scipy.cluster.hierarchy.linkage

scipy.cluster.hierarchy.**linkage**(*y*, *method='single'*, *metric='euclidean'*, *optimal_ordering=False*) [source] (https://github.com/scipy/scipy/blob/v1.2.0/scipy/cluster/hierarchy.py#L881-L1125)

Perform hierarchical/agglomerative clustering.

The input y may be either a 1d condensed distance matrix or a 2d array of observation vectors.

If y is a 1d condensed distance matrix, then y must be a $\binom{n}{2}$ sized vector where n is the number of original observations paired in the distance matrix. The behavior of this function is very similar to the MATLAB linkage function.

A $(n-1)$ by 4 matrix `Z` is returned. At the i-th iteration, clusters with indices `Z[i, 0]` and `Z[i, 1]` are combined to form cluster $n+i$. A cluster with an index less than n corresponds to one of the n original observations. The distance between clusters `Z[i, 0]` and `Z[i, 1]` is given by `Z[i, 2]`. The fourth value `Z[i, 3]` represents the number of original observations in the newly formed cluster.

The following linkage methods are used to compute the distance $d(s, t)$ between two clusters s and t. The algorithm begins with a forest of clusters that have yet to be used in the hierarchy being formed. When two clusters s and t from this forest are combined into a single cluster u, s and t are removed from the forest, and u is added to the forest. When only one cluster remains in the forest, the algorithm stops, and this cluster becomes the root.

A distance matrix is maintained at each iteration. The `d[i,j]` entry corresponds to the distance between cluster i and j in the original forest.

At each iteration, the algorithm must update the distance matrix to reflect the distance of the newly formed cluster u with the remaining clusters in the forest.

Suppose there are $|u|$ original observations $u[0], \ldots, u[|u|-1]$ in cluster u and $|v|$ original objects $v[0], \ldots, v[|v|-1]$ in cluster v. Recall s and t are combined to form cluster u. Let v be any remaining cluster in the forest that is not u.

The following are methods for calculating the distance between the newly formed cluster u and each v.

- method='single' assigns

$$d(u, v) = \min(dist(u[i], v[j]))$$

for all points i in cluster u and j in cluster v. This is also known as the Nearest Point Algorithm.

- method='complete' assigns

$$d(u, v) = \max(dist(u[i], v[j]))$$

for all points i in cluster u and j in cluster v. This is also known by the Farthest Point Algorithm or Voor Hees Algorithm.

- method='average' assigns

$$d(u, v) = \sum_{ij} \frac{d(u[i], v[j])}{(|u| * |v|)}$$

for all points i and j where $|u|$ and $|v|$ are the cardinalities of clusters u and v, respectively. This is also called the UPGMA algorithm.

- method='weighted' assigns

$$d(u, v) = (dist(s, v) + dist(t, v))/2$$

where cluster u was formed with cluster s and t and v is a remaining cluster in the forest. (also called WPGMA)

- method='centroid' assigns

$$dist(s, t) = ||c_s - c_t||_2$$

where c_s and c_t are the centroids of clusters s and t, respectively. When two clusters s and t are combined into a new cluster u, the new centroid is computed over all the original objects in clusters s and t. The distance then becomes the Euclidean distance between the centroid of u and the centroid of a remaining cluster v in the forest. This is also known as the UPGMC algorithm.

- method='median' assigns $d(s, t)$ like the `centroid` method. When two clusters s and t are combined into a new cluster u, the average of centroids s and t give the new centroid u. This is also known as the WPGMC algorithm.

- method='ward' uses the Ward variance minimization algorithm. The new entry $d(u, v)$ is computed as follows,

$$d(u, v) = \sqrt{\frac{|v| + |s|}{T} d(v, s)^2 + \frac{|v| + |t|}{T} d(v, t)^2 - \frac{|v|}{T} d(s, t)^2}$$

where u is the newly joined cluster consisting of clusters s and t, v is an unused cluster in the forest, $T = |v| + |s| + |t|$, and $| * |$ is the cardinality of its argument. This is also known as the incremental algorithm.

Warning: When the minimum distance pair in the forest is chosen, there may be two or more pairs with the same minimum distance. This implementation may choose a different minimum than the MATLAB version.

Parameters: **y : *ndarray***

A condensed distance matrix. A condensed distance matrix is a flat array containing the upper triangular of the distance matrix. This is the form that `pdist` returns. Alternatively, a collection of m observation vectors in n dimensions may be passed as an m by n array. All elements of the condensed distance matrix must be finite, i.e. no NaNs or infs.

method : *str, optional*

The linkage algorithm to use. See the `Linkage Methods` section below for full descriptions.

metric : *str or function, optional*

The distance metric to use in the case that y is a collection of observation vectors; ignored otherwise. See the `pdist` function for a list of valid distance metrics. A custom distance function can also be used.

optimal_ordering : *bool, optional*

If True, the linkage matrix will be reordered so that the distance between successive leaves is minimal. This results in a more intuitive tree structure when the data are visualized. defaults to False, because this algorithm can be slow, particularly on large datasets [2]. See also the **optimal_leaf_ordering** (scipy.cluster.hierarchy.optimal_leaf_ordering.html#scipy.cluster.hierarchy.optimal_leaf_ordering) function.
New in version 1.0.0.

Returns: **Z : *ndarray***

The hierarchical clustering encoded as a linkage matrix.

See also:

**scipy.spatial.distance.pdist
(scipy.spatial.distance.pdist.html#scipy.spatial.distance.pdist)**
pairwise distance metrics

Notes

1. For method ‘single’ an optimized algorithm based on minimum spanning tree is implemented. It has time complexity $O(n^2)$. For methods ‘complete’, ‘average’, ‘weighted’ and ‘ward’ an algorithm called nearest-neighbors chain is implemented. It also has time complexity $O(n^2)$. For other methods a naive algorithm is implemented with $O(n^3)$ time complexity. All algorithms use $O(n^2)$ memory. Refer to [1] for details about the algorithms.
2. Methods ‘centroid’, ‘median’ and ‘ward’ are correctly defined only if Euclidean pairwise metric is used. If *y* is passed as precomputed pairwise distances, then it is a user responsibility to assure that these distances are in fact Euclidean, otherwise the produced result will be incorrect.

References

[1] *(1, 2)* Daniel Mullner, “Modern hierarchical, agglomerative clustering algorithms”, arXiv:1109.2378v1 (https://arxiv.org/abs/1109.2378v1).

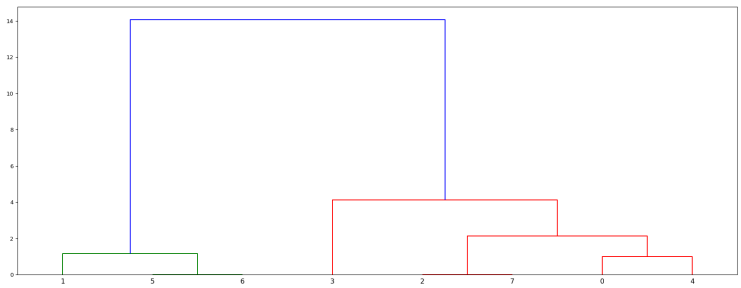
[2] *(1, 2)* Ziv Bar-Joseph, David K. Gifford, Tommi S. Jaakkola, “Fast optimal leaf ordering for hierarchical clustering”, 2001. Bioinformatics DOI:10.1093/bioinformatics/17.suppl_1.S22 (https://doi.org/10.1093/bioinformatics/17.suppl_1.S22)

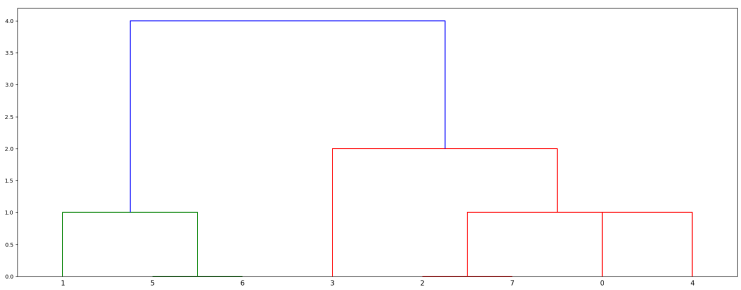
Examples

```
>>> from scipy.cluster.hierarchy import dendrogram, linkage
>>> from matplotlib import pyplot as plt
>>> X = [[i] for i in [2, 8, 0, 4, 1, 9, 9, 0]]
```

```
>>> Z = linkage(X, 'ward')
>>> fig = plt.figure(figsize=(25, 10))
>>> dn = dendrogram(Z)
```

```
>>> Z = linkage(X, 'single')
>>> fig = plt.figure(figsize=(25, 10))
>>> dn = dendrogram(Z)
>>> plt.show()
```





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