# Package 'genieclust'

January 17, 2023

```
Title Fast and Robust Hierarchical Clustering with Noise Points
Version 1.1.3
Date 2023-01-17
Description A retake on the Genie algorithm
      (Gagolewski, 2021 < DOI:10.1016/j.softx.2021.100722>) - a robust
      hierarchical clustering method
      (Gagolewski, Bartoszuk, Cena, 2016 < DOI:10.1016/j.ins.2016.05.003 > ).
      Now faster and more memory efficient; determining the whole hierarchy
      for datasets of 10M points in low dimensional Euclidean spaces or
      100K points in high-dimensional ones takes only 1-2 minutes.
      Allows clustering with respect to mutual reachability distances
      so that it can act as a noise point detector or a robustified version of
      'HDBSCAN*' (that is able to detect a predefined number of
      clusters and hence it does not dependent on the somewhat
      fragile 'eps' parameter).
      The package also features an implementation of economic inequity indices
      (the Gini, Bonferroni index), external cluster validity measures
      (e.g., the adjusted asymmetric accuracy and partition similarity scores
      such as the adjusted Rand, Fowlkes-Mallows, adjusted mutual information,
      and pair sets indices),
      and internal cluster validity indices (e.g., the Calinski-Harabasz,
      Davies-Bouldin, Ball-Hall, Silhouette, and generalised Dunn indices).
      See also the 'Python' version of 'genieclust' available on 'PyPI', which
      supports sparse data, more metrics, and even larger datasets.
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 (>= 1.0.4), stats, utils
```

Type Package

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```
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 genieclust-package
               The Genie Hierarchical Clustering Algorithm (with Extras)
Description
  See genie() for more details.
Author(s)
  Marek Gagolewski and other contributors
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.

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cluster\_validity

Internal Cluster Validity Measures

# **Description**

Implementation of a number of so-called cluster validity indices critically reviewed in (Gagolewski, Bartoszuk, Cena, 2021). See Section 2 therein and (Gagolewski, 2022) 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_index(X, y)

wcnn_index(X, y, M = 25L)
```

# **Arguments**

X	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, $X[i, ]; 1 \le y[i] \le K$ , where K is the number or clusters

M number of nearest neighbours

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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.

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

Ball G.H., Hall D.J., *ISODATA: A novel method of data analysis and pattern classification*, Technical report No. AD699616, Stanford Research Institute, 1965.

Bezdek J., Pal N., Some new indexes of cluster validity, *IEEE Transactions on Systems, Man, and Cybernetics, Part B* 28, 1998, 301-315, doi:10.1109/3477.678624.

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

Davies D.L., Bouldin D.W., A Cluster Separation Measure, *IEEE Transactions on Pattern Analysis and Machine Intelligence* PAMI-1 (2), 1979, 224-227, doi:10.1109/TPAMI.1979.4766909.

Dunn J.C., A Fuzzy Relative of the ISODATA Process and Its Use in Detecting Compact Well-Separated Clusters, *Journal of Cybernetics* 3(3), 1973, 32-57, doi:10.1080/01969727308546046.

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.

 $Gagolewski\ M., A\ Framework for\ Benchmarking\ Clustering\ Algorithms, 2022, \verb|https://clustering-benchmarks.gagolewski.com|.$ 

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.

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## **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  $\mathbf{x}$  and  $\mathbf{y}$  which represent two partitions of a set of n elements into, respectively, K and L nonempty and pairwise disjoint subsets.

For instance, x and y can be two clusterings of a dataset with n observations specified by two vectors of labels. These functions can be used as external cluster validity measures, where we assume that x is the reference (ground-truth) partition (compare Gagolewski, 2022).

```
adjusted_asymmetric_accuracy(x, y = NULL)
normalized_accuracy(x, y = NULL)
pair_sets_index(x, y = NULL, simplified = FALSE)
adjusted_rand_score(x, y = NULL)
rand_score(x, y = NULL)
adjusted_fm_score(x, y = NULL)
fm_score(x, y = NULL)
mi_score(x, y = NULL)
normalized_mi_score(x, y = NULL)
normalized_mi_score(x, y = NULL)
normalized_confusion_matrix(x, y = NULL)
normalizing_permutation(x, y = NULL)
```

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## **Arguments**

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))

y 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\*L confusion matrix)

simplified whether to assume E=1 in the definition of the pair sets index index, i.e., use Eq. (20) instead of (18); see (Rezaei, Franti, 2016).

#### **Details**

Each index except adjusted\_asymmetric\_accuracy() can act as a pairwise partition similarity score: it is 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 bijection of the set of possible labels, e.g., (1, 1, 2, 1) and (4, 4, 2, 4) represent the same 2-partition.

adjusted\_asymmetric\_accuracy() (Gagolewski, 2022) is an external cluster validity measure which assumes that the label vector x (or rows in the confusion matrix) represents the reference (ground truth) partition. It is a corrected-for-chance summary of the proportion of correctly classified points in each cluster (with cluster matching based on the solution to the maximal linear sum assignment problem; see normalized\_confusion\_matrix), given by:  $(\max_{\sigma} \sum_{i=1}^{K} (c_{i,\sigma(i)}/(c_{i,1} + ... + c_{i,K})) - 1)/(K-1)$ , where C is the confusion matrix.

normalized\_accuracy() is defined as  $(Accuracy(C_{\sigma}) - 1/max(K,L))/(1 - 1/max(K,L))$ , where  $C_{\sigma}$  is a version of the confusion matrix for given x and y with columns permuted based on the solution to the maximal linear sum assignment problem. The  $Accuracy(C_{\sigma})$  part is sometimes referred to as set-matching classification rate or pivoted accuracy.

pair\_sets\_index() gives the Pair Sets Index (PSI) adjusted for chance (Rezaei, Franti, 2016). Pairing is based on the solution to the linear sum assignment problem of a transformed version of the confusion matrix. Its simplified version assumes E=1 in the definition of the index, i.e., uses Eq. (20) instead of (18).

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 0.0 given two independent partitions. Due to the adjustment, the resulting index might also 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).

Note that both the (unadjusted) Rand and FM scores are bounded from below by 1/(K+1) if K=L, hence their adjusted versions are preferred.

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 (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 sole reordering of the columns of a confusion matrix can be determined by calling normalizing\_permutation().

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

#### Value

Each cluster validity measure is a single numeric value.

normalized\_confusion\_matrix() returns an integer matrix.

#### Author(s)

Marek Gagolewski and other contributors

#### References

Gagolewski M., A Framework for Benchmarking Clustering Algorithms, 2022, https://clustering-benchmarks.gagolewski.com.

Gagolewski M., Adjusted asymmetric accuracy: A well-behaving external cluster validity measure, 2022, under review (preprint), doi:10.48550/arXiv.2209.02935.

Hubert L., Arabie P., Comparing partitions, *Journal of Classification* 2(1), 1985, 193-218, esp. Eqs. (2) and (4).

Meila M., Heckerman D., An experimental comparison of model-based clustering methods, *Machine Learning* 42, 2001, pp. 9-29, doi:10.1023/A:1007648401407.

Rezaei M., Franti P., Set matching measures for external cluster validity, *IEEE Transactions on Knowledge and Data Mining* 28(8), 2016, 2173-2186.

Steinley D., Properties of the Hubert-Arabie adjusted Rand index, *Psychological Methods* 9(3), 2004, pp. 386-396, doi:10.1037/1082989X.9.3.386.

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
adjusted_asymmetric_accuracy(y_true, y_pred)
normalized_accuracy(y_true, y_pred)
pair_sets_index(y_true, y_pred)
pair_sets_index(y_true, y_pred, simplified=TRUE)
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)</pre>
```

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```
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)
```

emst\_mlpack

Euclidean Minimum Spanning Tree

# **Description**

Provides access to the implementation of the Dual-Tree Boruvka algorithm from the mlpack package (if available). It is based on kd-trees and is fast for (very) low-dimensional Euclidean spaces. For higher dimensional spaces (say, over 5 features) or other metrics, use the parallelised Prim-like algorithm implemented in mst().

## Usage

```
emst_mlpack(X, leaf_size = 1, naive = FALSE, verbose = FALSE)
```

## **Arguments**

X a numeric matrix (or an object coercible to one, e.g., a data frame with numeric-

like columns)

leaf\_size size of leaves in the kd-tree, controls the trade-off between speed and memory

consumption

naive logical; whether to use the naive, quadratic-time algorithm

verbose logical; whether to print diagnostic messages

## Value

An object of class mst, see mst() for details.

# Author(s)

Marek Gagolewski and other contributors

#### References

March W.B., Ram P., Gray A.G., Fast Euclidean Minimum Spanning Tree: Algorithm, Analysis, and Applications, *Proc. ACM SIGKDD'10*, 2010, 603-611, https://mlpack.org/papers/emst.pdf.

Curtin R.R., Edel M., Lozhnikov M., Mentekidis Y., Ghaisas S., Zhang S., mlpack 3: A fast, flexible machine learning library, *Journal of Open Source Software* 3(26), 2018, 726.

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#### 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.

gclust

Hierarchical Clustering Algorithm Genie

#### **Description**

A reimplementation of *Genie* - a robust and outlier resistant clustering algorithm (see Gagolewski, Bartoszuk, Cena, 2016). The Genie algorithm is based on a 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, a forced merge of a point group of the smallest size is performed. Its appealing simplicity goes hand in hand with its usability; Genie often outperforms other clustering approaches on benchmark data, such as https://github.com/gagolews/clustering-benchmarks.

The clustering can now also be computed with respect to the mutual reachability distance (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 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 c(i) is d(i,k) with k being the (M-1)-th nearest neighbour of i. This makes "noise" and "boundary" points being "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 robustified version of the HDBSCAN\* algorithm that is able to detect a predefined number of clusters. Hence it does not dependent on the DBSCAN's somewhat magical eps parameter or the HDBSCAN's min\_cluster\_size one.

```
gclust(d, ...)
## Default S3 method:
gclust(
    d,
    gini_threshold = 0.3,
    distance = c("euclidean", "12", "manhattan", "cityblock", "11", "cosine"),
    cast_float32 = TRUE,
    verbose = FALSE,
    ...
)

## S3 method for class 'dist'
gclust(d, gini_threshold = 0.3, verbose = FALSE, ...)
```

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```
## S3 method for class 'mst'
gclust(d, gini_threshold = 0.3, verbose = FALSE, ...)
genie(d, ...)
## Default S3 method:
genie(
 d,
  gini_threshold = 0.3,
  distance = c("euclidean", "12", "manhattan", "cityblock", "11", "cosine"),
  postprocess = c("boundary", "none", "all"),
  detect_noise = M > 1L,
  cast_float32 = TRUE,
  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,
)
## 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, see mst().

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... further arguments passed to other methods.

gini\_threshold threshold for the Genie correction, i.e., the Gini index of the cluster size distri-

bution; Threshold of 1.0 disables the correction. Low thresholds highly penalise

the formation of small clusters.

distance metric used to compute the linkage, one of: "euclidean" (synonym: "12"),

"manhattan" (a.k.a. "11" and "cityblock"), "cosine".

cast\_float32 logical; whether to compute the distances using 32-bit instead of 64-bit precision

floating-point arithmetic (up to 2x faster).

verbose logical; whether to print diagnostic messages and progress information.

k the desired number of clusters to detect, k = 1 with M > 1 acts as a noise point

detector.

M smoothing factor; M <= 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's amongst its adjacent vertex's M-1 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**

Note that, as in the case of all the distance-based methods, the standardisation of the input features is definitely worth giving a try.

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 (the algorithm we provide is parallelised, environment variable OMP\_NUM\_THREADS controls the number of threads in use). However, see emst\_mlpack() for a very fast alternative in the case of Euclidean spaces of (very) low dimensionality and M = 1.

Given an minimum spanning tree, the algorithm runs in  $O(n\sqrt{n})$  time. Therefore, if you want to test different gini\_thresholds, (or ks), it is best to explicitly compute the MST first.

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). Departures from ultrametricity are corrected by applying height = rev(cummin(rev(height))).

#### Value

gclust() computes the whole 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 with elements in 1,...,k, whose i-th element denotes the i-th input point's cluster identifier. Missing values (NA) denote noise points (if detect\_noise is TRUE).

# Author(s)

Marek Gagolewski and other contributors

inequity inequity

## 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.

Campello R.J.G.B., Moulavi D., Sander J., Density-based clustering based on hierarchical density estimates, *Lecture Notes in Computer Science* 7819, 2013, 160-172, doi:10.1007/978364237456-2\_14.

#### 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.

adjusted\_rand\_score() (amongst others) for external cluster validity measures (partition similarity scores).

## **Examples**

inequity

Inequity (Inequality) Measures

#### **Description**

gini\_index() gives the normalised Gini index, bonferroni\_index() implements the Bonferroni index, and devergottini\_index() implements the De Vergottini index.

```
gini_index(x)
bonferroni_index(x)
devergottini_index(x)
```

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# **Arguments**

Х

numeric vector of non-negative values

#### **Details**

These indices can be used to quantify the "inequity" of a numeric sample. They can be perceived as 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 inequity), 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  $x_i-h\geq x_j+h$  (taking from the "rich" and giving to the "poor") decreases the inequity.

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:

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

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,  $\sigma$  is an ordering permutation of  $(x_1, \ldots, x_n)$ .

Time complexity: O(n) for sorted (increasingly) data. Otherwise, the vector will be sorted.

## Value

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

#### Author(s)

Marek Gagolewski and other contributors

# References

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

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

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

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## 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**

mst

Minimum Spanning Tree of the Pairwise Distance Graph

# **Description**

An parallelised implementation of a Jarnik (Prim/Dijkstra)-like algorithm for determining a(\*) minimum spanning tree (MST) of a complete undirected graph representing a set of n points with weights given by a pairwise distance matrix.

(\*) Note that there might be multiple minimum trees spanning a given graph.

```
mst(d, ...)
## Default S3 method:
mst(
    d,
    distance = c("euclidean", "12", "manhattan", "cityblock", "11", "cosine"),
    M = 1L,
    cast_float32 = TRUE,
    verbose = FALSE,
    ...
)

## S3 method for class 'dist'
mst(d, M = 1L, verbose = FALSE, ...)
```

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# **Arguments**

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
 metric used to compute the linkage, one of: "euclidean" (synonym: "12"), "manhattan" (a.k.a. "11" and "cityblock"), "cosine"
 smoothing factor; M = 1 gives the selected distance; otherwise, the mutual reachability distance is used
 logical; whether to compute the distances using 32-bit instead of 64-bit precision floating-point arithmetic (up to 2x faster)
 verbose

#### **Details**

If d is a numeric matrix of size np, the n(n-1)/2 distances are computed on the fly, so that O(nM) memory is used.

The algorithm is parallelised; set the OMP\_NUM\_THREADS environment variable Sys.setenv to control the number of threads used.

Time complexity is  $O(n^2)$  for the method accepting an object of class dist and  $O(pn^2)$  otherwise.

If M>= 2, then the mutual reachability distance m(i,j) with 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 d(i,k) with k being the (M-1)-th nearest neighbour of i. This makes "noise" and "boundary" points being "pulled away" from each other. Genie++ clustering algorithm (see gclust) with respect to the mutual reachability distance gains the ability to identify some observations are noise points.

Note that the case M = 2 corresponds to the original distance, but we are determining the 1-nearest neighbours separately as well, which is a bit suboptimal; you can file a feature request if this makes your data analysis tasks too slow.

# Value

Matrix of class mst with n-1 rows and 3 columns: from, to and dist. It holds from < to. Moreover, dist is sorted nondecreasingly. The i-th row gives the i-th edge of the MST. (from[i], to[i]) defines the vertices (in 1,...,n) and dist[i] gives the weight, i.e., the distance between the corresponding points.

The method attribute gives the name of the distance used. The Labels attribute gives the labels of all the input points.

If M > 1, the nn attribute gives the indices of the M-1 nearest neighbours of each point.

#### Author(s)

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16 mst

## References

Jarnik V., O jistem problemu minimalnim, *Prace Moravske Prirodovedecke Spolecnosti* 6, 1930, 57-63.

Olson C.F., Parallel algorithms for hierarchical clustering, *Parallel Comput.* 21, 1995, 1313-1325.

Prim R., Shortest connection networks and some generalisations, *Bell Syst. Tech. J.* 36, 1957, 1389-1401.

Campello R.J.G.B., Moulavi D., Sander J., Density-based clustering based on hierarchical density estimates, *Lecture Notes in Computer Science* 7819, 2013, 160-172, doi:10.1007/978364237456-2\_14.

#### 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.

 $emst_mlpack()$  for a very fast alternative in case of (very) low-dimensional Euclidean spaces (and M = 1).

# **Examples**

```
library("datasets")
data("iris")
X <- iris[1:4]
tree <- mst(X)</pre>
```

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