Package 'StabMap'

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Type Package

Title Stabilised mosaic single cell data integration using unshared features

Version 1.6.0

Description StabMap performs single cell mosaic data integration by first building a mosaic data topology, and for each reference dataset, traverses the topology to project and predict data onto a common embedding. Mosaic data should be provided in a list format, with all relevant features included in the data matrices within each list object. The output of stabMap is a joint low-dimensional embedding taking into account all available relevant features. Expression imputation can also be performed using the StabMap embedding and any of the original data matrices for given reference and query cell lists.

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.runOps *Run a sequence of binary operations*

Description

Run a sequence of binary operations

Usage

```
.runOps(obj, ops, leftToRight = TRUE)
```

Arguments

obj	list of objects.
ops	list of operations (length should be 1 less than 'obj').
leftToRight	logical whether operations should be performed in order from left to right (default), or right to left.

Value

matrix or array output of the sequence of binary operations

adaptiveKNN *Adaptive k-Nearest Neighbour Classification*

Description

Adaptive k-Nearest Neighbour Classification for a k-nearest neighbour matrix, given class labels and local k values for the training data

Usage

```
adaptiveKNN(knn, class, k_local)
```

Arguments

knn	Is a k-nearest neighbour matrix, giving the indices of the training set that the query is closest to. Rows are the query cells, columns are the NNs. Typically output using BiocNeighbors::queryKNN(,,k = max(k_local)).
class	Is the labels associated with the training set.
k_local	Is an integer vector length of the training set, giving the local k to use if k_local is given as a single integer, then that value is used as k for all observations.

Value

A character vector of of classifications for the test set.

Examples

```
# Generate example data
data <- matrix(rpois(10 * 20, 10), 10, 20) # 10 genes, 20 cells
data_2 <- matrix(rpois(10 * 30, 10), 10, 30) # 10 genes, 30 cells

# Generate error matrix for k_local
E <- matrix(runif(100), 20, 5)
colnames(E) <- paste0("K_", 1:5)

# Define training class labels and adaptive k-values
class <- factor(rep(letters[1:2], each = 10))
k_local <- getAdaptiveK(E, labels = class)

knn <- BiocNeighbors::queryKNN(
  t(data), t(data_2),
  k = max(as.numeric(gsub("K_", "", k_local)))
)$index

# Adaptive KNN classification
test <- adaptiveKNN(
  knn, class, as.numeric(gsub("K_", "", k_local))
)
```

`allEqual` *allEqual*

Description

Checks if a vector is equal to its first element

Usage

```
allEqual(x)
```

Arguments

x	A vector.

Value

logical whether a a vector is equal to its first element.

`buildLabelsDataFrame` *buildLabelsDataFrame*

Description

Build dataframe for output from ‘classifyEmbedding‘

Usage

```
buildLabelsDataFrame(labels, resubstituted_labels, k_adaptive)
```

Arguments

`labels`	Is a named character vector with true labels.
`resubstituted_labels`	Is a named character vector with predicted labels.
`k_adaptive`	Is a named vector of the k-values, this could be a single integer when fixed.

Value

A dataframe with rows the same as resubstituted_labels and columns for input_labels, predicted_labels, and resubstituted_labels.

`classifyEmbedding` *Adaptive k-Nearest Neighbour Classification using the StabMap joint embedding*

Description

Performs adaptive k-nearest neighbour classification of discrete labels for a training set from a query set, leveraging the StabMap joint embedding. The training labels are defined in ‘labels‘, with all other rows of the embedding treated as the testing set.

Usage

```
classifyEmbedding(
  coords,
  labels,
  type = c("uniform_fixed", "adaptive_labels", "adaptive_local", "uniform_optimised"),
  k_values = 5,
  error_measure = c("simple_error", "balanced_error"),
  adaptive_nFold = 2,
  adaptive_nRep = 5,
  adaptive_local_nhood = 100,
  adaptive_local_smooth = 10,
  verbose = TRUE
)
```

Arguments

coords	A cells (rows) x dimensions data matrix, on which euclidean distances are to be calculated for KNN classification. Must have rownames. Typically, output from ‘stabMap()‘.
labels	A named character vector of labels for the training set.
type	A character of the type of adaptive KNN classification to be used. Must be one of "adaptive_local", "adaptive_labels", "uniform_optimised", or "uniform_fixed". Default is "uniform_fixed".
k_values	A numeric vector of potential k values. If type is "uniform_fixed", then the first value of k_values is used. Default is 5.
error_measure	Is the error type to use for selection of the best k. Must be one of "simple_error" or "balanced_error". "simple_error" weights all cells equally. "balanced_error" weights error by ‘labels‘ factors. Only affects error type for type == "uniform_optimised".
adaptive_nFold	Is the number of folds for adaptive selection cross-validation.
adaptive_nRep	Is the number of repetitions of adaptive selection cross-validation.
adaptive_local_nhood	Is the neighbourhood size for optimising locally.
adaptive_local_smooth	Is the number of neighbours to use for smoothing locally.
verbose	Logical whether to print repetition and fold number for adaptive selection cross-validation.

Value

Is a dataframe with rows the same as coords, and same rownames. Columns are: input_labels is the training labels that were provided in ‘labels‘ (NA is used as labels for the testing set), resubstituted_labels is predicted labels for all rows (including for the training data), predicted_labels is predicted labels for the testing set but true labels as provided in ‘labels‘ for the training set, k is the adaptive k value used for that each row of the training set.

Examples

```
set.seed(100)
# Simulate coordinates
coords <- matrix(rnorm(1000), 100, 10)
rownames(coords) <- paste0("cell_", seq_len(nrow(coords)))

# Define labels of the first 50 cells
labels <- rep(paste0("type_", letters[1:5]), 10)
names(labels) <- rownames(coords)[seq_along(labels)]

# Uniform fixed KNN classification
knn_out <- classifyEmbedding(
  coords, labels,
  type = "uniform_fixed", k_values = 5
)
```

```
table(knn_out$predicted_labels)

# Adaptive KNN classification using local error
knn_out <- classifyEmbedding(
coords, labels,
type = "adaptive_local",
k_values = 2:3,
adaptive_nFold = 5,
adaptive_nRep = 10
)
table(knn_out$predicted_labels)

knn_out <- classifyEmbedding(
  coords, labels,
  type = "adaptive_labels",
  k_values = 2:3,
  adaptive_nFold = 5,
  adaptive_nRep = 10
)
table(knn_out$predicted_labels)

# Adaptive KNN classification using uniform optimised with balanced error
knn_out <- classifyEmbedding(
  coords, labels,
  type = "uniform_optimised",
  k_values = 2:3,
  adaptive_nFold = 3,
  adaptive_nRep = 10,
  error_measure = "balanced_error"
)
table(knn_out$predicted_labels)
```

`combineBinaryErrors` *combineBinaryErrors*

Description

Combines binary error matrices by averaging error values across all matrices, for each entry (row and column combination)

Usage

```
combineBinaryErrors(E_list)
```

Arguments

`E_list`	A list containing matrices. Each matrix must have the same number of columns (k-values) and contain rownames (cells).

Value

A sparse error matrix.

`getAdaptiveK` *Adaptive k selection for KNN classification*

Description

Given an error matrix, identify the k that maximises the accuracy for cells belonging to a provided labelling/grouping. If no labelling given, expect a cell-cell similarity network to identify the k that maximises the accuracy for cells within that neighbourhood. If neither are given, simply treat all cells as if they have the same labelling/grouping

Usage

```
getAdaptiveK(E, labels = NULL, local = NULL, outputPerCell = TRUE, ...)
```

Arguments

`E`	An error matrix with rows corresponding to cells and columns corresponding to candidate k values, with values themselves corresponding to error values (either binary for single classification, or continuous after multiple classification).
`labels`	Group labels for cells.
`local`	A neighbourhood index representation, as typically output using BiocNeighbors::findKNN().
`outputPerCell`	Logical whether to return adaptive k for each cell, not just for each label type (used for when labels is given).
`...`	Includes return_colnames, whether to give the colnames of the best selected, or just the index, which is default TRUE.

Value

Vector of adaptive k values.

Examples

```
E <- matrix(runif(100), 20, 5)
colnames(E) <- paste0("K_", 1:5)

# generate cell labels
labels <- factor(rep(letters[1:2], each = 10))

# generate nearest neighbourhood index representation
data <- matrix(rpois(10 * 20, 10), 10, 20) # 10 genes, 20 cells
local <- BiocNeighbors::findKNN(t(data), k = 5, get.distance = FALSE)$index

best_k_labels <- getAdaptiveK(E,
```

```
  labels = labels
)
best_k_local <- getAdaptiveK(E,
  local = local
)
```

---

getArgMin *getArgMin*

Description

For each row in a matrix calculate the first index which gives the minimum value

Usage

```
getArgMin(M, return_colnames = TRUE, identicalNA = TRUE)
```

Arguments

M	A matrix.
return_colnames	Logical whether to return column names of matrix (default TRUE). Otherwise return index.
identicalNA	Logical whether to return NA if all values in a row are identical (default TRUE).

Value

A vector containing the first index or column name of the minimum values for each row of the matrix.

---

getBestColumn *getBestColumn*

Description

Identifies the index of the column of a matrix with the minimum mean. If balanced_labels is given then calculate the balanced mean

Usage

```
getBestColumn(E, balanced_labels = NULL)
```

Arguments

E	An error matrix.
balanced_labels	Class labels for each row (cell) of E.

Value

The index of the best performing column of E

`getBinaryError` *getBinaryError*

Description

For potential k values, generate a binary error matrix from KNN label classification

Usage

```
getBinaryError(knn, k_values, class_train, class_true)
```

Arguments

knn	Is a k-nearest neighbour matrix, giving the indices of the training set that the query is closest to. Rows are the query cells, columns are the NNs, should be a large value. Typically output using BiocNeighbors::queryKNN(,,k = max(k_values)).
k_values	Is an integer vector of the values of k to consider for extracting accuracy. If k_values has names then pass these to colnames of E.
class_train	Is a factor or character vector of classes that corresponds to the indices given within knn.
class_true	Is a factor or character vector that corresponds to the rows of knn. If class_true has names then pass these to rownames of E.

Value

A sparse binary error matrix.

`getBinaryErrorFromPredictions` *getBinaryErrorFromPredictions*

Description

Compute binary error between predicted labels and true labels

Usage

```
getBinaryErrorFromPredictions(pred, labels)
```

Arguments

`pred`	Is a matrix of class label predictions.
`labels`	Is a named vector of true labels.

Value

A sparse binary error matrix.

`getModeFirst` *getModeFirst*

Description

Identify the mode of x up to the first index

Usage

```
getModeFirst(x, first)
```

Arguments

`x`	A character or a factor.
`first`	An integer.

Value

A character of the mode of x.

getQueryK *getQueryK*

Description

For each cell in the query data, use the 1NN's adaptive k value (of the reference data) to identify the local best k value

Usage

```
getQueryK(knn, k_local)
```

Arguments

knn	Is a k-nearest neighbour matrix, giving the indices of the training set that the query is closest to. Rows are the query cells, columns are the NNs, should be a large value. Typically output using BiocNeighbors::queryKNN(„k = max(k_local)).
k_local	Is an integer vector length of the reference set, giving the local k to use. If k_local is given as a single integer, then that value is used as k for all observations.

Value

An integer vector with local k to use for each query cell.

gm_mean *gm_mean*

Description

Calculate the geometric mean

Usage

```
gm_mean(x, na.rm = TRUE)
```

Arguments

x	A vector.
na.rm	A logical value indicating whether NA values should be stripped before calculating the geometric mean.

Value

A numeric.

imputeEmbedding *Impute values using StabMap joint embedding*

Description

Performs naive imputation of values from the list of mosaic data and joint embedding from StabMap.

Usage

```
imputeEmbedding(
  assay_list,
  embedding,
  reference = Reduce(union, lapply(assay_list, colnames)),
  query = Reduce(union, lapply(assay_list, colnames)),
  neighbours = 5,
  fun = mean
)
```

Arguments

assay_list	List of mosaic data from which to perform imputation.
embedding	Joint embedding from which to extract nearest neighbour relationships.
reference	Character vector of cell names to treat as reference cells.
query	Character vector of cell names to treat as query cells.
neighbours	Number of nearest neighbours to consider (default 5).
fun	function (default 'mean') to aggregate nearest neighbours' imputed values.

Value

List containing imputed values from each assay_list data matrix which contains reference cells.

Examples

```
set.seed(2021)
assay_list <- mockMosaicData()
lapply(assay_list, dim)

# stabMap
out <- stabMap(assay_list,
  ncomponentsReference = 20,
  ncomponentsSubset = 20
)

# impute values
imp <- imputeEmbedding(assay_list, out)

# inspect the imputed values
```

```
lapply(imp, dim)
imp[[1]][1:5, 1:5]
```

`isUnequal` *isUnequal*

Description

Checks if elements of 2 vectors are unequal

Usage

```
isUnequal(x, y)
```

Arguments

`x`	A vector.
`y`	A vector.

Value

An integer vector. 1 for unequal. 0 for equal

`mockMosaicData` *mockMosaicData*

Description

Mock up a mosaic data list using simulated data, for use in documentation examples.

Usage

```
mockMosaicData(
  names = c("D1", "D2", "D3"),
  ncells = c(50, 50, 50),
  ngenes = list(1:150, 76:225, 151:300),
  fun = "rnorm",
  ...
)
```

Arguments

`names`	character vector of mock datasets.
`ncells`	integer vector of cells in each mock dataset.
`ngenes`	list containing integer vectors of features measured in each mock dataset.
`fun`	name of function to simulate data, default "rnorm".
`...`	further arguments passed to ‘fun‘.

Value

assay_list a list of data matrices with rownames (features) specified.

Examples

```
set.seed(2021)
assay_list <- mockMosaicData()
lapply(assay_list, dim)

# simulate data from another distribution
assay_list <- mockMosaicData(fun = "rnbinom", size = 5, prob = 0.5)
lapply(assay_list, dim)
```

`mosaicDataTopology` *mosaicDataTopology*

Description

Generate mosaic data topology network as an igraph object.

Usage

```
mosaicDataTopology(assay_list)
```

Arguments

`assay_list`	a list of data matrices with rownames (features) specified.

Value

igraph weighted network with nodes corresponding to `assay_list` elements, and edges present if the matrices share at least one rowname. Edge weights correspond to the number of shared rownames among data matrices.

Examples

```
set.seed(2021)
assay_list <- mockMosaicData()
mdt <- mosaicDataTopology(assay_list)
mdt
plot(mdt)
```

mosaicDataUpSet *mosaicDataUpSet*

Description

Plots feature overlaps of mosaic data as an UpSet plot.

Usage

```
mosaicDataUpSet(assay_list, plot = FALSE, ...)
```

Arguments

assay_list	a list of data matrices with rownames (features) specified.
plot	logical (default FALSE) whether the UpSet plot should be printed.
...	further arguments passed to ‘upset‘ from the ‘UpSetR‘ package.

Value

UpSet object displaying degree of overlap of rownames (features) among each of the data matrices in assay_list. Set bars correspond to the number of cells/samples present in each data matrix.

Examples

```
set.seed(2021)
assay_list <- mockMosaicData()
lapply(assay_list, dim)
mosaicDataUpSet(assay_list)

# additional arguments from UpSetR::upset()
mosaicDataUpSet(assay_list, empty.intersections = TRUE)
```

queryNamedKNN *queryNamedKNN*

Description

queryNamedKNN

Usage

```
queryNamedKNN(coords_reference, coords_query, k)
```

Arguments

coords_reference	coords_reference
coords_query	coords_query
k	k

Value

matrix

`reWeightEmbedding` *Re-weight StabMap embedding*

Description

Re-weights embedding according to given weights for each reference dataset. This gives more or less weighting to each contributing dataset and method (PCA or LDA),

Usage

```
reWeightEmbedding(embedding, weights = NULL, factor = 1e+06)
```

Arguments

embedding	Joint embedding as output from stabMap.
weights	(optional) named numeric vector giving relative weights for each reference dataset.
factor	numeric multiplicative value to offset near-zero values.

Value

matrix of same dimensions as ‘embedding‘.

Examples

```
set.seed(2021)
assay_list <- mockMosaicData()
lapply(assay_list, dim)

# specify which datasets to use as reference coordinates
reference_list <- c("D1", "D3")

# specify some sample labels to distinguish using linear discriminant
# analysis (LDA)
labels_list <- list(
  D1 = rep(letters[1:5], length.out = ncol(assay_list[["D1"]]))
)
```

```
# stabMap
out <- stabMap(assay_list,
  reference_list = reference_list,
  labels_list = labels_list,
  ncomponentsReference = 20,
  ncomponentsSubset = 20
)

# look at the scale of each component and discriminant
boxplot(out, las = 2, outline = FALSE)

# re-weight embedding for less contribution from LDs and equal contribution
# from PCs of both references
out_reweighted <- reWeightEmbedding(
  out,
  weights = c("D1_LD" = 0.5, "D1_PC" = 1, "D3_PC" = 1)
)

# look at the new scale of each component and discriminant
boxplot(out_reweighted, las = 2, outline = FALSE)
```

`selectFeatures` *selectFeatures*

Description

For a given assay and set of features, perform variance ranking and select a subset of features

Usage

```
selectFeatures(assay, features, maxFeatures)
```

Arguments

`assay`	An assay matrix rows are features, columns are cells
`features`	Character vector of the current features that are selected
`maxFeatures`	Integer of the number of maxFeatures to select

Value

A character vector of the selected features according to variance ranking.

smoothLocal *smoothLocal*

Description

Smooth out the adaptive k values. Can be smoothed by computing the arithmetic or geometric mean of the adaptive k-values for each cells neighbourhood

Usage

```
smoothLocal(best_k, local, smooth = 10, mean_type = "geometric")
```

Arguments

best_k	Is a named vector of local best k values
local	Is a KNN matrix, with rows same as best_k and values indices of best_k.
smooth	An integer of k-nearest neighbours to smooth over.
mean_type	Character indicating to calculate the 'geometric' or 'arithmetic' mean.

Value

A numeric vector of smoothed adaptive k-values.

stabMap *Stabilised mosaic single cell data integration using unshared features*

Description

stabMap performs mosaic data integration by first building a mosaic data topology, and for each reference dataset, traverses the topology to project and predict data onto a common principal component (PC) or linear discriminant (LD) embedding.

Usage

```
stabMap(
  assay_list,
  labels_list = NULL,
  reference_list = NULL,
  reference_features_list = lapply(assay_list, rownames),
  reference_scores_list = NULL,
  ncomponentsReference = 50,
  ncomponentsSubset = 50,
  suppressMessages = TRUE,
  projectAll = FALSE,
  restrictFeatures = FALSE,
```

```
  maxFeatures = 1000,
  plot = TRUE,
  scale.center = TRUE,
  scale.scale = TRUE,
  SE_assay_names = "logcounts",
  BPPARAM = SerialParam(),
  verbose = TRUE
)
```

Arguments

assay_list	A list of data matrices with rownames (features) specified.
labels_list	(optional) named list containing cell labels
reference_list	Named list containing logical values whether the data matrix should be considered as a reference dataset, alternatively a character vector containing the names of the reference data matrices. If NULL, defaults to: sapply(names(assay_list), function(x) TRUE, simplify = FALSE)
reference_features_list	List of features to consider as reference data (default is all available features).
reference_scores_list	Named list of reference scores (default NULL). If provided, matrix of cells (rows with rownames given) and dimensions (columns with colnames given) are used as the reference low-dimensional embedding to target, as opposed to performing PCA or LDA on the input reference data.
ncomponentsReference	Number of principal components for embedding reference data, given either as an integer or a named list for each reference dataset.
ncomponentsSubset	Number of principal components for embedding query data prior to projecting to the reference, given either as an integer or a named list for each reference dataset.
suppressMessages	Logical whether to suppress messages (default TRUE).
projectAll	Logical whether to re-project reference data along with query (default FALSE).
restrictFeatures	logical whether to restrict to features used in dimensionality reduction of reference data (default FALSE). Overall it's recommended that this be FALSE for single-hop integrations and TRUE for multi-hop integrations.
maxFeatures	Maximum number of features to consider for predicting principal component scores (default 1000).
plot	Logical whether to plot mosaic data UpSet plot and mosaic data topology networks (default TRUE).
scale.center	Logical whether to re-center data to a mean of 0 (default FALSE).
scale.scale	Logical whether to re-scale data to standard deviation of 1 (default FALSE).

SE_assay_names	Either a string indicating the name of the assays for the SummarizedExperiment objects in assay_list or a named list of assay names, where the names corrispond to the names SE objects in assay_list (default "logcounts")
BPPARAM	a BiocParallelParam object specifying how parallelisation should be performed
verbose	Logical whether console output is provided (default TRUE)

Value

matrix containing common embedding with rows corresponding to cells, and columns corresponding to PCs or LDs for reference dataset(s).

Examples

```
set.seed(2021)
assay_list <- mockMosaicData()
lapply(assay_list, dim)

# specify which datasets to use as reference coordinates
reference_list <- c("D1", "D3")

# specify some sample labels to distinguish using linear discriminant
# analysis (LDA)
labels_list <- list(
  D1 = rep(letters[1:5], length.out = ncol(assay_list[["D1"]]))
)

# examine the topology of this mosaic data integration
mosaicDataUpSet(assay_list)
plot(mosaicDataTopology(assay_list))

# stabMap
out <- stabMap(assay_list,
  reference_list = reference_list,
  labels_list = labels_list,
  ncomponentsReference = 20,
  ncomponentsSubset = 20
)

head(out)
```

---

vectorSubset *vectorSubset*

Description

vectorSubset

Usage

```
vectorSubset(vec, mat)
```

Arguments

vec	vec
mat	mat

Value

matrix

%pred% *Binary operator for model predictions on data*

Description

This function performs model predictions via the `predict` function for each column of data.

Usage

```
data %pred% models
```

Arguments

data	is a matrix with rows corresponding to features, and columns corresponding to cells/observations
models	is a list of univariate outcome models with the features as explanatory variables

Value

a matrix with rows equal to `length(models)` and columns corresponding to cells/observations

---

%projpred% *Project and/or predict data using feature weights or a LDA model object*

Description

This function takes a data matrix a and, depending on the class of b, projects the data using feature weights, or predicts new values using linear discriminant analysis (LDA) model object, or both.

Usage

```
a %projpred% b
```

Arguments

a	a matrix with colnames specified
b	a matrix with rownames specified, or a lda model object, or a list containing a matrix and/or a lda model object.

Value

matrix

%*1% *Sorted matrix multiplication with intercept column*

Description

This function first binds a column filled with 1s named `intercept` to `a`, then performs rownames and colnames-aware (`%**%`) matrix multiplication with `b`.

Usage

```
a %*1% b
```

Arguments

a	a matrix with rownames specified
b	a matrix with colnames specified

Value

matrix

%**% *Sorted matrix multiplication*

Description

This function multiplies two matrices but first reorders the rows of the second matrix to match the columns of the first matrix

Usage

```
X %**% Y
```

Arguments

X	a matrix with colnames specified.
Y	a matrix with rownames specified. Alternatively, a list assumed to contain two objects, a matrix with rownames specified, and a vector of scaling values for subtraction.

Value

matrix

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