# Package 'poem'

July 18, 2025

Title POpulation-based Evaluation Metrics

# Version 1.1.2

#### Description

This package provides a comprehensive set of external and internal evaluation metrics. It includes metrics for assessing partitions or fuzzy partitions derived from clustering results, as well as for evaluating

subpopulation identification results within embeddings or graph representations. Addition-

ally, it provides metrics for

comparing spatial domain detection results against ground truth labels, and tools for visualizing spatial errors.

#### BugReports https://github.com/RoseYuan/poem/issues

License GPL (>= 3)

#### URL https://roseyuan.github.io/poem/

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```

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.check\_duplicated\_samples

Check Duplicated Samples

### Description

Checks for duplicated samples in matrix X.

# Usage

```
.check_duplicated_samples(X, threshold = 1e-09)
```

### Arguments

Х	Numeric matrix of samples.
threshold	Numeric, the distance threshold to consider samples as duplicates.

### Value

None

.compute\_cluster\_core\_distance Compute Cluster Core Distance

# Description

Computes the core distance for each point in a cluster.

### Usage

.compute\_cluster\_core\_distance(dists, d)

#### Arguments

dists	Numeric matrix of distances.
d	Integer, the dimensionality.

# Value

Numeric vector of core distances for each point.

.compute\_cross\_dists Compute Cross Distances

### Description

Computes the cross distances between two sets of indices in matrix X.

### Usage

```
.compute_cross_dists(X, inds_a, inds_b, distance)
```

### Arguments

Х	Numeric matrix of samples.
inds_a	Integer vector of indices for the first set.
inds_b	Integer vector of indices for the second set.
distance	String specifying the distance metric.

#### Value

Numeric matrix of cross distances.

.compute\_mutual\_reach\_dists

Compute Mutual Reachability Distances

### Description

Computes the mutual reachability distances between points.

### Usage

```
.compute_mutual_reach_dists(dists, d)
```

# Arguments

dists	Numeric matrix of distances.
d	Float, the dimensionality.

### Value

A list containing core distances and mutual reachability distances.

.compute\_pair\_to\_pair\_dists

Compute Pair to Pair Distances

### Description

Compute the pairwise distances between points in matrix X.

### Usage

```
.compute_pair_to_pair_dists(X, distance = "euclidean")
```

### Arguments

Х	Numeric matrix.
distance	String specifying the metric to compute the distances.

#### Value

Numeric matrix of pairwise distances with self-distances set to Inf.

.convert\_singleton\_clusters\_to\_noise Convert Singleton Clusters to Noise

# Description

Converts clusters containing a single instance to noise.

### Usage

```
.convert_singleton_clusters_to_noise(labels, noise_id)
```

# Arguments

labels	Integer vector of cluster IDs.
noise_id	Integer, the ID for noise.

### Value

Integer vector with singleton clusters converted to noise.

```
.fn_density_separation
```

```
Density Separation of a Pair of Clusters
```

### Description

Computes the density separation between two clusters.

### Usage

```
.fn_density_separation(
    cls_i,
    cls_j,
    dists,
    internal_core_dists_i,
    internal_core_dists_j
)
```

### Arguments

cls_i	Integer, first cluster index.
cls_j	Integer, second cluster index.
dists internal_core_c	Numeric matrix of distances. lists_i
	Numeric vector of core distances for cluster i.
internal_core_c	lists_j
	Numeric vector of core distances for cluster j.

# Value

A list containing the cluster indices and their density separation.

```
.fn_density_sparseness
```

Density Sparseness of a Cluster

### Description

Computes the density sparseness for a given cluster.

### Usage

```
.fn_density_sparseness(cls_inds, dists, d, use_igraph_mst)
```

### Arguments

cls_inds	Integer vector of cluster indices.
dists	Numeric matrix of distances.
d	Integer, the dimensionality.
use_igraph_mst	Logical flag to use MST implementation in igraph. Currently only mst from
	igraph is implemented.

### Value

A list containing the density sparseness, internal core distances, and internal node indices.

.get\_internal\_objects Get Internal Objects

# Description

Computes the internal nodes and edges using Minimum Spanning Tree.

#### Usage

```
.get_internal_objects(mutual_reach_dists, use_igraph_mst = TRUE)
```

#### Arguments

mutual_reach_di	sts
	Numeric matrix representing mutual reachability distances.
use_igraph_mst	Logical flag to use MST implementation in igraph. Currently only mst from igraph is implemented.

# Value

A list containing the indices of internal nodes and their edge weights.

.get_submatrix	Get Sub matrix		
----------------	----------------	--	--

#### Description

Extract a sub matrix from a matrix based on optional row and column indices.

### Usage

```
.get_submatrix(arr, inds_a = NULL, inds_b = NULL)
```

### Arguments

arr	Numeric matrix.
inds_a	Optional integer vector for row indices.
inds_b	Optional integer vector for column indices.

# Value

Numeric matrix representing the sub matrix.

#### CDbw

# Description

Computes the CDbw-index (Halkidi and Vazirgiannis 2008; Halkidi, Vazirgiannis and Hennig, 2015). This function is directly copied from the fpc CRAN package and was written by Christian Hennig. It is included here to reduce the package dependencies (since fpc has a few not-so-light dependencies that aren't required here).

### Usage

```
CDbw(
    x,
    labels,
    r = 10,
    s = seq(0.1, 0.8, by = 0.1),
    clusterstdev = TRUE,
    trace = FALSE
)
```

### Arguments

x	Something that can be coerced into a numerical matrix, with elements as rows.
labels	A vector of integers with length =nrow(x) indicating the cluster for each observation.
r	Number of cluster border representatives.
S	Vector of shrinking factors.
clusterstdev	Logical. If TRUE, the neighborhood radius for intra-cluster density is the within- cluster estimated squared distance from the mean of the cluster; otherwise it is the average of these over all clusters.
trace	Logical; whether to print processing info.

#### Value

A vector with the following values (see refs for details):

cdbw	value of CDbw index (the higher the better).
cohesion	cohesion.
compactness	compactness.
sep	separation.

### Author(s)

Christian Hennig

#### CHAOS

#### References

Halkidi, M. and Vazirgiannis, M. (2008) A density-based cluster validity approach using multi-representatives. Pattern Recognition Letters 29, 773-786.

Halkidi, M., Vazirgiannis, M. and Hennig, C. (2015) Method-independent indices for cluster validation. In C. Hennig, M. Meila, F. Murtagh, R. Rocci (eds.) Handbook of Cluster Analysis, CRC Press/Taylor & Francis, Boca Raton.

#### Examples

```
d1 <- mockData()
CDbw(d1[,seq_len(2)], d1[,3])</pre>
```

CHAOS

Calculate CHAOS score

#### Description

CHAOS score measures the clustering performance by calculating the mean length of the graph edges in the 1-nearest neighbor (1NN) graph for each cluster, averaged across clusters. Lower CHAOS score indicates better spatial domain clustering performance.

#### Usage

CHAOS(labels, location, BNPARAM = NULL)

#### Arguments

labels	Cluster labels.
location	A numeric data matrix containing location information, where rows are points and columns are location dimensions.
BNPARAM	BNPARAM object passed to findKNN specifying the kNN approximation method to use. Defaults to exact for small datasets, and Annoy for larger ones.

# Value

A numeric value for CHAOS score.

#### Examples

```
data(sp_toys)
data <- sp_toys
CHAOS(data$label, data[,c("x", "y")])
CHAOS(data$p1, data[,c("x", "y")])
CHAOS(data$p2, data[,c("x", "y")])</pre>
```

### Description

Compute the DBCV (Density-Based Clustering Validation) metric.

# Usage

```
dbcv(
 X,
 labels,
 distance = "euclidean",
 noise_id = -1,
 check_duplicates = FALSE,
 use_igraph_mst = TRUE,
 BPPARAM = BiocParallel::SerialParam(),
 ...
```

### Arguments

Х	Numeric matrix of samples.	
labels	Integer vector of cluster IDs.	
distance	String specifying the distance metric. "sqeuclidean", or possible method in stats::dist(). By default "euclidean".	
noise_id	Integer, the cluster ID in y for noise (default -1).	
check_duplicates		
	Logical flag to check for duplicate samples.	
use_igraph_mst	Logical flag to use igraph's MST implementation. Currently only mst from igraph is implemented.	
BPPARAM	BiocParallel params for multithreading (default none)	
	Ignored	

#### Details

This implementation will not fully reproduce the results of other existing implementations (e.g. https://github.com/FelSiq/DBCV) due to the different algorithms used for computing the Minimum Spanning Tree.

### Value

A list:	
VCS	Numeric vector of validity index for each cluster.
dbcv	Numeric value representing the overall DBCV metric.

### References

Davoud Moulavi, et al. 2014; 10.1137/1.9781611973440.96.

# dbcv

### ELSA

### Examples

```
data(noisy_moon)
data <- noisy_moon
dbcv(data[, c("x", "y")], data$kmeans_label)
dbcv(data[, c("x", "y")], data$hdbscan_label)</pre>
```

ELSA

#### Calculate ELSA scores

### Description

Calculating the Entropy-based Local indicator of Spatial Association (ELSA) scores, which consist of Ea, Ec and the overall ELSA.

### Usage

ELSA(labels, location, k = 10)

### Arguments

labels	Cluster labels.
location	A numerical matrix containing the location information, with rows as samples and columns as location dimensions.
k	Number of nearest neighbors.

#### Value

A dataframe containing the Ea, Ec and ELSA for all samples in the dataset.

### References

Naimi, Babak, et al., 2019; 10.1016/j.spasta.2018.10.001

# Examples

```
data(sp_toys)
data <- sp_toys
ELSA(data$label, data[,c("x", "y")], k=6)
ELSA(data$p1, data[,c("x", "y")], k=6)
ELSA(data$p2, data[,c("x", "y")], k=6)</pre>
```

emb2knn

### Description

Computes k nearest neighbors from embedding.

### Usage

```
emb2knn(x, k, BNPARAM = NULL)
```

### Arguments

х	A numeric matrix (with features as columns and items as rows) from which nearest neighbors will be computed.
k	The number of nearest neighbors.
BNPARAM	A BiocNeighbors parameter object to compute kNNs. Ignored unless the input is a matrix or data.frame. If omitted, the Annoy approximation will be used if there are more than 500 elements.

### Value

A knn list.

# Examples

d1 <- mockData()
emb2knn(as.matrix(d1[,seq\_len(2)]),k=5)</pre>

emb2snn

Computes shared nearest neighbors from embedding

### Description

computes shared nearest neighbors from embedding.

# Usage

```
emb2snn(x, k, type = "rank", BNPARAM = NULL)
```

# Arguments

x	A numeric matrix (with features as columns and items as rows) from which nearest neighbors will be computed.
k	The number of nearest neighbors.
type	A string specifying the type of weighting scheme to use for shared neighbors. Possible choices include "rank", "number", and "jaccard". See type in bluster::neighborsToSNNGr for details.
BNPARAM	A BiocNeighbors parameter object to compute kNNs. Ignored unless the input is a matrix or data.frame. If omitted, the Annoy approximation will be used if there are more than 500 elements.

### findSpatialKNN

# Value

An igraph object.

### Examples

```
d1 <- mockData()
emb2snn(as.matrix(d1[,seq_len(2)]),k=5)</pre>
```

findSpatialKNN Find the k nearest spatial neighbors

# Description

For a given dataset, find the k nearest neighbors for each object based on their spatial locations, with the option of handling ties.

### Usage

```
findSpatialKNN(
   location,
   k,
   keep_ties = TRUE,
   useMedianDist = FALSE,
   BNPARAM = NULL
)
```

# Arguments

location	A numeric data matrix containing location information, where rows are points and columns are location dimensions.
k	The number of nearest neighbors to look at.
keep_ties	A Boolean indicating if ties are counted once or not. If TRUE, neighbors of the same distances will be included even if it means returning more than k neighbors.
useMedianDist	Use the median distance of the k nearest neighbor as maximum distance to be included. Ignored if keep_ties=FALSE.
BNPARAM	BNPARAM object passed to findKNN specifying the kNN approximation method to use. Defaults to exact for small datasets, and Annoy for larger ones.

# Value

A list of indices.

# Examples

```
data(sp_toys)
data <- sp_toys
findSpatialKNN(data[,c("x", "y")], k=6)</pre>
```

FMeasure

#### Description

Compute the F measure between two clustering results. This is directly copied from the package FlowSOM.

#### Usage

FMeasure(true, pred, silent = TRUE)

### Arguments

true	Array containing real cluster labels for each sample
pred	Array containing predicted cluster labels for each sample
silent	Logical, if FALSE, print some information about precision and recall

### Value

F measure score

fuzzyHardMetrics Compute fuzzy-hard versions of pair-sorting partition metrics

# Description

Computes fuzzy-hard versions of pair-sorting partition metrics to compare a hard clustering with both a fuzzy and hard truth. This was especially designed for cases where the fuzzy truth represents an uncertainty of a hard truth. Briefly put, the maximum of the pair concordance between the clustering and either the hard or the fuzzy truth is used, and the hard truth is used to compute completeness. See fuzzyPartitionMetrics for the more standard implementation of the metrics.

### Usage

```
fuzzyHardMetrics(
    hardTrue,
    fuzzyTrue,
    hardPred,
    nperms = NULL,
    returnElementPairAccuracy = FALSE,
    lowMemory = NULL,
    verbose = TRUE,
    BPPARAM = BiocParallel::SerialParam()
)
```

# Arguments

hardTrue	An atomic vector coercible to a factor or integer vector containing the true hard labels. Must have the same length as hardPred.	
fuzzyTrue	A object coercible to a numeric matrix with membership probability of elements (rows) in clusters (columns). Must have the same number of rows as the length of hardTrue. Also note that the columns of fuzzyTrue should be in the order of the levels (or integer values) of hardTrue.	
hardPred	An atomic vector coercible to a factor or integer vector containing the predicted hard labels.	
nperms	The number of permutations (for correction for chance). If NULL (default), a first set of 10 permutations will be run to estimate whether the variation across permutations is above 0.0025, in which case more (max 1000) permutations will be run.	
returnElementPairAccuracy		
	Logical. If TRUE, returns the per-element pair accuracy instead of the various parition-level and dataset-level metrics. Default FALSE.	
lowMemory	Logical; whether to use the slower, low-memory algorithm. By default this is enabled if the projected memory usage is higher than ~2GB.	
verbose	Logical; whether to print info and warnings, including the standard error of the mean across permutations (giving an idea of the precision of the adjusted metrics).	
BPPARAM	BiocParallel params for multithreading (default none)	

# Value

A list of metrics:

NDC	Hullermeier's NDC (fuzzy rand index)
ACI	Ambrosio's Adjusted Concordance Index (ACI), i.e. a permutation-based fuzzy version of the adjusted Rand index.
fuzzyWH	Fuzzy Wallace Homogeneity index
fuzzyWC	Fuzzy Wallace Completeness index
fuzzyAWH	Adjusted fuzzy Wallace Homogeneity index
fuzzyAWC	Adjusted fuzzy Wallace Completeness index

# Author(s)

Pierre-Luc Germain

# References

Hullermeier et al. 2012; 10.1109/TFUZZ.2011.2179303; D'Ambrosio et al. 2021; 10.1007/s00357-020-09367-0

# See Also

fuzzyPartitionMetrics().

### Examples

```
# generate a fuzzy truth:
fuzzyTrue <- matrix(c(</pre>
  0.95, 0.025, 0.025,
  0.98, 0.01, 0.01,
 0.96, 0.02, 0.02,
 0.95, 0.04, 0.01,
 0.95, 0.01, 0.04,
 0.99, 0.005, 0.005,
 0.025, 0.95, 0.025,
 0.97, 0.02, 0.01,
 0.025, 0.025, 0.95),
 ncol = 3, byrow=TRUE)
# a hard truth:
hardTrue <- apply(fuzzyTrue,1,FUN=which.max)</pre>
# some predicted labels:
hardPred <- c(1,1,1,1,1,1,2,2,2)
fuzzyHardMetrics(hardTrue, fuzzyTrue, hardPred, nperms=3)
```

fuzzyHardMetrics2 Compute fuzzy-hard metrics with lower memory requirement

#### Description

This is a slightly slower, but low-memory version of fuzzyHardMetrics.

### Usage

```
fuzzyHardMetrics2(
  hardTrue,
  fuzzyTrue,
  hardPred,
  nperms = 10,
  returnElementPairAccuracy = FALSE,
  verbose = TRUE,
  BPPARAM = BiocParallel::SerialParam()
)
```

#### Arguments

hardTrue	An atomic vector coercible to a factor or integer vector containing the true hard labels. Must have the same length as hardPred.
fuzzyTrue	A object coercible to a numeric matrix with membership probability of elements (rows) in clusters (columns). Must have the same number of rows as the length of hardTrue. Also note that the columns of fuzzyTrue should be in the order of the levels (or integer values) of hardTrue.
hardPred	An atomic vector coercible to a factor or integer vector containing the predicted hard labels.
nperms	The number of permutations (for correction for chance). If NULL (default), a first set of 10 permutations will be run to estimate whether the variation across permutations is above 0.0025, in which case more (max 1000) permutations will be run.

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returnElementPairAccuracy	
	Logical. If TRUE, returns the per-element pair accuracy instead of the various parition-level and dataset-level metrics. Default FALSE.
verbose	Logical; whether to print info and warnings, including the standard error of the mean across permutations (giving an idea of the precision of the adjusted metrics).
BPPARAM	BiocParallel params for multithreading (default none)

# Value

A list of metrics:

NDC	Hullermeier's NDC (fuzzy rand index)
ACI	Ambrosio's Adjusted Concordance Index (ACI), i.e. a permutation-based fuzzy version of the adjusted Rand index.
fuzzyWH	Fuzzy Wallace Homogeneity index
fuzzyWC	Fuzzy Wallace Completeness index
fuzzyAWH	Adjusted fuzzy Wallace Homogeneity index
fuzzyAWC	Adjusted fuzzy Wallace Completeness index

### Author(s)

Pierre-Luc Germain

# References

Hullermeier et al. 2012; 10.1109/TFUZZ.2011.2179303; D'Ambrosio et al. 2021; 10.1007/s00357-020-09367-0

### See Also

fuzzyHardMetrics()

# Examples

```
# generate a fuzzy truth:
fuzzyTrue <- matrix(c(</pre>
0.95, 0.025, 0.025,
0.98, 0.01, 0.01,
0.96, 0.02, 0.02,
0.95, 0.04, 0.01,
0.95, 0.01, 0.04,
0.99, 0.005, 0.005,
0.025, 0.95, 0.025,
0.97, 0.02, 0.01,
0.025, 0.025, 0.95),
ncol = 3, byrow=TRUE)
# a hard truth:
hardTrue <- apply(fuzzyTrue,1,FUN=which.max)</pre>
# some predicted labels:
hardPred <- c(1,1,1,1,1,1,2,2,2)
poem:::fuzzyHardMetrics2(hardTrue, fuzzyTrue, hardPred, nperms=3)
```

```
fuzzyHardSpotConcordance
```

*Per-element maximal concordance between a hard and a fuzzy partition* 

### Description

Per-element maximal concordance between a hard clustering and hard and fuzzy ground truth labels.

### Usage

```
fuzzyHardSpotConcordance(
   hardTrue,
   fuzzyTrue,
   hardPred,
   useNegatives = TRUE,
   verbose = TRUE
)
```

#### Arguments

hardTrue	A vector of true cluster labels
fuzzyTrue	A object coercible to a numeric matrix with membership probability of elements (rows) in clusters (columns). Must have the same number of rows as the length of hardTrue.
hardPred	A vector of predicted cluster labels
useNegatives	Logical; whether to include negative pairs in the concordance score (tends to result in a larger overall concordance and lower dynamic range of the score). Default TRUE.
verbose	Logical; whether to print expected memory usage for large datasets.

#### Value

A numeric vector of concordance scores for each element of hardPred

### Examples

```
# generate a fuzzy truth:
fuzzyTrue <- matrix(c(
    0.95, 0.025, 0.025,
    0.98, 0.01, 0.01,
    0.96, 0.02, 0.02,
    0.95, 0.04, 0.01,
    0.95, 0.01, 0.04,
    0.99, 0.005, 0.005,
    0.025, 0.95, 0.025,
    0.97, 0.02, 0.01,
    0.025, 0.025, 0.95),
    ncol = 3, byrow=TRUE)
# a hard truth:
```

```
hardTrue <- apply(fuzzyTrue,1,FUN=which.max)
# some predicted labels:
hardPred <- c(1,1,1,1,1,2,2,2)
fuzzyHardSpotConcordance(hardTrue, fuzzyTrue, hardPred)</pre>
```

fuzzyPartitionMetrics Compute fuzzy-fuzzy versions of pair-sorting partition metrics

### Description

Computes fuzzy versions of pair-sorting partition metrics. This is largely based on the permutationbased implementation by Antonio D'Ambrosio from the ConsRankClass package, modified to also compute the fuzzy versions of the adjusted Wallace indices, implement multithreading, and adjust the number of permutations according to their variability.

# Usage

```
fuzzyPartitionMetrics(
    P,
    Q,
    computeWallace = TRUE,
    nperms = NULL,
    verbose = TRUE,
    returnElementPairAccuracy = FALSE,
    BPPARAM = BiocParallel::SerialParam(),
    tnorm = c("product", "min", "lukasiewicz")
)
```

#### Arguments

Р	A object coercible to a numeric matrix with membership probability of elements (rows) in ground-truth classes (columns).
Q	A object coercible to a numeric matrix with membership probability of elements (rows) in predicted clusters (columns). Must have the same number of rows as P.
computeWallace	Logical; whether to compute the individual fuzzy versions of the Wallace indices (increases running time).
nperms	The number of permutations (for correction for chance). If NULL (default), a first set of 10 permutations will be run to estimate whether the variation across permutations is above 0.0025, in which case more (max 1000) permutations will be run.
verbose	Logical; whether to print info and warnings, including the standard error of the mean across permutations (giving an idea of the precision of the adjusted metrics).
returnElementPa	airAccuracy
	Logical. If TRUE, returns the per-element pair accuracy instead of the various parition-level and dataset-level metrics. Default FALSE.
BPPARAM	BiocParallel params for multithreading (default none)
tnorm	Which type of t-norm operation to use for class membership of pairs (either product, min, or lukasiewicz) when calculating the Wallace indices. Does not influence the NDC/ACI metrics.

### Value

When returnElementPairAccuracy is FALSE, return a list of metrics:

NDC	Hullermeier's NDC (fuzzy rand index)
ACI	Ambrosio's Adjusted Concordance Index (ACI), i.e. a permutation-based fuzzy version of the adjusted Rand index.
fuzzyWH	Fuzzy Wallace Homogeneity index
fuzzyWC	Fuzzy Wallace Completeness index
fuzzyAWH	Adjusted fuzzy Wallace Homogeneity index
fuzzyAWC	Adjusted fuzzy Wallace Completeness index

### Author(s)

Pierre-Luc Germain

#### References

Hullermeier et al. 2012; 10.1109/TFUZZ.2011.2179303; D'Ambrosio et al. 2021; 10.1007/s00357-020-09367-0

# Examples

# generate fuzzy partitions:

```
getEmbeddingClassMetrics
```

getEmbeddingClassMetrics

# Description

Computes class-level, embedding-based metrics.

# Usage

```
getEmbeddingClassMetrics(
    x,
    labels,
    metrics = c("meanSW", "minSW", "pnSW", "dbcv"),
    distance = "euclidean",
    ...
)
```

#### Arguments

x	A data frame or matrix (with features as columns and items as rows) from which the metrics will be computed.
labels	A vector containing the labels of the predicted clusters. Must be a vector of characters, integers, numerics, or a factor, but not a list.
metrics	The metrics to compute.
distance	The distance metric to use (default euclidean).
	Optional arguments. See details.

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# Value

A data.frame of metrics for each node/element of x.

 ${\tt getEmbeddingElementMetrics}$ 

getEmbeddingElementMetrics

### Description

Computes element-level, embedding-based metrics.

# Usage

```
getEmbeddingElementMetrics(
    x,
    labels,
    metrics = c("SW"),
    distance = "euclidean",
    ...
)
```

### Arguments

x	A data frame or matrix (with features as columns and items as rows) from which the metrics will be computed.
labels	A vector containing the labels of the predicted clusters. Must be a vector of characters, integers, numerics, or a factor, but not a list.
metrics	The metrics to compute. Currently, only the silhouette width is supported at the node-level.
distance	The distance metric to use (default euclidean).
	Optional arguments. See details.

# Value

A data.frame of metrics for each node/element of x.

getEmbeddingGlobalMetrics

getEmbeddingGlobalMetrics

# Description

Computes dataset-level, embedding-based metrics.

### Usage

```
getEmbeddingGlobalMetrics(
    x,
    labels,
    metrics = c("meanSW", "meanClassSW", "pnSW", "minClassSW", "cdbw", "cohesion",
        "compactness", "sep", "dbcv"),
    distance = "euclidean",
    ...
)
```

### Arguments

x	A data.frame or matrix (with features as columns and items as rows) from which the metrics will be computed.
labels	A vector containing the labels of the predicted clusters. Must be a vector of characters, integers, numerics, or a factor, but not a list.
metrics	The metrics to compute.
distance	The distance metric to use (default euclidean).
	Optional arguments. See details.

# Value

A data.frame (with 1 row) of metrics.

getEmbeddingMetrics Compute embedding-based metrics

### Description

Computes embedding-based metrics for the specified level.

### Usage

```
getEmbeddingMetrics(
    x,
    labels,
    metrics = NULL,
    distance = "euclidean",
    level = "class",
    ...
)
```

### Arguments

x	A data.frame or matrix (with features as columns and items as rows) from which the metrics will be computed.
labels	A vector containing the labels of the predicted clusters. Must be a vector of characters, integers, numerics, or a factor, but not a list.
metrics	The metrics to compute. See details.

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distance	The distance metric to use (default euclidean).
level	The level to calculate the metrics. Options include "element", "class" and "dataset".
	Optional arguments. See details.

#### Details

The allowed values for metrics depend on the value of level:

- If level = "element", the allowed metrics are: "SW".
- If level = "class", the allowed metrics are: "meanSW", "minSW", "pnSW", "dbcv".
- If level = "dataset", the allowed metrics are: "meanSW", "meanClassSW", "pnSW", "minClassSW", "cdbw", "cohesion", "compactness", "sep", "dbcv".

The function(s) that the optional arguments ... passed to depend on the value of level:

- If level = "element", optional arguments are passed to stats::dist().
- If level = "class", optional arguments are passed to dbcv().
- If level = "dataset", optional arguments are passed to dbcv() or CDbw().

### Value

A data.frame of metrics.

### Examples

```
d1 <- mockData()
getEmbeddingMetrics(d1[,seq_len(2)], labels=d1$class,
metrics=c("meanSW", "minSW", "pnSW", "dbcv"), level="class")</pre>
```

getFuzzyLabel Get fuzzy representation of labels

### Description

Get fuzzy representation of labels according to the spatial neighborhood label composition.

#### Usage

```
getFuzzyLabel(labels, location, k = 6, alpha = 0.5, ...)
```

#### Arguments

labels	An anomic vector of cluster labels
location	A matrix or data.frame of coordinates
k	The wished number of nearest neighbors
alpha	The parameter to control to what extend the spot itself contribute to the class composition calculation. "equal" means it is weighted the same as other neighbors. A numeric value between 0 and 1 means the weight of the frequency contribution for the spot itself, and the frequency contribution for its knn is then $1-alpha$ . By default 0.5.
•••	Passed to findSpatialKNN().

### Value

A matrix of fuzzy memberships.

### Examples

```
data(sp_toys)
data <- sp_toys
getFuzzyLabel(data$label, data[,c("x", "y")], k=6)
```

getFuzzyPartitionElementMetrics

getFuzzyPartitionElementMetrics

### Description

Computes a selection of external fuzzy clustering evaluation metrics at the element level.

### Usage

```
getFuzzyPartitionElementMetrics(
  hardTrue = NULL,
  fuzzyTrue = NULL,
  hardPred = NULL,
  fuzzyPred = NULL,
  fuzzy_true = TRUE,
  fuzzy_pred = FALSE,
  metrics = c("fuzzySPC"),
  useNegatives = TRUE,
  verbose = TRUE,
  usePairs = TRUE
)
```

#### Arguments

hardTrue	A vector of true cluster labels
fuzzyTrue	A object coercible to a numeric matrix with membership probability of elements (rows) in clusters (columns). Must have the same number of rows as the length of hardTrue.
hardPred	A vector of predicted cluster labels
fuzzyPred	A object coercible to a numeric matrix with membership probability of elements (rows) in clusters (columns).
fuzzy_true	Logical; whether the truth is fuzzy.
fuzzy_pred	Logical; whether the prediction is fuzzy.
metrics	The metrics to compute. Currently only "fuzzySPC" is included at the element level.
useNegatives	Logical; whether to include negative pairs in the concordance score (tends to result in a larger overall concordance and lower dynamic range of the score). Default TRUE.
verbose	Logical; whether to print expected memory usage for large datasets.
usePairs	Logical; whether to compute over pairs instead of elements. Only useful when fuzzy_true=TRUE and fuzzy_pred=FALSE.

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getFuzzyPartitionMetrics

# Value

A dataframe of metric values.

```
getFuzzyPartitionMetrics
```

Compute external metrics for fuzzy clusterings

#### Description

Computes a selection of external fuzzy clustering evaluation metrics.

### Usage

```
getFuzzyPartitionMetrics(
  hardTrue = NULL,
  fuzzyTrue = NULL,
  hardPred = NULL,
  fuzzyPred = NULL,
  metrics = c("fuzzyWH", "fuzzyAWH", "fuzzyWC", "fuzzyAWC"),
  level = "class",
  nperms = NULL,
  verbose = TRUE,
  BPPARAM = BiocParallel::SerialParam(),
  useNegatives = TRUE,
  usePairs = NULL,
  lowMemory = NULL,
  ...
)
```

### Arguments

hardTrue	An atomic vector coercible to a factor or integer vector containing the true hard labels.
fuzzyTrue	A object coercible to a numeric matrix with membership probability of elements (rows) in clusters (columns).
hardPred	An atomic vector coercible to a factor or integer vector containing the predicted hard labels.
fuzzyPred	A object coercible to a numeric matrix with membership probability of elements (rows) in clusters (columns).
metrics	The metrics to compute. See details.
level	The level to calculate the metrics. Options include "element", "class" and "dataset".
nperms	The number of permutations (for correction for chance). If NULL (default), a first set of 10 permutations will be run to estimate whether the variation across permutations is above 0.0025, in which case more (max 1000) permutations will be run.
verbose	Logical; whether to print info and warnings, including the standard error of the mean across permutations (giving an idea of the precision of the adjusted metrics).

BPPARAM	BiocParallel params for multithreading (default none)
useNegatives	Logical; whether to include negative pairs in the concordance score (tends to result in a larger overall concordance and lower dynamic range of the score). Default TRUE.
usePairs	Logical; whether to compute over pairs instead of elements Recommended and TRUE by default.
lowMemory	Logical, whether to use a low memory mode. This is only useful whenhardTrue and fuzzyPred is used. If TRUE, the function will compute the metrics in a low memory mode, which is slower but uses less memory. If FALSE, the function will compute the metrics in a high memory mode, which is faster but uses more memory. By default it is set automatically based on the size of the input data. See fuzzyHardMetrics.
	Optional arguments for fuzzyPartitionMetrics: tnorm. Only useful when fuzzyTrue and fuzzyPred is used.

### Details

The allowed values for metrics depend on the value of level:

- If level = "element", the allowed metrics are: "fuzzySPC".
- If level = "class", the allowed metrics are: "fuzzyWH", "fuzzyAWH", "fuzzyWC", "fuzzyAWC".
- If level = "dataset", the allowed metrics are: "fuzzyRI", "fuzzyARI", "fuzzyWH", "fuzzyAWH", "fuzzyWC", "fuzzyAWC".

### Value

A dataframe of metric results.

### Examples

```
# generate fuzzy partitions:
m1 <- matrix(c(0.95, 0.025, 0.025,
               0.98, 0.01, 0.01,
               0.96, 0.02, 0.02,
               0.95, 0.04, 0.01,
               0.95, 0.01, 0.04,
               0.99, 0.005, 0.005,
               0.025, 0.95, 0.025,
               0.97, 0.02, 0.01,
               0.025, 0.025, 0.95),
               ncol = 3, byrow=TRUE)
m2 <- matrix(c(0.95, 0.025, 0.025,
               0.98, 0.01, 0.01,
               0.96, 0.02, 0.02,
               0.025, 0.95, 0.025,
               0.02, 0.96, 0.02,
               0.01, 0.98, 0.01,
               0.05, 0.05, 0.95,
               0.02, 0.02, 0.96,
               0.01, 0.01, 0.98),
               ncol = 3, byrow=TRUE)
colnames(m1) <- colnames(m2) <- LETTERS[seq_len(3)]</pre>
getFuzzyPartitionMetrics(fuzzyTrue=m1,fuzzyPred=m2, level="class")
```

```
# generate a fuzzy truth:
fuzzyTrue <- matrix(c(</pre>
  0.95, 0.025, 0.025,
 0.98, 0.01, 0.01,
 0.96, 0.02, 0.02,
 0.95, 0.04, 0.01,
  0.95, 0.01, 0.04,
  0.99, 0.005, 0.005,
  0.025, 0.95, 0.025,
  0.97, 0.02, 0.01,
  0.025, 0.025, 0.95),
 ncol = 3, byrow=TRUE)
# a hard truth:
hardTrue <- apply(fuzzyTrue,1,FUN=which.max)</pre>
# some predicted labels:
hardPred <- c(1,1,1,1,1,1,2,2,2)
getFuzzyPartitionMetrics(hardPred=hardPred, hardTrue=hardTrue,
fuzzyTrue=fuzzyTrue, nperms=3, level="class")
getFuzzyPartitionMetrics(hardTrue=hardPred, hardPred=hardTrue,
fuzzyPred=fuzzyTrue, nperms=3, level="class")
```

getGraphClassMetrics getGraphClassMetrics

#### Description

Computes a selection of supervised graph evaluation metrics using ground truth class labels. The metrics are reported (as average) per class.

### Usage

```
getGraphClassMetrics(
  х,
  labels.
  metrics = c("SI", "NP", "AMSP", "PWC", "NCE"),
  directed = NULL,
)
## S4 method for signature 'list'
getGraphClassMetrics(x, labels, metrics, directed = NULL, k = NULL, ...)
## S4 method for signature 'data.frame'
getGraphClassMetrics(
  х,
  labels,
  metrics,
  directed = NULL,
  k,
  shared = FALSE,
  . . .
)
```

```
## S4 method for signature 'matrix'
getGraphClassMetrics(
  х,
  labels,
  metrics,
  directed = NULL,
  k,
  shared = FALSE,
  . . .
)
## S4 method for signature 'igraph'
getGraphClassMetrics(
  х,
  labels,
  metrics = c("SI", "NP", "AMSP", "PWC", "NCE"),
  directed = NULL,
  • • •
)
## S4 method for signature 'dist'
getGraphClassMetrics(
  х,
  labels,
  metrics = c("SI", "NP", "AMSP", "PWC", "NCE"),
  directed = NULL,
  • • •
)
```

### Arguments

x	Either an igraph object, a list of nearest neighbors (see details below), or a data.frame or matrix (with features as columns and items as rows) from which nearest neighbors will be computed.
labels	Either a factor or a character vector indicating the true class label of each element (i.e. row or vertex) of x.
metrics	The metrics to compute. See details.
directed	Logical; whether to compute the metrics in a directed fashion. If left to NULL, conventional choices will be made per metric (adhesion, cohesion, PWC AMSP undirected, others directed).
	Optional arguments for emb2knn() or emb2snn().
k	The number of nearest neighbors to compute and/or use. Can be omitted if x is a graph or list of nearest neighbors.
shared	Logical; whether to use a shared nearest neighbor network instead of a nearest neighbor network. Ignored if x is not an embedding or dist object.

### Value

A data.frame of metrics for each class.

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getGraphElementMetrics

getGraphElementMetrics

#### Description

Computes a selection of supervised graph evaluation metrics using ground truth class labels. The metrics are reported (as average) per node/element.

#### Usage

```
getGraphElementMetrics(x, labels, directed = NULL, ...)
## S4 method for signature 'list'
getGraphElementMetrics(x, labels, metrics, directed = NULL, k = NULL, ...)
## S4 method for signature 'data.frame'
getGraphElementMetrics(
  х,
  labels,
  metrics,
  directed = NULL,
  k,
  shared = FALSE,
  . . .
)
## S4 method for signature 'matrix'
getGraphElementMetrics(
  х,
  labels,
  metrics,
  directed = NULL,
  k,
  shared = FALSE,
)
## S4 method for signature 'igraph'
getGraphElementMetrics(x, labels, directed = NULL, ...)
## S4 method for signature 'dist'
getGraphElementMetrics(x, labels, directed = NULL, ...)
```

### Arguments

х	Either an igraph object, a list of nearest neighbors (see details below), or a
	data.frame or matrix (with features as columns and items as rows) from which
	nearest neighbors will be computed.
labels	Either a factor or a character vector indicating the true class label of each element (i.e. row or vertex) of x.

Logical; whether to compute the metrics in a directed fashion. If left to NULL, conventional choices will be made per metric (adhesion, cohesion, PWC AMSP undirected, others directed).
Optional arguments for emb2knn() or emb2snn().
The metrics to compute. See details.
The number of nearest neighbors to compute and/or use. Can be omitted if x is a graph or list of nearest neighbors.
Logical; whether to use a shared nearest neighbor network instead of a nearest neighbor network. Ignored if x is not an embedding or dist object.

# Value

A data.frame of metrics for each node/element of x.

getGraphMetrics Compute graph-based metrics

# Description

Computes a selection of graph evaluation metrics using class labels.

### Usage

```
getGraphMetrics(
    x,
    labels,
    metrics = NULL,
    directed = NULL,
    k = 10,
    shared = FALSE,
    level = "class",
    ....
)
```

# Arguments

x	Either an igraph object, a list of nearest neighbors (see details below), or a data.frame or matrix (with features as columns and items as rows) from which nearest neighbors will be computed.
labels	Either a factor or a character vector indicating the true class label of each element (i.e. row or vertex) of x.
metrics	The metrics to compute. See details.
directed	Logical; whether to compute the metrics in a directed fashion. If left to NULL, conventional choices will be made per metric (adhesion, cohesion, PWC AMSP undirected, others directed).
k	The number of nearest neighbors to compute and/or use. Can be omitted if x is a graph or list of nearest neighbors.
shared	Logical; whether to use a shared nearest neighbor network instead of a nearest neighbor network. Ignored if $x$ is not an embedding or dist object.

level	The level to calculate the metrics. Options include "element", "class" and "dataset".
	Optional arguments for emb2knn() or emb2snn().

#### Details

The allowed values for metrics depend on the value of level:

- If level = "element", the allowed metrics are: "SI","ISI","NP", "NCE" (see below for details).
- If level = "class", the allowed metrics are:
  - "SI": Simpson's Index.
  - "ISI": Inverse Simpson's Index
  - "NP": Neighborhood Purity
  - "AMSP": Adjusted Mean Shortest Path
  - "PWC": Proportion of Weakly Connected
  - "NCE": Neighborhood Class Enrichment
  - "adhesion": adhesion of a graph, is the minumum number of nodes that must be removed to split a graph.
  - "cohesion": cohesion of a graph, is the minumum number of edges that must be removed to split a graph.
- If level = "dataset", the allowed metrics are: "SI","ISI", "NP","AMSP","PWC","NCE", "adhesion","cohesion".

### Value

A data.frame of metrics.

### Examples

```
d1 <- mockData()
getGraphMetrics(d1[,seq_len(2)], labels=d1$class, level="class")</pre>
```

getNeighboringPairConcordance

Per-element local concordance between a clustering and a ground truth

#### Description

Per-element local concordance between a clustering and a ground truth

### Usage

```
getNeighboringPairConcordance(
   true,
   pred,
   location,
   k = 20L,
   useNegatives = FALSE,
   distWeights = TRUE,
   BNPARAM = NULL
)
```

### Arguments

true	A vector of true class labels
pred	A vector of predicted clusters
location	A matrix or data.frame with spatial dimensions as columns. Alternatively, a nearest neighbor object as produced by findKNN.
k	Approximate number of nearest neighbors to consider
useNegatives	Logical; whether to include the concordance of negative pairs in the score (default FALSE).
distWeights	Logical; whether to weight concordance by distance (default TRUE).
BNPARAM	A BiocNeighbors parameter object to compute kNNs. Ignored unless the input is a matrix or data.frame. If omitted, the Annoy approximation will be used if there are more than 500 elements.

### Value

A vector of concordance scores

### Examples

```
data(sp_toys)
data <- sp_toys
getNeighboringPairConcordance(data$label, data$p1, data[,c("x", "y")], k=6)</pre>
```

getPairConcordance *Per-element pair concordance score* 

### Description

Per-element pair concordance between a clustering and a ground truth. Note that by default, negative pairs (i.e. that are split in both the predicted and true groupings) are not counted. To count it (as in the standard Rand Index), use useNegatives=TRUE.

# Usage

```
getPairConcordance(
  true,
  pred,
  usePairs = TRUE,
  useNegatives = FALSE,
  adjust = FALSE
)
```

### Arguments

true	A vector of true class labels
pred	A vector of predicted clusters
usePairs	Logical; whether to compute over pairs instead of elements Recommended and TRUE by default.

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#### getPartitionClassMetrics

useNegatives	Logical; whether to include the consistency of negative pairs in the score (default FALSE).
adjust	Logical; whether to adjust for chance. Only implemented for useNegatives=FALSE (doesn't make sense on a element-level otherwise).

### Value

A vector of concordance scores

getPartitionClassMetrics

getPartitionClassMetrics

### Description

Computes a selection of external evaluation metrics for partition. The metrics are reported per class.

# Usage

```
getPartitionClassMetrics(
  true,
  pred,
  metrics = c("WC", "WH", "AWC", "AWH", "FM")
)
```

### Arguments

true	A vector containing the labels of the true classes. Must be a vector of characters, integers, numerics, or a factor, but not a list.
pred	A vector containing the labels of the predicted clusters. Must be a vector of characters, integers, numerics, or a factor, but not a list.
metrics	The metrics to compute. If omitted, main metrics will be computed.

### Value

A dataframe of metrics.

getPartitionElementMetrics

getPartitionElementMetrics

# Description

Computes a selection of external evaluation metrics for partition. The metrics are reported per element.

### Usage

```
getPartitionElementMetrics(
  true,
  pred,
  metrics = c("SPC"),
  usePairs = TRUE,
  useNegatives = TRUE
)
```

### Arguments

true	A vector of true class labels
pred	A vector of predicted clusters
metrics	The metrics to compute.
usePairs	Logical; whether to compute over pairs instead of elements Recommended and TRUE by default.
useNegatives	Logical; whether to include the consistency of negative pairs in the score (default FALSE).

### Value

A dataframe of metrics.

```
getPartitionGlobalMetrics
```

getPartitionGlobalMetrics

# Description

Computes a selection of external evaluation metrics for partition. The metrics are reported per dataset.

### Usage

```
getPartitionGlobalMetrics(
    true,
    pred,
    metrics = c("RI", "WC", "WH", "ARI", "NCR", "AWC", "AWH", "MI", "AMI", "VI", "EH",
        "EC", "VM", "FM"),
    ...
)
```

# Arguments

true	A vector containing the labels of the true classes. Must be a vector of characters, integers, numerics, or a factor, but not a list.
pred	A vector containing the labels of the predicted clusters. Must be a vector of characters, integers, numerics, or a factor, but not a list.

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### getPartitionMetrics

metrics	The metrics to compute. If omitted, main metrics will be computed. See below for more details.
	Optional arguments for MI, VI, or VM. See clevr::mutual_info(), clevr::variation_info() and clevr::v_measure() for more details.

# Value

A dataframe of metric results. Possible metrics are:

RI	Rand Index
WC	Wallace Completeness
WH	Wallace Homogeneity
ARI	Adjusted Rand Index
AWC	Adjusted Wallace Completeness
AWH	Adjusted Wallace Homogeneity
NCR	Normalized class size Rand index
MI	Mutual Information
AMI	Adjusted Mutual Information
VI	Variation of Information
EH	(Entropy-based) Homogeneity
EC	(Entropy-based) Completeness
VM	V-measure
FM	F-measure/weighted average F1 score
VDM	Van Dongen Measure
MHM	Meila-Heckerman Measure
MMM	Maximum-Match Measure
Mirkin	Mirkin Metric
Accuracy	Set Matching Accuracy

getPartitionMetrics Compute partition-based metrics

# Description

Computes a selection of external evaluation metrics for partition.

# Usage

```
getPartitionMetrics(true, pred, metrics = NULL, level = "class", ...)
```

# Arguments

true	A vector containing the labels of the true classes. Must be a vector of characters, integers, numerics, or a factor, but not a list.
pred	A vector containing the labels of the predicted clusters. Must be a vector of characters, integers, numerics, or a factor, but not a list.
metrics	The metrics to compute. If omitted, main metrics will be computed. See details.
level	The level to calculate the metrics. Options include "element", "class" and "dataset".
	Optional arguments for MI, VI, or VM. See clevr::mutual_info(), clevr::variation_info() and clevr::v_measure() for more details.

#### Details

The allowed values for metrics depend on the value of level:

- If level = "element", the allowed metrics are:
  - "SPC": Spot-wise Pair Concordance.
  - "ASPC": Adjusted Spot-wise Pair Concordance.
- If level = "class", the allowed metrics are: "WC", "WH", "AWC", "AWH", "FM" (see below for details).
- If level = "dataset", the allowed metrics are:
  - "RI": Rand Index
  - "WC": Wallace Completeness
  - "WH": Wallace Homogeneity
  - "ARI": Adjusted Rand Index
  - "AWC": Adjusted Wallace Completeness
  - "AWH": Adjusted Wallace Homogeneity
  - "NCR": Normalized class size Rand index
  - "MI": Mutual Information
  - "AMI": Adjusted Mutual Information
  - "VI": Variation of Information
  - "EH": (Entropy-based) Homogeneity
  - "EC": (Entropy-based) Completeness
  - "VM": V-measure
  - "FM": F-measure/weighted average F1 score
  - "VDM": Van Dongen Measure
  - "MHM": Meila-Heckerman Measure
  - "MMM": Maximum-Match Measure
  - "Mirkin": Mirkin Metric
  - "Accuracy": Set Matching Accuracy

# Value

A data.frame of metrics.
#### getSpatialClassExternalMetrics

#### Examples

```
true <- rep(LETTERS[seq_len(3)], each=10)
pred <- c(rep("A", 8), rep("B", 9), rep("C", 3), rep("D", 10))
getPartitionMetrics(true, pred, level="class")
getPartitionMetrics(true, pred, level="dataset")</pre>
```

# getSpatialClassExternalMetrics

```
Compute class-level external evaluation metrics for spatially-resolved data
```

# Description

Computes a selection of external clustering evaluation metrics for spatial data at the class/cluster level.

#### Usage

```
getSpatialClassExternalMetrics(
  true,
  pred,
  location,
  k = 6,
  alpha = 0.5,
  metrics = c("nsWH", "nsAWH", "nsWC", "nsAWC"),
  fuzzy_true = TRUE,
  fuzzy_pred = FALSE,
  lowMemory = NULL,
  ...
)
```

true	A vector containing the labels of the true classes. Must be a vector of characters, integers, numerics, or a factor, but not a list.
pred	A vector containing the labels of the predicted clusters. Must be a vector of characters, integers, numerics, or a factor, but not a list.
location	A matrix or data.frame of coordinates
k	The number of neighbors used when calculating the fuzzy class memberships for fuzzy metrics.
alpha	The parameter to control to what extend the spot itself contribute to the class composition calculation. "equal" means it is weighted the same as other neighbors. A numeric value between 0 and 1 means the weight of the frequency contribution for the spot itself, and the frequency contribution for its knn is then 1-alpha. By default 0.5.
metrics	a vector of metric names to compute.
fuzzy_true	Logical; whether to compute fuzzy class memberships for true.
fuzzy_pred	Logical; whether to compute fuzzy class memberships for pred.

	getSpatialClassInternalMetrics
lowMemory	Logical, whether to use a low memory mode. This is only useful whenhardTrue and fuzzyPred is used. If TRUE, the function will compute the metrics in a low memory mode, which is slower but uses less memory. If FALSE, the function will compute the metrics in a high memory mode, which is faster but uses more memory. By default it is set automatically based on the size of the input data. See fuzzyHardMetrics.
	Optional params for fuzzyPartitionMetrics or findSpatialKNN.

# Value

A data.frame of metrics.

```
getSpatialClassInternalMetrics
Compute class-level internal evaluation metrics for spatially-resolved
data
```

# Description

Computes a selection of internal clustering evaluation metrics for spatial data for each class.

# Usage

```
getSpatialClassInternalMetrics(
  labels,
  location,
  k = 6,
  metrics = c("CHAOS", "PAS", "ELSA"),
  ...
)
```

# Arguments

labels	A vector containing the labels to be evaluated.
location	A numerical matrix containing the location information, with rows as samples and columns as location dimensions.
k	The size of the spatial neighborhood to look at for each spot. This is used for calculating PAS and ELSA scores.
metrics	Possible metrics: "CHAOS", "PAS" and "ELSA".
	Optional params for PAS().

# Value

A dataframe of metric values.

getSpatialElementExternalMetrics

getSpatialElementExternalMetrics

# Description

Computes a selection of external clustering evaluation metrics for spatial data at the element level.

#### Usage

```
getSpatialElementExternalMetrics(
  true,
  pred,
  location,
  k = 6,
  alpha = 0.5,
  metrics = c("nsSPC", "NPC", "SpatialSPC"),
  fuzzy_true = TRUE,
  fuzzy_pred = FALSE,
  ...
)
```

# Arguments

true	A vector containing the labels of the true classes. Must be a vector of characters, integers, numerics, or a factor, but not a list.
pred	A vector containing the labels of the predicted clusters. Must be a vector of characters, integers, numerics, or a factor, but not a list.
location	A matrix or data.frame of coordinates
k	The number of neighbors used when calculating the fuzzy class memberships for fuzzy metrics, or when calculating the weighted accuracy.
alpha	The parameter to control to what extend the spot itself contribute to the class composition calculation. "equal" means it is weighted the same as other neighbors. A numeric value between 0 and 1 means the weight of the frequency contribution for the spot itself, and the frequency contribution for its knn is then 1-alpha. By default 0.5.
metrics	a vector of metric names to compute.
fuzzy_true	Logical; whether to compute fuzzy class memberships for true.
fuzzy_pred	Logical; whether to compute fuzzy class memberships for pred.
	Optional params for getFuzzyPartitionElementMetrics() or findSpatialKNN().

# Value

A data.frame of metrics.

```
getSpatialElementInternalMetrics
```

Compute spot-level internal evaluation metrics for spatially-resolved data

#### Description

Computes a selection of internal clustering evaluation metrics for spatial data at each spot level.

# Usage

```
getSpatialElementInternalMetrics(
  labels,
  location,
  k = 6,
  metrics = c("PAS", "ELSA"),
   ...
)
```

#### Arguments

labels	A vector containing the labels to be evaluated.
location	A numerical matrix containing the location information, with rows as samples and columns as location dimensions.
k	The size of the spatial neighborhood to look at for each spot. This is used for calculating PAS and ELSA scores.
metrics	Possible metrics: "PAS" and "ELSA".
	Optional params for PAS().

# Value

A dataframe containing the metric values for all samples in the dataset. If PAS is calculated, the value is a Boolean about the abnormality of a spot. If ELSA is calculated, Ea, Ec and ELSA for all spots will be returned.

getSpatialExternalMetrics

Calculate Spatial External Metrics

# Description

A generic function to calculate spatial external metrics. It can be applied to raw components (true, pred, location) or directly to a SpatialExperiment object.

# Usage

```
getSpatialExternalMetrics(
  object = NULL,
  true,
  pred,
  location = NULL,
  k = 6,
  alpha = 0.5,
  level = "class",
  metrics = NULL,
  fuzzy_true = TRUE,
  fuzzy_pred = FALSE,
  . . .
)
## S4 method for signature 'missing'
getSpatialExternalMetrics(
  object = NULL,
  true,
  pred,
  location = NULL,
  k = 6,
  alpha = 0.5,
  level = "class",
  metrics = NULL,
  fuzzy_true = TRUE,
  fuzzy_pred = FALSE,
  . . .
)
## S4 method for signature 'SpatialExperiment'
getSpatialExternalMetrics(
  object = NULL,
  true,
  pred,
  location = NULL,
  k = 6,
  alpha = 0.5,
  level = "class",
  metrics = NULL,
  fuzzy_true = TRUE,
  fuzzy_pred = FALSE,
  • • •
)
```

object	The main input. Can be a SpatialExperiment object or missing (when using true, pred, and location directly).
true	When object is missing: a vector containing the labels of the true classes. Must be a vector of characters, integers, numerics, or a factor, but not a list. When
	object is a SpatialExperiment object: the column name in colData(object)

pred	containing the true labels. When object is missing: a vector containing the labels of the predicted clus-
p. 02	ters. Must be a vector of characters, integers, numerics, or a factor, but not a list. When object is a SpatialExperiment object: the column name in colData(object) containing the predicted labels.
location	A matrix or data.frame of coordinates
k	The number of neighbors used when calculating the fuzzy class memberships for fuzzy metrics, or when calculating the weighted accuracy.
alpha	The parameter to control to what extend the spot itself contribute to the class composition calculation. "equal" means it is weighted the same as other neighbors. A numeric value between 0 and 1 means the weight of the frequency contribution for the spot itself, and the frequency contribution for its knn is then 1-alpha. By default 0.5.
level	The level to calculate the metrics. Options include "element", "class" and "dataset".
metrics	The metrics to compute. See details.
fuzzy_true	Logical; whether to compute fuzzy class memberships for true.
fuzzy_pred	Logical; whether to compute fuzzy class memberships for pred.
•••	Additional arguments passed to specific methods.

# Details

The allowed values for metrics depend on the value of level:

- If level = "element", the allowed metrics are: "nsSPC", "NPC", "SpatialSPC".
- If level = "class", the allowed metrics are: "nsWH", "nsAWH", "nsWC", "nsAWC".
- If level = "dataset", the allowed metrics are: "nsRI", "nsARI", "nsWH", "nsWWH", "nsWC", "nsAWC", "nsAccuracy", "SpatialRI", "SpatialARI".

#### Value

A data.frame of metrics based on the specified input.

#### Examples

getSpatialGlobalExternalMetrics

Compute dataset-level external evaluation metrics for spatiallyresolved data

# Description

Computes a selection of external clustering evaluation metrics for spatial data at the dataset level. Options include a series of fuzzy pair-counting metrics and set matching-based accuracy.

# Usage

```
getSpatialGlobalExternalMetrics(
    true,
    pred,
    location,
    k = 6,
    alpha = 0.5,
    metrics = c("nsRI", "nsARI", "nsWH", "nsAWH", "nsWC", "nsAWC", "nsAccuracy",
        "SpatialRI", "SpatialARI"),
    fuzzy_true = TRUE,
    fuzzy_pred = FALSE,
    lowMemory = NULL,
    ...
)
```

true	A vector containing the labels of the true classes. Must be a vector of characters, integers, numerics, or a factor, but not a list.
pred	A vector containing the labels of the predicted clusters. Must be a vector of characters, integers, numerics, or a factor, but not a list.
location	A matrix or data.frame of coordinates
k	The number of neighbors used when calculating the fuzzy class memberships for fuzzy metrics, or when calculating the weighted accuracy.
alpha	The parameter to control to what extend the spot itself contribute to the class composition calculation. "equal" means it is weighted the same as other neighbors. A numeric value between $\emptyset$ and 1 means the weight of the frequency contribution for the spot itself, and the frequency contribution for its knn is then 1-alpha. By default $\emptyset$ . 5.
metrics	a vector of metric names to compute.
fuzzy_true	Logical; whether to compute fuzzy class memberships for true.
fuzzy_pred	Logical; whether to compute fuzzy class memberships for pred.
lowMemory	Logical, whether to use a low memory mode. This is only useful whenhardTrue and fuzzyPred is used. If TRUE, the function will compute the metrics in a low memory mode, which is slower but uses less memory. If FALSE, the function will compute the metrics in a high memory mode, which is faster but uses more memory. By default it is set automatically based on the size of the input data. See fuzzyHardMetrics.
	Optional params for fuzzyPartitionMetrics or findSpatialKNN.

# Value

A data.frame of metrics.

```
getSpatialGlobalInternalMetrics
```

Compute dataset-level internal evaluation metrics for spatially-resolved data

#### Description

Computes a selection of internal clustering evaluation metrics for spatial data at the dataset level. MPC, PC and PE are internal metrics for fuzzy clustering, and their implementations in package fclust are used.

# Usage

```
getSpatialGlobalInternalMetrics(
   labels,
   location,
   k = 6,
   metrics = c("PAS", "ELSA", "CHAOS"),
   ...
)
```

#### Arguments

labels	A vector containing the labels to be evaluated.
location	A numerical matrix containing the location information, with rows as samples and columns as location dimensions.
k	The size of the spatial neighborhood to look at for each spot. This is used for calculating PAS and ELSA scores.
metrics	The metrics to compute. See below for more details.
	Optional arguments for PAS().

# Value

A named vector containing metric values. Possible metrics are:

PAS	Proportion of abnormal spots (PAS score).
ELSA	Entropy-based Local indicator of Spatial Association (ELSA score).
CHAOS	Spatial Chaos Score.
MPC	Modified partition coefficient
PC	Partition coefficient
PE	Partition entropy

# References

Yuan, Zhiyuan, et al., 2024; 10.1038/s41592-024-02215-8 Naimi, Babak, et al., 2019; 10.1016/j.spasta.2018.10.001 Wang, et al., 2022; 10.1016/j.ins.2022.11.010

getSpatialInternalMetrics

#### Description

A generic function to compute a selection of internal clustering evaluation metrics for spatial data. It can be applied to raw components (labels, location) or directly to a SpatialExperiment object.

#### Usage

```
getSpatialInternalMetrics(
  object = NULL,
  labels,
  location = NULL,
  k = 6,
  level = "class",
  metrics = c("CHAOS", "PAS", "ELSA"),
  . . .
)
## S4 method for signature 'missing'
getSpatialInternalMetrics(
  object = NULL,
  labels,
  location = NULL,
  k = 6,
  level = "class",
  metrics = c("CHAOS", "PAS", "ELSA"),
  . . .
)
## S4 method for signature 'SpatialExperiment'
getSpatialInternalMetrics(
  object = NULL,
  labels,
  location = NULL,
  k = 6,
  level = "class",
  metrics = c("CHAOS", "PAS", "ELSA"),
  . . .
)
```

- objectThe main input. Can be a SpatialExperiment object or missing (when using<br/>labels, and location directly).
- labels When object is missing: a vector containing the labels of the predicted clusters. Must be a vector of characters, integers, numerics, or a factor, but not a list. When object is a SpatialExperiment object: the column name in colData(object) containing the labels.

location	A numerical matrix containing the location information, with rows as samples and columns as location dimensions.
k	The size of the spatial neighborhood to look at for each spot. This is used for calculating PAS and ELSA scores.
level	The level to calculate the metrics. Options include "element", "class" and "dataset".
metrics	The metrics to compute. See details.
	Optional params for PAS().

# Details

The allowed values for metrics depend on the value of level:

- If level = "element", the allowed metrics are: "PAS", "ELSA".
- If level = "class", the allowed metrics are: "CHAOS", "PAS", "ELSA".
- If level = "dataset", the allowed metrics are:
  - "PAS": Proportion of abnormal spots (PAS score)
  - "ELSA": Entropy-based Local indicator of Spatial Association (ELSA score)
  - "CHAOS": Spatial Chaos Score.
  - "MPC": Modified partition coefficient
  - "PC": Partition coefficient
  - "PE": Partition entropy

# Value

A data.frame of metrics.

#### Examples

knnComposition Com

# Description

For a given dataset with locations and labels, compute the label composition of the neighborhood for each sample.

# Usage

```
knnComposition(location, k = 6, labels, alpha = 0.5, ...)
```

#### Arguments

location	A numeric data matrix containing location information, where rows are points and columns are location dimensions.
k	The number of nearest neighbors to look at.
labels	A vector containing the label for the dataset.
alpha	The parameter to control to what extend the spot itself contribute to the class composition calculation. "equal" means it is weighted the same as other neighbors. A numeric value between 0 and 1 means the weight of the frequency contribution for the spot itself, and the frequency contribution for its knn is then 1-alpha. By default 0.5.
	Optional arguments for findSpatialKNN().

# Value

A numerical matrix indicating the composition, where rows correspond to samples and columns correspond to the classes in label.

#### Examples

```
data(sp_toys)
data <- sp_toys
knnComposition(data[,c("x", "y")], k=6, data$label)</pre>
```

```
Match two partitions using Hungarian algorithm
```

#### Description

Match sets from a partitions to a reference partition using the Hungarian algorithm to optimize F1 scores.

# Usage

```
matchSets(pred, true, forceMatch = TRUE, returnIndices = is.integer(true))
```

#### Arguments

pred	An integer or factor of cluster labels
true	An integer or factor of reference labels
forceMatch	Logical; whether to enforce a match for every set of pred
returnIndices	Logical; whether to return indices rather than levels

# Value

A vector of matching sets (i.e. level) from true for every set (i.e. level) of pred.

<pre>metric_info</pre>	Metrics Information	
------------------------	---------------------	--

# Description

A dataframe storing the information of all metrics. The code to generate the dataset is at system.file('inst/scripts/', 'metric\_info.R', package='poem').

# Usage

metric\_info

#### Format

metric\_info: A data frame.

mockData

Generate mock multidimensional data

#### Description

Generates mock multidimensional data of a given number of classes of points, for testing.

# Usage

```
mockData(
    Ns = c(25, 15),
    classDiff = 2,
    Sds = 1,
    ndims = 2,
    spread = c(1, 2),
    rndFn = rnorm
)
```

### Arguments

Ns	A vector of more than one positive integers specifying the number of elements of each class.
classDiff	The distances between the classes. If there are more than 2 classes, this can be a dist object or a symmetric matrix of length(Ns)-1columns/rows where the lower triangle indicates the desired distances between classes.
Sds	The standard deviation. Can either be a fixed value, a value per class, or a matrix of values for each class (rows) and dimension (column).
ndims	The number of dimensions to generate (default 2).
spread	The spread of the points. Can either be a fixed value, a value per class, or a matrix of values for each class (rows) and dimension (col).
rndFn	The random function, by default rnorm, but should also work for rlnorm and similar.

# Value

A data.frame with coordinates and a class column.

#### Examples

d <- mockData()</pre>

nnWeightedAccuracy nnWeightedAccuracy

# Description

Computes an accuracy score which weighs elements/spots that are misclassified by the proportion of their (spatial) neighborhood that is not of the element/spot's predicted class. This reduces the weight of misclassifications happening at the boundary between domains.

# Usage

```
nnWeightedAccuracy(true, pred, location, k = 5, ...)
```

#### Arguments

true	True class labels (vector coercible to factor)
pred	Predicted labels (vector coercible to factor)
location	The spatial coordinates to compute the nearest neighbors.
k	Number of nearest neighbors
	Optional params passed to findSpatialKNN().

# Value

A scalar representing the weighted accuracy.

noisy\_moon

#### Description

A simple toy dataset consists of two interleaving half circles. The code to generate the dataset is at system.file('inst/scripts/', 'noisy\_moon.R', package='poem').

#### Usage

noisy\_moon

#### Format

noisy\_moon:

A data frame with 100 rows and 5 columns:

x, y Coordinates of each observations.

label Ground truth labels. Either 1 or 2.

**kmeans\_label** Predicted clustering labels using kmeans with 2 centers.

hdbscan\_label Predicted clustering labels using hdbscan with minPts = 5.

PAS

Calculate PAS score

# Description

PAS score measures the clustering performance by calculating the randomness of the spots that located outside of the spatial region where it was clustered to. Lower PAS score indicates better spatial domian clustering performance.

#### Usage

```
PAS(labels, location, k = 10, ...)
```

# Arguments

labels	Cluster labels.
location	A numerical matrix containing the location information, with rows as samples and columns as location dimensions.
k	Number of nearest neighbors.
	Optional params for findSpatialKNN().

# Value

A numeric value for PAS score, and a boolean vector about the abnormal spots.

#### setMatchingAccuracy

#### Examples

```
data(sp_toys)
data <- sp_toys
PAS(data$label, data[,c("x", "y")], k=6)
PAS(data$p1, data[,c("x", "y")], k=6)
PAS(data$p2, data[,c("x", "y")], k=6)</pre>
```

setMatchingAccuracy The non-spatially-weighted counterpart of nnWeightedAccuracy

# Description

The non-spatially-weighted counterpart of nnWeightedAccuracy

#### Usage

setMatchingAccuracy(true, pred)

#### Arguments

true	True class labels (vector coercible to factor)
pred	Predicted labels (vector coercible to factor)

### Value

A scalar representing the weighted accuracy.

silhouetteWidths silhouetteWidths

#### Description

Computes the silhouette widths. If the dataset is sufficiently small for the cluster::silhouette implementation to work, this will be used. Otherwise a slower chunked implementation is used.

# Usage

```
silhouetteWidths(x, labels)
```

#### Arguments

х	A numeric matrix or data.frame with observations as rows.
labels	An integer/factor vector of clustering labels, or length equal to the number of
	rows in x.

# Value

A numeric vector of silhouette widths for each element of x.

### Examples

```
# generate dummy data
m <- matrix(rnorm(100*3),ncol=3)
labels <- sample.int(3,100,replace=TRUE)
# calculate SWs:
sw <- silhouetteWidths(m, labels)</pre>
```

spatialARI

Spatially aware ARI from Yan, Yinqiao, et al. (2025).

#### Description

Computes the spatial Rand Index and spatial ARI (Yan, Feng and Luo, 2025). Note that by default, the decay functions are different from those of the original publication (see details for more information), but the latter can be replicated with original=TRUE.

#### Usage

```
spatialARI(
 true,
 pred,
  location,
 normCoords = TRUE,
 lambda = 0.8,
 fbeta = 4,
 hbeta = 1,
 spotWise = FALSE,
 nChunks = NULL,
 original = FALSE,
  f = function(x) {
     lambda * exp(-x * fbeta)
},
 h = function(x) {
     lambda * (1 - exp(-x * hbeta))
}
)
```

#### Arguments

true	A vector of true class labels
pred	A vector of predicted clusters
location	A matrix of spatial coordinates, with dimensions as columns
normCoords	Logical; whether to normalize the coordinates to 0-1.
lambda	The alpha used in the f and h functions (default 0.8) in Yan, Feng and Luo, 2025.
fbeta, hbeta	Additional factors used in the exponential decay functions (see details). A higher value means a faster decay. These are ignored if original=TRUE.
spotWise	Logical; whether to return the spot-wise spatial concordance (not adjusted for chance).

nChunks	The number of processing chunks. If NULL, this will be determined automati- cally based on the size of the dataset, so as to remain below 2GB RAM usage.
original	Logical; whether to use the original h/f functions from Yan, Feng and Luo (de-fault FALSE). If set to TRUE, the arguments fbeta, hbeta, f and h are ignored.
f	The f function, which determines the positive contribution of pairs that are in different partitions in the reference, but grouped together in the clustering, based on the distance between mates.
h	The h function, which determines the positive contribution of pairs that are in the same partition in the reference, but different ones in the clustering, based on the distance between mates.

#### Details

This is a reimplementation of the method from the spARI package, made more scalable (i.e. a bit slower but more memory-efficient) through chunk-based processing, extensible to more than 2 dimensions, and with some additional options. Note that by default, this will not produce the same results as the original method: to do so, set original=TRUE. In our exploration of the method and its behavior, we found the decay to be too slow, and we therefore 1) do not square the distances, and 2) introduced a beta parameter in each function which allows to scale it (a higher beta parameter means a faster decay).

By default, chunking to keep RAM usage roughly below 2GB. Higher speed can be achieved (at higher memory costs) for larger datasets by limiting the number of chunks. The memory usage if done in a single chunk should be roughly 4e-5\*nrow(location)^2 Mb, and this scales down linearly with the number of chunks.

#### Value

A vector containing the spatial Rand Index (spRI) and spatial adjusted Rand Index (spARI). Alternatively, if spotWise=TRUE, a vector of spatial pair concordances for each spot.

#### Author(s)

Pierre-Luc Germain

#### References

Yan, Feng and Luo, biorxiv 2025, https://doi.org/10.1101/2025.03.25.645156

#### Examples

```
data(sp_toys)
spatialARI(true=sp_toys$label, pred=sp_toys$p2, location = sp_toys[,1:2])
```

sp\_toys

Toy examples of spatial data

#### Description

Toy examples of spatial data. The code to generate the dataset is at system.file('inst/scripts/', 'sp\_toys.R', package='poem').

#### Usage

sp\_toys

# Format

sp\_toys:A data frame with 240 rows and 11 columns, representing a 16 x 15 array of spots:x, y Coordinates of each spots.row, col The row and column index of each spots.

**label** Ground truth labels. Either 1 or 2.

**p1-p6** Hypothetical predicted spatial clustering labels.

toyExamples Toy embedding examples

#### Description

Toy example 2D embeddings of elements of different classes, with varying mixing and spread. Graphs 1-3 all have 20 elements of each of 4 classes, but that are mixed in different fashion in the embedding space. Graphs 4-7 all have 100 elements of class1 and 60 of class2, and the class1 elements vary in their spread. The code to generate the dataset is at system.file('inst/scripts/', 'graph\_example.R', package='poem').

# Usage

toyExamples

# Format

toyExamples:

A data frame.

graph The name of the embedding to which the element belongs.

**x**, **y** Coordinates in the 2D embedding.

class The class to which the element belongs.

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