vectors $\mathbf{x}_i$ and $\mathbf{x}_j$.

Dendrogram

- A dendrogram is an effective means of representing the sequence of clusterings produced by an agglomerative algorithm.

$\{\{\boldsymbol{x}_1\},\{\boldsymbol{x}_2\},\{\boldsymbol{x}_3\},\{\boldsymbol{x}_4\},\{\boldsymbol{x}_5\}\}$

$\{\{\boldsymbol{x}_1, \boldsymbol{x}_2\},\{\boldsymbol{x}_3\},\{\boldsymbol{x}_4\},\{\boldsymbol{x}_5\}\}$

$\{\{\boldsymbol{x}_1, \boldsymbol{x}_2\},\{\boldsymbol{x}_3\},\{\boldsymbol{x}_4, \boldsymbol{x}_5\}\}$

$\{\{\boldsymbol{x}_1, \boldsymbol{x}_2\},\{\boldsymbol{x}_3, \boldsymbol{x}_4, \boldsymbol{x}_5\}\}$

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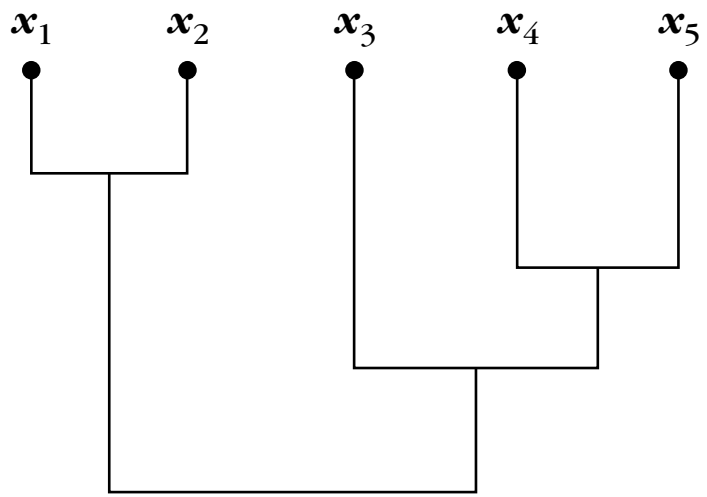
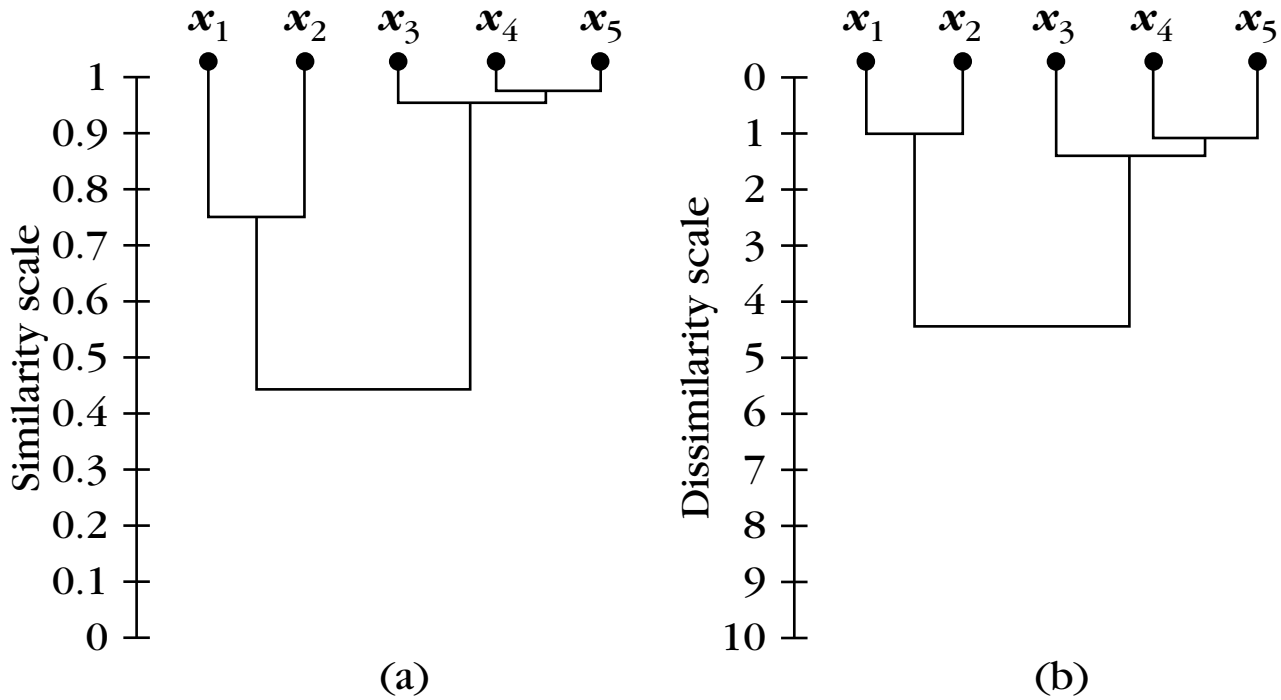


Proximity Dendrogram

- A proximity dendrogram is a dendrogram that takes into account the level of proximity where two clusters are merged for the first time. We distinguish between similarity and dissimilarity dendrograms.



Matrix Updating Algorithmic Scheme (MUAS)

- Initialisation
  - $\mathbb{R}_0 = \{\{\mathbf{x}_i\}, i = 1, \ldots, N\}$
  - $P_0 = P(X)$
  - $t = 0$
- Repeat:
  - $t = t + 1$
  - Find C_i, C_j such that $d(C_i, C_j) = \min_{r,s=1,\ldots,N; r \neq s} d(C_r, C_s)$
  - Merge C_i, C_j into a single cluster C_q and form $\mathbb{R}_t = \{\mathbb{R}_{t-1} \setminus \{C_i, C_j\}\} \cup \{C_q\}$
  - Define a proximity matrix P_t from P_{t-1}
- Until $\mathbb{R}_{N-1}$ clustering is formed, that is, all feature vectors lie in the same cluster.

Overview

General Idea

- The divisive algorithms follow the reverse strategy from that of the agglomerative schemes.
- At the first step, we search for the best possible partition of X into two clusters. The straightforward method is to consider all possible $2^{N-1} - 1$ partitions of X into two sets and to select the optimum according to a prespecified criterion.
- This procedure is then applied iteratively to each of the two sets produced in the previous stage.
- The final clustering consists o N clusters, each containing a single vector of X.

Generalised Divisive Scheme (GDS) - Assumptions

- The t-th clustering contains $t + 1$ clusters.
- C_{tj} denotes the j-th cluster of the t-th clustering $\mathbb{R}_t$.
- $g(C_i, C_j)$ is a dissimilarity function[1] defined for all possible pairs of clusters.
- The initial clustering $\mathbb{R}_0$ contains only the set of X.

Generalised Divisive Scheme (GDS)

- Initialisation
  - Choose $\mathbb{R}_0 = \{X\}$ as the initial clustering, e. g., $C_{01} = X$.
  - $t = 0$
- Repeat:
  - $t = t + 1$
  - For $i = 1$ to t
    - Among all possible pairs of clusters (C_r, C_s) that form a partition of $C_{t-1,i}$ find the pair $(C^1_{t-1,i}, C^2_{t-1,i})$ that gives the maximum value for g.
  - Next i
  - From the t pairs defined in the previous step choose the one that maximises g. Suppose that this is $(C^1_{t-1,i}, C^2_{t-1,i})$.
  - The new clustering is $\mathbb{R}_t = \{\mathbb{R}_{t-1} \setminus \{C_{t-1,j}\}\} \cup \{C^1_{t-1,j}, C^2_{t-1,j}\}$
  - Relabel the clusters of $\mathbb{R}_t$
- Until each vector lies in a single distinct cluster.