Perform hierarchical/agglomerative clustering.

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

If y is a 1-D 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.