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# Single-linkage clustering

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In [statistics](#), **single-linkage clustering** is one of several methods of [hierarchical clustering](#). It is based on grouping clusters in bottom-up fashion (agglomerative clustering), at each step combining two clusters that contain the closest pair of elements not yet belonging to the same cluster as each other.

A drawback of this method is that it tends to produce long thin clusters in which nearby elements of the same cluster have small distances, but elements at opposite ends of a cluster may be much farther from each other than to elements of other clusters. This may lead to difficulties in defining classes that could usefully subdivide the data. <sup>[1]</sup>

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## Overview of agglomerative clustering methods [\[edit\]](#)

In the beginning of the agglomerative clustering process, each element is in a cluster of its own. The clusters are then sequentially combined into larger clusters, until all elements end up being in the same cluster. At each step, the two clusters separated by the shortest distance are combined. The definition of 'shortest distance' is what differentiates between the different agglomerative clustering methods.

In single-linkage clustering, the distance between two clusters is determined by a single element pair, namely those two elements (one in each cluster) that are closest to each other. The shortest of these links that remains at any step causes the fusion of the two clusters whose elements are involved. The method is also known as **nearest neighbour clustering**. The result of the clustering can be visualized as a [dendrogram](#), which shows the sequence of cluster fusion and the distance at which each fusion took place.<sup>[2]</sup>

Mathematically, the linkage function – the distance  $D(X, Y)$  between clusters  $X$  and  $Y$  – is described by the expression

$$D(X, Y) = \min_{x \in X, y \in Y} d(x, y),$$

where  $X$  and  $Y$  are any two sets of elements considered as clusters, and  $d(x, y)$  denotes the distance between the two elements  $x$  and  $y$ .

## Naive algorithm [\[edit\]](#)

The following algorithm is an [agglomerative](#) scheme that erases rows and columns in a proximity matrix as old clusters are merged into new ones. The  $N \times N$  proximity matrix  $D$  contains all distances  $d(i, j)$ . The clusterings are assigned sequence numbers  $0, 1, \dots, (n - 1)$  and  $L(k)$  is the level of the  $k$ th clustering. A cluster with sequence number  $m$  is denoted  $(m)$  and the proximity between clusters  $(r)$  and  $(s)$  is denoted  $d[(r), (s)]$ .

The algorithm is composed of the following steps:

- Begin with the disjoint clustering having level  $L(0) = 0$  and sequence number  $m = 0$ .
- Find the most similar pair of clusters in the current clustering, say pair  $(r), (s)$ , according to  $d[(r), (s)] = \min d[(i), (j)]$  where the minimum is over all pairs of clusters in the current clustering.
- Increment the sequence number:  $m = m + 1$ . Merge clusters  $(r)$  and  $(s)$  into a single cluster to form the next clustering  $m$ . Set the level of this clustering to  $L(m) = d[(r), (s)]$
- Update the proximity matrix,  $D$ , by deleting the rows and columns corresponding to clusters  $(r)$  and  $(s)$  and adding a row and column corresponding to the newly formed cluster. The proximity between the new cluster, denoted  $(r, s)$  and old cluster  $(k)$  is defined as  $d[(k), (r, s)] = \min d[(k), (r)], d[(k), (s)]$ .
- If all objects are in one cluster, stop. Else, go to step 2.

## Other linkages [edit]

The naive algorithm for single linkage clustering is essentially the same as [Kruskal's algorithm](#) for [minimum spanning trees](#). However, in single linkage clustering, the order in which clusters are formed is important, while for minimum spanning trees what matters is the set of pairs of points that form distances chosen by the algorithm.

Alternative linkage schemes include [complete linkage clustering](#), [average linkage clustering](#), and [Ward's method](#). In the naive algorithm for agglomerative clustering, implementing a different linkage scheme may be accomplished simply by using a different formula to calculate inter-cluster distances in the algorithm.. The formula that should be adjusted has been highlighted using bold text. However, more efficient algorithms such as the one described below do not generalize to all linkage schemes in the same way.

## Faster algorithms [edit]

The naive algorithm for single-linkage clustering is easy to understand but slow, with time complexity  $O(n^3)$ .<sup>[3]</sup> In 1973, R. Sibson proposed an algorithm with time complexity  $O(n^2)$  and space complexity  $O(n)$  (both optimal) known as SLINK. The slink algorithm represents a clustering on a set of  $n$  numbered items by two functions. These functions are both determined by finding the smallest cluster  $C$  that contains both item  $i$  and at least one larger-numbered item. The first function,  $\pi$ , maps item  $i$  to the largest-numbered item in cluster  $C$ . The second function,  $\lambda$ , maps item  $i$  to the distance associated with the creation of cluster  $C$ . Storing these functions in two arrays that map each item number to its function value takes space  $O(n)$ , and this information is sufficient to determine the clustering itself. As Sibson shows, when a new item is added to the set of items, the updated functions representing the new single-linkage clustering for the augmented set, represented in the same way, can be constructed from the old clustering in time  $O(n)$ . The SLINK algorithm then loops over the items, one by one, adding them to the representation of the clustering.<sup>[4][5]</sup>

An alternative algorithm, running in the same optimal time and space bounds, is based on the equivalence between the naive algorithm and Kruskal's algorithm for minimum spanning trees. Instead of using Kruskal's algorithm, one can use [Prim's algorithm](#), in a variation without priority queues that takes time  $O(n^2)$  and space  $O(n)$  to construct the minimum spanning tree (but not the clustering) of the given items and distances. Then, applying Kruskal's algorithm to the sparse graph formed by the edges of the minimum spanning tree produces the clustering itself in an additional time  $O(n \log n)$  and space  $O(n)$ .<sup>[6]</sup>

## References [edit]

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## External links [edit]

- Single linkage clustering algorithm implementation in Ruby (A14R)
- Linkages used in Matlab

Categories: Data clustering algorithms

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