

Reference: (Project from NUS CS5228 Knowledge Discovery and Data Mining)

The algorithm of Agglomerative Hierarchical Clustering is summarized as follows:

Input: Data points $X = \{(x_1, y_1), (x_2, y_2), \dots, (x_N, y_N)\}$; $x_i \in \mathbf{R}$ and $y_i \in \mathbf{R}$ are the coordinates.

Output: Clustering history: a list of pairs of the cluster ID, $H = \{(i_1, j_1), (i_2, j_2), \dots\}$, that indicates which pair of clusters are merged first; for example, $\{(1, 3), (2, 4), \dots\}$ indicates that (C_1, C_3) are merged first, then (C_2, C_4) are merged, ...

Steps:

1. $C_i \leftarrow \{(x_i, y_i)\}$, for $i \in \{1, \dots, N\}$, # current clusters $\leftarrow N$
2. Compute $ProximityMatrix[i, j]$, for $i, j \in \{1, \dots, N\}$
3. $ClusterIndexSet = \{1, \dots, N\}$; $H = []$
4. Repeat:
 - Find (p, q) with $\underset{i, j \in ClusterIndexSet}{\operatorname{argmin}} ProximityMatrix[i, j]$
 - Merge (C_p, C_q) together as C_{N+1}
 - Update $ProximityMatrix[i, N+1]$, for each $i \in ClusterIndexSet$
 - Append (p, q) into H
 - $N \leftarrow N + 1$
 - Remove p from $ClusterIndexSet$
 - Remove q from $ClusterIndexSet$
 - Insert N into $ClusterIndexSet$
5. Return H