Package 'genieclust'

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TypePackageTitleFast and Robust Hierarchical Clustering with Noise Point

Detection

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Description The Genie algorithm

(Gagolewski, 2021 <DOI:10.1016/j.softx.2021.100722>) is a robust and outlier-resistant hierarchical clustering method (Gagolewski, Bartoszuk, Cena, 2016 <DOI:10.1016/j.ins.2016.05.003>). This package features its faster and more powerful version. It allows clustering with respect to mutual reachability distances, enabling it to act as a noise point detector or a version of 'HDBSCAN*' that can identify a predefined number of clusters. The package also features an implementation of the Gini and Bonferroni inequality indices, external cluster validity measures (e.g., the normalised clustering accuracy, the adjusted Rand index, the Fowlkes-Mallows index, and normalised mutual information), and internal cluster validity indices (e.g., the Calinski-Harabasz, Davies-Bouldin, Ball-Hall, Silhouette, and generalised Dunn indices). The 'Python' version of 'genieclust' is available via 'PyPI'.

BugReports https://github.com/gagolews/genieclust/issues

URL https://genieclust.gagolewski.com/,

https://clustering-benchmarks.gagolewski.com/,
https://github.com/gagolews/genieclust

License AGPL-3 Imports Rcpp, stats, utils, quitefastmst Suggests datasets, LinkingTo Rcpp Encoding UTF-8 SystemRequirements OpenMP, C++17 RoxygenNote 7.3.2 NeedsCompilation yes

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Index

cluster_validity Internal Cluster Validity Measures

Description

Implementation of cluster validity indices reviewed in (Gagolewski, Bartoszuk, Cena, 2021). See Section 2 therein for the respective definitions.

The greater the index value, the more *valid* (whatever that means) the assessed partition. For consistency, the Ball-Hall and Davies-Bouldin indexes as well as the within-cluster sum of squares (WCSS) take negative values.

Usage

```
calinski_harabasz_index(X, y)
dunnowa_index(
    X,
    y,
    M = 25L,
    owa_numerator = "SMin:5",
    owa_denominator = "Const"
)
generalised_dunn_index(X, y, lowercase_d, uppercase_d)
negated_ball_hall_index(X, y)
```

```
negated_davies_bouldin_index(X, y)
```

negated_wcss_index(X, y)

silhouette_index(X, y)

silhouette_w_index(X, y)

wcnn_index(X, y, M = 25L)

Arguments

Х	numeric matrix with n rows and d columns, representing n points in a d-dimensional space	
У	vector of n integer labels, representing a partition whose <i>quality</i> is to be assessed; y[i] is the cluster ID of the i-th point, X[i,]; 1 <= y[i] <= K, where K is the number or clusters	
М	number of nearest neighbours	
owa_numerator,owa_denominator		
	single string specifying the OWA operators to use in the definition of the DuNN index; one of: "Mean", "Min", "Max", "Const", "SMin:D", "SMax:D", where D is an integer defining the degree of smoothness	
lowercase_d	an integer between 1 and 5, denoting $d_1,, d_5$ in the definition of the generalised Dunn (Bezdek-Pal) index (numerator: min, max, and mean pairwise intracluster distance, distance between cluster centroids, weighted point-centroid distance, respectively)	
uppercase_d	an integer between 1 and 3, denoting D_1 ,, D_3 in the definition of the gener- alised Dunn (Bezdek-Pal) index (denominator: max and min pairwise intraclus- ter distance, average point-centroid distance, respectively)	

Value

A single numeric value (the more, the *better*).

Author(s)

Marek Gagolewski and other contributors

References

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Calinski, T., Harabasz, J., A dendrite method for cluster analysis, *Communications in Statistics* 3(1), 1974, 1-27, doi:10.1080/03610927408827101.

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Gagolewski, M., Bartoszuk, M., Cena, A., Are cluster validity measures (in)valid?, *Information Sciences* 581, 620-636, 2021, doi:10.1016/j.ins.2021.10.004; preprint: https://raw.githubusercontent.com/gagolews/bibliography/master/preprints/2021cvi.pdf.

Gagolewski, M., A Framework for Benchmarking Clustering Algorithms, *SoftwareX* 20, 2022, 101270, doi:10.1016/j.softx.2022.101270, https://clustering-benchmarks.gagolewski.com.

Rousseeuw, P.J., Silhouettes: A Graphical Aid to the Interpretation and Validation of Cluster Analysis, *Computational and Applied Mathematics* 20, 1987, 53-65, doi:10.1016/03770427(87)901257.

See Also

The official online manual of genieclust at https://genieclust.gagolewski.com/

Gagolewski, M., **genieclust**: Fast and robust hierarchical clustering, *SoftwareX* 15:100722, 2021, doi:10.1016/j.softx.2021.100722

Examples

```
X <- as.matrix(iris[,1:4])
X[,] <- jitter(X) # otherwise we get a non-unique solution
y <- as.integer(iris[[5]])
calinski_harabasz_index(X, y) # good
calinski_harabasz_index(X, sample(1:3, nrow(X), replace=TRUE)) # bad</pre>
```

compare_partitions	External Cluster Validity Measures and Pairwise Partition Similarity
	Scores

Description

The functions described in this section quantify the similarity between two label vectors x and y which represent two partitions of a set of n elements into, respectively, K and L nonempty and pairwise disjoint subsets; for a review, refer to the paper by Gagolewski (2025).

For instance, x and y can represent two clusterings of a dataset with n observations specified by two vectors of labels. The functions described here can be used as external cluster validity measures, where we assume that x is a reference (ground-truth) partition whilst y is the vector of predicted cluster memberships.

All indices except normalized_clustering_accuracy() can act as a pairwise partition similarity score: they are symmetric, i.e., index(x, y) == index(y, x).

Each index except $mi_score()$ (which computes the mutual information score) outputs 1 given two identical partitions. Note that partitions are always defined up to a permutation (bijection) of the set of possible labels, e.g., (1, 1, 2, 1) and (4, 4, 2, 4) represent the same 2-partition.

Usage

```
normalized_clustering_accuracy(x, y = NULL)
normalized_pivoted_accuracy(x, y = NULL)
pair_sets_index(x, y = NULL, simplified = FALSE, clipped = TRUE)
adjusted_rand_score(x, y = NULL, clipped = FALSE)
rand_score(x, y = NULL)
adjusted_fm_score(x, y = NULL, clipped = FALSE)
fm_score(x, y = NULL)
mi_score(x, y = NULL)
normalized_mi_score(x, y = NULL, clipped = FALSE)
normalized_mi_score(x, y = NULL, clipped = FALSE)
normalized_confusion_matrix(x, y = NULL)
normalizing_permutation(x, y = NULL)
```

Arguments

x	an integer vector of length n (or an object coercible to) representing a K-partition of an n-set (e.g., a reference partition), or a confusion matrix with K rows and L columns (see table(x, y))
У	an integer vector of length n (or an object coercible to) representing an L-partition of the same set (e.g., the output of a clustering algorithm we wish to compare with x), or NULL (if x is an $K \times L$ confusion matrix)
simplified	whether to assume E=1 in the definition of the pair sets index index, i.e., use Eq. (20) in (Rezaei, Franti, 2016) instead of Eq. (18)
clipped	whether the result should be clipped to the unit interval, i.e., [0, 1]

Details

normalized_clustering_accuracy() is an asymmetric external cluster validity measure proposed by Gagolewski (2025). It assumes that the label vector x (or rows in the confusion matrix) represents the reference (ground truth) partition. It is the average proportion of correctly classified points in each cluster above the worst case scenario representing the uniform membership assignment, with the cluster ID matching based on the solution to the maximal linear sum assignment problem; see normalized_confusion_matrix). The index is given by: $\max_{\sigma} \frac{1}{K} \sum_{j=1}^{K} \frac{c_{\sigma(j),j} - c_{\sigma(j),.}/K}{c_{\sigma(j),.} - c_{\sigma(j),.}/K}$, where *C* is a confusion matrix with *K* rows and *L* columns, σ is a permutation of the set $\{1, \ldots, \max(K, L)\}$,

and $c_{i,.} = c_{i,1} + ... + c_{i,L}$ is the i-th row sum, under the assumption that $c_{i,j} = 0$ for i > K or j > L and 0/0 = 0.

normalized_pivoted_accuracy() is defined as $(\max_{\sigma} \sum_{j=1}^{\max(K,L)} \frac{c_{\sigma(j),j}/n-1/\max(K,L)}{1-1/\max(K,L)})$, where σ is a permutation of the set $\{1, \ldots, \max(K,L)\}$, and n is the sum of all elements in C. For non-square matrices, missing rows/columns are assumed to be filled with 0s.

pair_sets_index() (PSI) was introduced by Rezaei and Franti (2016). The simplified PSI assumes E=1 in the definition of the index, i.e., uses Eq. (20) in the said paper instead of Eq. (18). For non-square matrices, missing rows/columns are assumed to be filled with 0s.

rand_score() gives the Rand score (the "probability" of agreement between the two partitions) and adjusted_rand_score() is its version corrected for chance (see Hubert, Arabie, 1985): its expected value is 0 given two independent partitions. Due to the adjustment, the resulting index may be negative for some inputs.

Similarly, fm_score() gives the Fowlkes-Mallows (FM) score and adjusted_fm_score() is its adjusted-for-chance version; (see Hubert, Arabie, 1985).

mi_score(), adjusted_mi_score() and normalized_mi_score() are information-theoretic scores, based on mutual information, see the definition of AMI_{sum} and NMI_{sum} in the paper by Vinh et al. (2010).

normalized_confusion_matrix() computes the confusion matrix and permutes its rows and columns so that the sum of the elements of the main diagonal is the largest possible (by solving the maximal assignment problem). The function only accepts $K \leq L$. The reordering of the columns of a confusion matrix can be determined by calling normalizing_permutation().

Also note that the built-in table() function determines the standard confusion matrix.

Value

Each cluster validity measure is a single numeric value.

normalized_confusion_matrix() returns a numeric matrix.

normalizing_permutation() returns a vector of indexes.

Author(s)

Marek Gagolewski and other contributors

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Gagolewski, M., A framework for benchmarking clustering algorithms, *SoftwareX* 20, 2022, 101270, doi:10.1016/j.softx.2022.101270, https://clustering-benchmarks.gagolewski.com.

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Vinh, N.X., Epps, J., Bailey, J., Information theoretic measures for clusterings comparison: Variants, properties, normalization and correction for chance, *Journal of Machine Learning Research* 11, 2010, 2837-2854.

See Also

The official online manual of genieclust at https://genieclust.gagolewski.com/

Gagolewski, M., **genieclust**: Fast and robust hierarchical clustering, *SoftwareX* 15:100722, 2021, doi:10.1016/j.softx.2021.100722

Examples

```
y_true <- iris[[5]]
y_pred <- kmeans(as.matrix(iris[1:4]), 3)$cluster
normalized_clustering_accuracy(y_true, y_pred)
normalized_pivoted_accuracy(y_true, y_pred)
pair_sets_index(y_true, y_pred)
pair_sets_index(y_true, y_pred)
adjusted_rand_score(y_true, y_pred)
rand_score(table(y_true, y_pred)) # the same
adjusted_fm_score(y_true, y_pred)
fm_score(y_true, y_pred)
mi_score(y_true, y_pred)
normalized_mi_score(y_true, y_pred)
adjusted_mi_score(y_true, y_pred)
normalized_confusion_matrix(y_true, y_pred)
normalizing_permutation(y_true, y_pred)
```

gclust

Hierarchical Clustering Algorithm Genie

Description

A reimplementation of *Genie* - a robust and outlier resistant clustering algorithm by Gagolewski, Bartoszuk, and Cena (2016). The Genie algorithm is based on the minimum spanning tree (MST) of the pairwise distance graph of a given point set. Just like the single linkage, it consumes the edges of the MST in an increasing order of weights. However, it prevents the formation of clusters of highly imbalanced sizes; once the Gini index (see gini_index()) of the cluster size distribution raises above gini_threshold, the merging of a point group of the smallest size is enforced.

The clustering can also be computed with respect to the mutual reachability distances (based, e.g., on the Euclidean metric), which is used in the definition of the HDBSCAN* algorithm (see Campello et al., 2013). If M > 1, then the mutual reachability distance m(i, j) with a smoothing factor M is used instead of the chosen "raw" distance d(i, j). It holds $m(i, j) = \max(d(i, j), c(i), c(j))$, where the core distance c(i) is the distance to the *i*-th point's (M - 1)-th nearest neighbour. This makes "noise" and "boundary" points being more "pulled away" from each other.

The Genie correction together with the smoothing factor M > 1 (note that M = 2 corresponds to the original distance) gives a version of the HDBSCAN* algorithm that is able to detect a predefined number of clusters. Hence it does not dependent on the DBSCAN's eps parameter or the HDBSCAN's min_cluster_size one.

Usage

```
gclust(d, ...)
## Default S3 method:
gclust(
  d,
  gini_threshold = 0.3,
  distance = c("euclidean", "12", "manhattan", "cityblock", "11", "cosine"),
  verbose = FALSE,
  . . .
)
## S3 method for class 'dist'
gclust(d, gini_threshold = 0.3, verbose = FALSE, ...)
## S3 method for class 'mst'
gclust(d, gini_threshold = 0.3, verbose = FALSE, ...)
genie(d, ...)
## Default S3 method:
genie(
 d,
 k,
  gini_threshold = 0.3,
  distance = c("euclidean", "12", "manhattan", "cityblock", "11", "cosine"),
 M = 1L.
  postprocess = c("boundary", "none", "all"),
  detect_noise = M > 1L,
  verbose = FALSE,
  . . .
)
## S3 method for class 'dist'
genie(
  d,
  k,
  gini_threshold = 0.3,
 M = 1L,
  postprocess = c("boundary", "none", "all"),
  detect_noise = M > 1L,
  verbose = FALSE,
  . . .
```

gclust

```
)
## S3 method for class 'mst'
genie(
    d,
    k,
    gini_threshold = 0.3,
    postprocess = c("boundary", "none", "all"),
    detect_noise = FALSE,
    verbose = FALSE,
    ...
)
```

Arguments

d	a numeric matrix (or an object coercible to one, e.g., a data frame with numeric- like columns) or an object of class dist (see dist), or an object of class mst (mst)
	further arguments passed to mst()
gini_threshold	threshold for the Genie correction, i.e., the Gini index of the cluster size dis- tribution; threshold of 1.0 leads to the single linkage algorithm; low thresholds highly penalise the formation of small clusters
distance	<pre>metric used to compute the linkage, one of: "euclidean" (synonym: "12"), "manhattan" (a.k.a. "11" and "cityblock"), "cosine"</pre>
verbose	logical; whether to print diagnostic messages and progress information
k	the desired number of clusters to detect, $k=1$ with $M>1\ {\rm acts}$ as a noise point detector
М	smoothing factor; $M \leq 2$ gives the selected distance; otherwise, the mutual reachability distance is used
postprocess	one of "boundary" (default), "none" or "all"; in effect only if $M > 1$. By default, only "boundary" points are merged with their nearest "core" points (A point is a boundary point if it is a noise point and it is amongst its adjacent vertex's $(M - 1)$ -th nearest neighbours). To force a classical k-partition of a data set (with no notion of noise), choose "all"
detect_noise	whether the minimum spanning tree's leaves should be marked as noise points, defaults to TRUE if $M>1$ for compatibility with HDBSCAN*

Details

As in the case of all the distance-based methods, the standardisation of the input features is definitely worth giving a try. Oftentimes, more sophisticated feature engineering (e.g., dimensionality reduction) will lead to more meaningful results.

If d is a numeric matrix or an object of class dist, mst() will be called to compute an MST, which generally takes at most $O(n^2)$ time. However, by default, a faster algorithm based on K-d trees is selected automatically for low-dimensional Euclidean spaces; see mst_euclid from the **quitefastmst** package.

Once a minimum spanning tree is determined, the Genie algorithm runs in $O(n\sqrt{n})$ time. If you want to test different gini_thresholds or ks, it is best to compute the MST first explicitly.

According to the algorithm's original definition, the resulting partition tree (dendrogram) might violate the ultrametricity property (merges might occur at levels that are not increasing w.r.t. a between-cluster distance). gclust() automatically corrects departures from ultrametricity by applying height = rev(cummin(rev(height))).

Value

gclust() computes the entire clustering hierarchy; it returns a list of class hclust; see hclust. Use cutree to obtain an arbitrary k-partition.

genie() returns a k-partition - a vector whose i-th element denotes the i-th input point's cluster label between 1 and k If detect_noise is TRUE, missing values (NA) denote noise points.

Author(s)

Marek Gagolewski and other contributors

References

Gagolewski, M., Bartoszuk, M., Cena, A., Genie: A new, fast, and outlier-resistant hierarchical clustering algorithm, *Information Sciences* 363, 2016, 8-23, doi:10.1016/j.ins.2016.05.003

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Gagolewski, M., Cena, A., Bartoszuk, M., Brzozowski, L., Clustering with minimum spanning trees: How good can it be?, *Journal of Classification* 42, 2025, 90-112, doi:10.1007/s00357024-094831

See Also

The official online manual of genieclust at https://genieclust.gagolewski.com/

Gagolewski, M., **genieclust**: Fast and robust hierarchical clustering, *SoftwareX* 15:100722, 2021, doi:10.1016/j.softx.2021.100722

mst() for the minimum spanning tree routines

normalized_clustering_accuracy() (amongst others) for external cluster validity measures

Examples

```
library("datasets")
data("iris")
X <- jitter(as.matrix(iris[2:3]))
h <- gclust(X)
y_pred <- cutree(h, 3)
y_test <- as.integer(iris[,5])
plot(X, col=y_pred, pch=y_test, asp=1, las=1)
adjusted_rand_score(y_test, y_pred)
normalized_clustering_accuracy(y_test, y_pred)</pre>
```

inequality

```
y_pred2 <- genie(X, 3, M=5) # clustering wrt 5-mutual reachability distance
plot(X[,1], X[,2], col=y_pred2, pch=y_test, asp=1, las=1)
noise <- is.na(y_pred2) # noise/boundary points
points(X[noise, ], col="gray", pch=10)
normalized_clustering_accuracy(y_test[!noise], y_pred2[!noise])</pre>
```

inequality

Inequality Measures

Description

gini_index() gives the normalised Gini index, bonferroni_index() implements the Bonferroni index, and devergottini_index() implements the De Vergottini index.

Usage

gini_index(x)

bonferroni_index(x)

devergottini_index(x)

Arguments

Х

numeric vector of non-negative values

Details

These indices can be used to quantify the "inequality" of a sample. They can be conceived as normalised measures of data dispersion. For constant vectors (perfect equity), the indices yield values of 0. Vectors with all elements but one equal to 0 (perfect inequality), are assigned scores of 1. They follow the Pigou-Dalton principle (are Schur-convex): setting $x_i = x_i - h$ and $x_j = x_j + h$ with h > 0 and $x_i - h \ge x_j + h$ (taking from the "rich" and giving to the "poor") decreases the inequality.

These indices have applications in economics, amongst others. The Genie clustering algorithm uses the Gini index as a measure of the inequality of cluster sizes.

The normalised Gini index is given by:

$$G(x_1,\ldots,x_n) = \frac{\sum_{i=1}^n (n-2i+1)x_{\sigma(n-i+1)}}{(n-1)\sum_{i=1}^n x_i}.$$

The normalised Bonferroni index is given by:

$$B(x_1,\ldots,x_n) = \frac{\sum_{i=1}^n (n - \sum_{j=1}^i \frac{n}{n-j+1}) x_{\sigma(n-i+1)}}{(n-1) \sum_{i=1}^n x_i}.$$

inequality

The normalised De Vergottini index is given by:

$$V(x_1, \dots, x_n) = \frac{1}{\sum_{i=2}^n \frac{1}{i}} \left(\frac{\sum_{i=1}^n \left(\sum_{j=i}^n \frac{1}{j} \right) x_{\sigma(n-i+1)}}{\sum_{i=1}^n x_i} - 1 \right)$$

Here, σ is an ordering permutation of (x_1, \ldots, x_n) .

Value

The value of the inequality index, a number in [0, 1].

Author(s)

Marek Gagolewski and other contributors

References

Bonferroni, C., Elementi di Statistica Generale, Libreria Seber, Firenze, 1930.

Gini, C., Variabilita e Mutabilita, Tipografia di Paolo Cuppini, Bologna, 1912.

See Also

The official online manual of genieclust at https://genieclust.gagolewski.com/

Gagolewski, M., **genieclust**: Fast and robust hierarchical clustering, *SoftwareX* 15:100722, 2021, doi:10.1016/j.softx.2021.100722

Examples

```
gini_index(c(2, 2, 2, 2, 2, 2)) # no inequality
gini_index(c(0, 0, 10, 0, 0)) # one has it all
gini_index(c(7, 0, 3, 0, 0)) # give to the poor, take away from the rich
gini_index(c(6, 0, 3, 1, 0)) # (a.k.a. the Pigou-Dalton principle)
bonferroni_index(c(2, 2, 2, 2, 2, 2))
bonferroni_index(c(0, 0, 10, 0, 0))
bonferroni_index(c(7, 0, 3, 0, 0))
bonferroni_index(c(6, 0, 3, 1, 0))
devergottini_index(c(2, 2, 2, 2, 2, 2))
devergottini_index(c(7, 0, 3, 0, 0))
devergottini_index(c(7, 0, 3, 0, 0))
devergottini_index(c(7, 0, 3, 0, 0))
```

Description

Determine a(*) minimum spanning tree (MST) of the complete undirected graph representing a set of n points whose weights correspond to the pairwise distances between the points.

Usage

```
mst(d, ...)
## Default S3 method:
mst(
    d,
    distance = c("euclidean", "l2", "manhattan", "cityblock", "l1", "cosine"),
    M = 1L,
    verbose = FALSE,
    ...
)
## S3 method for class 'dist'
```

mst(d, M = 1L, verbose = FALSE, ...)

Arguments

d	either a numeric matrix (or an object coercible to one, e.g., a data frame with numeric-like columns) or an object of class dist; see dist
	further arguments passed to or from other methods, in particular, to mst_euclid from the quitefastmst package
distance	<pre>metric used in the case where d is a matrix; one of: "euclidean" (synonym: "12"), "manhattan" (a.k.a. "11" and "cityblock"), "cosine"</pre>
М	smoothing factor; M = 1 selects the requested distance; otherwise, the corresponding degree-M mutual reachability distance is used; M should be rather small, say, ≤ 20
verbose	logical; whether to print diagnostic messages and progress information

Details

(*) Note that if the distances are non unique, there might be multiple minimum trees spanning a given graph.

If d is a matrix and the use of Euclidean distance is requested (the default), then mst_euclid is called to determine the MST. It is quite fast in spaces of low intrinsic dimensionality, even for 10M points.

Otherwise, a much slower implementation of the Jarník (Prim/Dijkstra)-like method, which requires $O(n^2)$ time, is used. The algorithm is parallelised; the number of threads is determined by the

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mst

OMP_NUM_THREADS environment variable. As a rule of thumb, datasets up to 100k points should be processed relatively quickly.

If M > 1, then the mutual reachability distance m(i, j) with the smoothing factor M (see Campello et al. 2013) is used instead of the chosen "raw" distance d(i, j). It holds $m(i, j) = \max\{d(i, j), c(i), c(j)\}$, where c(i) is the core distance, i.e., the distance between the *i*-th point and its (M-1)-th nearest neighbour. This makes "noise" and "boundary" points being "pulled away" from each other. The Genie clustering algorithm (see gclust) with respect to the mutual reachability distance can mark some observations as noise points.

Value

Returns a numeric matrix of class mst with n-1 rows and three columns: from, to, and dist sorted nondecreasingly. Its i-th row specifies the i-th edge of the MST which is incident to the vertices from[i] and to[i] with from[i] < to[i] (in 1,...,n) and dist[i] gives the corresponding weight, i.e., the distance between the point pair.

The Size attribute specifies the number of points, n. The Labels attribute gives the labels of the input points, if available. The method attribute provides the name of the distance function used.

If M > 1, the nn.index attribute gives the indices of the M-1 nearest neighbours of each point and nn.dist provides the corresponding distances, both in the form of an n by M - 1 matrix.

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See Also

The official online manual of genieclust at https://genieclust.gagolewski.com/

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mst

mst_euclid

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