

Single Linkage Clustering

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Single Linkage Criterion

In Single Linkage Criterion of Agglomerative Hierarchical clustering, The distance between the elements of each cluster is minimised. As the Naive single linkage clustering has a worst case time complexity of $O(N^3)$. It becomes useless for large data which are frequently used in the field of bioinformatics

Hence Nearest-neighbor chain algorithm is being used here

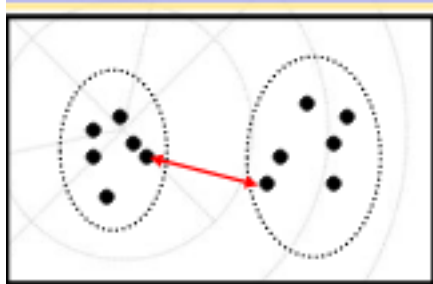
Nearest-neighbor chain algorithm

In the theory of cluster analysis, the nearest-neighbor chain algorithm is an algorithm that can speed up several methods for agglomerative hierarchical clustering. And Single Linkage Clustering is one of them.

The Algorithm

- Initialize the set of active clusters to consist of n one-point clusters, one for each input point.
- Let S be a stack data structure, initially empty, the elements of which will be active clusters.
- While there is more than one cluster in the set of clusters:
- If S is empty, choose an active cluster arbitrarily and push it onto S .
- Let C be the active cluster on the top of S . Compute the distances from C to all other clusters, and let D be the nearest other cluster.
- If D is already in S , it must be the immediate predecessor of C . Pop both clusters from S and merge them.
- Otherwise, if D is not already in S , push it onto S .

Here The cost function used is the minimum distance between the nearest cluster element.



As single linkage criterion can be implemented by using the Lance and William Algorithm

$$d(h,k) = \alpha_i d(i,k) + \alpha_j d(j,k) + \beta d(i,j) + \gamma |d(i,k) - d(j,k)| \quad (1)$$

TABLE 2
Parameter Values for Combinatorial SAHN Clustering Methods

Clustering Method	α_i	α_j	β	γ
Single linkage (Nearest neighbor)	1/2	1/2	0	-1/2
Complete linkage (Furthest neighbor)	1/2	1/2	0	1/2
Group Average (UPGMA)	$\frac{n_i}{n_i+n_j}$	$\frac{n_j}{n_i+n_j}$	0	0
Weighted Average (WPGMA)	1/2	1/2	0	0
Unweighted Centroid (UPGMC)	$\frac{n_i}{n_i+n_j}$	$\frac{n_j}{n_i+n_j}$	$\frac{-n_i n_j}{(n_i+n_j)^2}$	0
Weighted Centroid (WPGMC)	1/2	1/2	-1/4	0
Minimum Variance (Ward)	$\frac{n_i+n_k}{n_i+n_j+n_k}$	$\frac{n_j+n_k}{n_i+n_j+n_k}$	$\frac{-n_k}{n_i+n_j+n_k}$	0
Flexible (Lance and Williams)	$\frac{1-\beta}{2}$	$\frac{1-\beta}{2}$	$\beta < 1$	0

NOTE: n_i is the number of objects in cluster i .

Hence by tuning the cost function of FusedClasses.cpp

```
FusionCost = 0.5 * (MyValue() - abs(MyValue() - MyMatrix->Value(NextAvailableIndex,
NextAvailableIndex))) + MyMatrix->Value(NextAvailableIndex, NextAvailableIndex));
```

References: <https://users.cs.duke.edu/~edels/Papers/1984-J-05-HierarchicalClustering.pdf> http://www.lx.it.pt/~afred/tutorials/B_Clustering_Algorithms.pdf <http://orion.lcg.ufjf.br/Dr.Dobbs/books/book5/chap16.htm> https://en.wikipedia.org/wiki/Nearest-neighbor_chain_algorithm