Package ‘scClassify’

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Type Package
Title scClassify: single-cell Hierarchical Classification
Version 1.14.0
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Description scClassify is a multiscale classification framework for single-cell RNA-seq data based on ensemble learning and cell type hierarchies, enabling sample size estimation required for accurate cell type classification and joint classification of cells using multiple references.
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The scClassifyTrainModel class

Description

The scClassifyTrainModel class is designed to store training model for scClassify

Usage

```r
scClassifyTrainModel(
  name,
  cellTypeTree,
  cellTypeTrain,
  features,
  model,
  modelweights,
  metaData
)
```
Arguments

name Name of the training dataset
cellTypeTree A list indicate a cell type tree
cellTypeTrain A vector of cell type in training dataset
features A vector of character indicates the features that are trained for this data
model A list stored the training model, including the features that are selected and the cell expression matrix that are used for training
modelweights A vector of numeric indicates the weights of each model
metaData A DataFrame stored meta data of training model

Value

A scClassifyTrainModel object

Author(s)

Yingxin Lin

### cellTypeTrain

*Accessors of cellTypeTrain for scClassifyTrainModel*

#### Description

Methods to access various components of the ‘scClassifyTrainModel’ object.

#### Usage

```
cellTypeTrain(x)
```

#### Arguments

x A ‘scClassifyTrainModel’ object.

#### Value

cellTypeTrain of the scClassifyTrainModel slot

#### Examples

```
data(trainClassExample_xin)
cellTypeTrain(trainClassExample_xin)
```
cellTypeTree

Accessors of cellTypeTree for scClassifyTrainModel

Description
Methods to access various components of the 'scClassifyTrainModel' object.

Usage

cellTypeTree(x)

Arguments

x A 'scClassifyTrainModel' object.

Value
cellTypeTree of the scClassifyTrainModel slot

Examples

data(trainClassExample_xin)
cellTypeTree(trainClassExample_xin)

features

Accessors of features for scClassifyTrainModel

Description
Methods to access various components of the 'scClassifyTrainModel' object.

Usage

features(x)

Arguments

x A 'scClassifyTrainModel' object.

Value

features of the scClassifyTrainModel slot

Examples

data(trainClassExample_xin)
features(trainClassExample_xin)
getN

**Function to get the required N given by the accuracy and the learning curve model**

**Description**

Function to get the required N given by the accuracy and the learning curve model

**Usage**

getN(res, acc = 0.9)

**Arguments**

- **res**: model results returned by `learning_curve` function
- **acc**: accuracy that are quired

**Value**

sample size that are required

**Examples**

```r
set.seed(2019)
n <- seq(20, 10000, 100)
accMat <- do.call(cbind, lapply(1:length(n), function(i){
tmp_n <- rep(n[i], 50)
y <- -2/(tmp_n^0.8) + 0.95 + rnorm(length(tmp_n), 0, 0.02)
}))
res <- learningCurve(accMat = accMat, n)
N <- getN(res, acc = 0.9)
```

---

**learningCurve**

*Fit learning curve for accuracy matrix*

**Description**

Fit learning curve for accuracy matrix
Usage

learningCurve(
  accMat,  
  n,  
  auto_initial = TRUE,  
  a = NULL,  
  b = NULL,  
  c = NULL,  
  d_list = NULL,  
  fitmodel = c("nls", "nls_mix", "gam"),  
  plot = TRUE,  
  verbose = TRUE
)

Arguments

  accMat     Matrix of accuracy rate where column indicate different sample size  
  n          Vector indicates the sample size  
  auto_initial  whether automatical initialise  
  a          input the parameter a starting point  
  b          input the parameter a starting point  
  c          input the parameter a starting point  
  d_list     range of d  
  fitmodel   "nls", "nls_mix", "gam"  
  plot       indicates whether plot or not  
  verbose    indicates whether verbose or not

Value

  list of results

Author(s)

  Yingxin Lin

Examples

  set.seed(2019)  
  n <- seq(20, 10000, 100)  
  accMat <- do.call(cbind, lapply(1:length(n), function(i){  
    tmp_n <- rep(n[i], 50)  
    y <- -2/(tmp_n^0.8) + 0.95 + rnorm(length(tmp_n), 0, 0.02)  
  }))  
  res <- learningCurve(accMat = accMat, n)  
  N <- getN(res, acc = 0.9)
### Description

Methods to access various components of the `scClassifyTrainModel` object.

### Usage

```r
model(x)
```

### Arguments

- **x**: A `scClassifyTrainModel` object.

### Value

model of the scClassifyTrainModel slot

### Examples

```r
data(trainClassExample_xin)
model(trainClassExample_xin)
```

---

### Description

Methods to access various components of the `scClassifyTrainModel` object.

### Usage

```r
modelweights(x)
```

### Arguments

- **x**: A `scClassifyTrainModel` object.

### Value

modelweights of the scClassifyTrainModel slot

### Examples

```r
data(trainClassExample_xin)
modelweights(trainClassExample_xin)
```
name

**Accessors of name for scClassifyTrainModel**

**Description**

Methods to access various components of the 'scClassifyTrainModel' object.

**Usage**

```r
name(x)
```

**Arguments**

- **x**
  
  A 'scClassifyTrainModel' object.

**Value**

name of the scClassifyTrainModel slot

**Examples**

```r
data(trainClassExample_xin)
name(trainClassExample_xin)
```

---

**plotCellTypeTree**

To plot cell type tree

**Description**

To plot cell type tree

**Usage**

```r
plotCellTypeTree(cutree_list, group_level = NULL)
```

**Arguments**

- **cutree_list**
  
  A list indicates the hierarchical cell type tree

- **group_level**
  
  Indicate whether plot or not

**Value**

A ggplot object visualising the HOPACH tree
predict_scClassify

Examples

data("trainClassExample_xin")

plotCellTypeTree(cellTypeTree(trainClassExample_xin))

predict_scClassify	Testing scClassify model

Description

Testing scClassify model

Usage

predict_scClassify(
  exprsMat_test,
  trainRes,
  cellTypes_test = NULL,
  k = 10,
  prob_threshold = 0.7,
  cor_threshold_static = 0.5,
  cor_threshold_high = 0.7,
  features = "limma",
  algorithm = "WKNN",
  similarity = "pearson",
  cutoff_method = c("dynamic", "static"),
  weighted_ensemble = FALSE,
  weights = NULL,
  parallel = FALSE,
  BPPARAM = BiocParallel::SerialParam(),
  verbose = FALSE
)

Arguments

  exprsMat_test  A list or a matrix indicates the log-transformed expression matrices of the query datasets
  trainRes      A 'scClassifyTrainModel' or a 'list' indicates scClassify trained model
  cellTypes_test A list or a vector indicates cell types of the query datasets (Optional).
  k             An integer indicates the number of neighbour
  prob_threshold A numeric indicates the probability threshold for KNN/WKNN/DWKNN.
  cor_threshold_static  A numeric indicates the static correlation threshold.
  cor_threshold_high    A numeric indicates the highest correlation threshold
predict_scClassify

features A vector indicates the gene selection method, set as "limma" by default. This should be one or more of "limma", "DV", "DD", "chisq", "BI".

algorithm A vector indicates the KNN method that are used, set as "WKNN" by default. This should be one or more of "WKNN", "KNN", "DWKNN".

similarity A vector indicates the similarity measure that are used, set as "pearson" by default. This should be one or more of "pearson", "spearman", "cosine", "jaccard", "kendall", "binomial", "weighted_rank", "manhattan"

cutoff_method A vector indicates the method to cutoff the correlation distribution. Set as "dynamic" by default.

weighted_ensemble A logical input indicates in ensemble learning, whether the results is combined by a weighted score for each base classifier.

weights A vector indicates the weights for ensemble

parallel A logical input indicates whether running in parallel or not

BPPARAM A BiocParallelParam class object from the BiocParallel package is used. Default is SerialParam().

verbose A logical input indicates whether the intermediate steps will be printed

Value

list of results

Author(s)

Yingxin Lin

Examples

data("scClassify_example")
wang_cellTypes <- scClassify_example$wang_cellTypes
eexprsMat_wang_subset <- scClassify_example$eexprsMat_wang_subset
data("trainClassExample_xin")
pred_res <- predict_scClassify(exprsMat_test = eexprsMat_wang_subset, trainRes = trainClassExample_xin, cellTypes_test = wang_cellTypes, algorithm = "WKNN", features = c("limma"), similarity = c("pearson"), prob_threshold = 0.7, verbose = TRUE)
**predict_scClassifyJoint**

Testing scClassify model (joint training)

**Description**

Testing scClassify model (joint training)

**Usage**

```r
predict_scClassifyJoint(
  exprsMat_test,
  trainRes,
  cellTypes_test = NULL,
  k = 10,
  prob_threshold = 0.7,
  cor_threshold_static = 0.5,
  cor_threshold_high = 0.7,
  features = "limma",
  algorithm = "WKNN",
  similarity = "pearson",
  cutoff_method = c("dynamic", "static"),
  parallel = FALSE,
  BPPARAM = BiocParallel::SerialParam(),
  verbose = FALSE
)
```

**Arguments**

- `exprsMat_test`: A list or a matrix indicates the expression matrices of the testing datasets
- `trainRes`: A `scClassifyTrainModel` or a `list` indicates scClassify training model
- `cellTypes_test`: A list or a vector indicates cell types of the testing datasets (Optional).
- `k`: An integer indicates the number of neighbour
- `prob_threshold`: A numeric indicates the probability threshold for KNN/WKNN/DWKNN.
- `cor_threshold_static`: A numeric indicates the static correlation threshold.
- `cor_threshold_high`: A numeric indicates the highest correlation threshold.
- `features`: A vector indicates the method to select features, set as "limma" by default. This should be one or more of "limma", "DV", "DD", "chisq", "BI".
- `algorithm`: A vector indicates the KNN method that are used, set as "WKNN" by default. This should be one or more of "WKNN", "KNN", "DWKNN".
- `similarity`: A vector indicates the similarity measure that are used, set as "pearson" by default. This should be one or more of "pearson", "spearman", "cosine", "jaccard", "kendall", "binomial", "weighted_rank", "manhattan"
cutoff_method  A vector indicates the method to cutoff the correlation distribution. Set as "dynamic" by default.
parallel  A logical input indicates whether running in parallel or not
BPPARAM  A BiocParallelParam class object from the BiocParallel package is used. Default is SerialParam().
verbose  A logical input indicates whether the intermediate steps will be printed

Value
list of results

Author(s)
Yingxin Lin

Examples

data("scClassify_example")
wang_cellTypes <- scClassify_example$wang_cellTypes
eexprsMat_wang_subset <- scClassify_example$eexprsMat_wang_subset
data("trainClassExample_xin"")
data("trainClassExample_wang")

trainClassExampleJoint <- scClassifyTrainModelList(trainClassExample_wang, trainClassExample_xin)

pred_res_joint <- predict_scClassifyJoint(exprsMat_test = exprsMat_wang_subset, trainRes = trainClassExampleJoint, cellTypes_test = wang_cellTypes, algorithm = "WKNN", features = c("limma"), similarity = c("pearson"), prob_threshold = 0.7, verbose = FALSE)

table(pred_res_joint$jointRes$cellTypes, wang_cellTypes)

---

runHOPACH  Create HOPACH tree

Description
A function generating HOPACH tree using the average expression matrix for each cell type.

Usage

runHOPACH(data, plot = TRUE, kmax = 5)
Arguments

- **data**: A matrix of average expression matrix (each row indicates the gene, each column indicates the cell type)
- **plot**: Indicate whether plot or not
- **kmax**: Integer between 1 and 9 specifying the maximum number of children at each node in the tree.

Value

Return a list where

- cutree_list: A list indicates the hierarchical cell type tree
- plot: A ggplot visualise the cell type tree

Author(s)

Yingxin Lin

References


Examples

data("scClassify_example")
wang_cellTypes <- factor(scClassify_example$wang_cellTypes)
exprsMat_wang_subset <- scClassify_example$exprsMat_wang_subset
avgMat_wang <- apply(exprsMat_wang_subset, 1, function(x)
aggregate(x, list(wang_cellTypes), mean)$x)
rownames(avgMat_wang) <- levels(wang_cellTypes)
res_hopach <- runHOPACH(avgMat_wang)
res_hopach$plot
Usage

runSampleCal(
    exprsMat,
    cellTypes,
    n_list = c(20, 40, 60, 80, 100, seq(200, 500, 100)),
    num_repeat = 20,
    level = NULL,
    cellType_tree = NULL,
    BPPARAM = BiocParallel::SerialParam(),
    subset_test = FALSE,
    num_test = NULL,
    ...
)

Arguments

exprsMat       A matrix of expression matrix of pilot dataset (log-transformed, or normalised)
cellTypes      A vector of cell types of pilot dataset
n_list         A vector of integer indicates the sample size to run.
num_repeat     An integer indicates the number of run for each sample size will be repeated.
level          An integer indicates the accuracy rate is calculate based on the n-th level from top of cell type tree. If it is NULL (by default), it will be the bottom of the cell type tree. It can not be larger than the total number of levels of the tree.
cellType_tree  A list indicates the cell type tree (optional), if it is NULL, the accuracy rate is calculate based on the provided cellTypes.
BPPARAM        A BiocParallelParam class object from the BiocParallel package is used. Default is SerialParam().
subset_test    A logical input indicates whether we used a subset of data (fixed number for each sample size) to test instead of all remaining data. By default, it is FALSE.
num_test       An integer indicates the size of the test data.
...             other parameter from scClassify

Value

A matrix of accuracy matrix, where columns corresponding to different sample sizes, rows corresponding to the number of repetition.

Examples

data("scClassify_example")
xin_cellTypes <- scClassify_example$xin_cellTypes
driveMat_xin_subset <- scClassify_example$exprsMat_xin_subset

driveMat_xin_subset <- as(driveMat_xin_subset, "dgCMatrix")
set.seed(2019)
accMat <- runSampleCal(driveMat_xin_subset,
scClassify

xin_cellTypes,
n_list = seq(20, 100, 20),
num_repeat = 5, BPPARAM = BiocParallel::SerialParam()

scClassify  
Train and test scClassify model

Description

Train and test scClassify model

Usage

scClassify(
  exprsMat_train = NULL,
  cellTypes_train = NULL,
  exprsMat_test = NULL,
  cellTypes_test = NULL,
  tree = "HOPACH",
  algorithm = "WKNN",
  selectFeatures = "limma",
  similarity = "pearson",
  cutoff_method = c("dynamic", "static"),
  weighted_ensemble = FALSE,
  weights = NULL,
  weighted_jointClassification = TRUE,
  cellType_tree = NULL,
  k = 10,
  topN = 50,
  hopach_kmax = 5,
  pSig = 0.01,
  prob_threshold = 0.7,
  cor_threshold_static = 0.5,
  cor_threshold_high = 0.7,
  returnList = TRUE,
  parallel = FALSE,
  BPPARAM = BiocParallel::SerialParam(),
  verbose = FALSE
)

Arguments

exprsMat_train  A matrix of log-transformed expression matrix of reference dataset

cellTypes_train  
A vector of cell types of reference dataset

exprsMat_test  A list or a matrix indicates the expression matrices of the query datasets
cellTypes_test A list or a vector indicates cell types of the query datasets (Optional).
tree A vector indicates the method to build hierarchical tree, set as "HOPACH" by default. This should be one of "HOPACH" and "HC" (using hclust).
algorithm A vector indicates the KNN method that are used, set as "WKNN" by default. This should be one or more of "WKNN", "KNN", "DWKNN".
selectFeatures A vector indicates the gene selection method, set as "limma" by default. This should be one or more of "limma", "DV", "DD", "chisq", "BI" and "Cepo".
similarity A vector indicates the similarity measure that are used, set as "pearson" by default. This should be one or more of "pearson", "spearmcan", "cosine", "jaccard", "kendall", "binomial", "weighted_rank", "manhattan"
cutoff_method A vector indicates the method to cutoff the correlation distribution. Set as "dynamic" by default.
weighted_ensemble A logical input indicates in ensemble learning, whether the results is combined by a weighted score for each base classifier.
weights A vector indicates the weights for ensemble
weighted_jointClassification A logical input indicates in joint classification using multiple training datasets, whether the results is combined by a weighted score for each training model.

A list indicates the cell type tree provided by user. (By default, it is NULL) (Only for one training data input)
k An integer indicates the number of neighbour
topN An integer indicates the top number of features that are selected
hopach_kmax An integer between 1 and 9 specifying the maximum number of children at each node in the HOPACH tree.
pSig A numeric indicates the cutoff of pvalue for features
prob_threshold A numeric indicates the probability threshold for KNN/WKNN/DWKNN.
cor_threshold_static A numeric indicates the static correlation threshold.
cor_threshold_high A numeric indicates the highest correlation threshold
returnList A logical input indicates whether the output will be class of list
parallel A logical input indicates whether running in parallel or not
BPPARAM A BiocParallelParam class object from the BiocParallel package is used. Default is SerialParam().
verbose A logical input indicates whether the intermediate steps will be printed

Value
A list of the results, including testRes storing the results of the testing information, and trainRes storing the training model information.
Author(s)
Yingxin Lin

Examples

data("scClassify_example")
xin_cellTypes <- scClassify_example$xin_cellTypes
eexprsMat_xin_subset <- scClassify_example$exprsMat_xin_subset
wang_cellTypes <- scClassify_example$wang_cellTypes
eexprsMat_wang_subset <- scClassify_example$exprsMat_wang_subset

scClassify_res <- scClassify(exprsMat_train = eexprsMat_xin_subset, cellTypes_train = xin_cellTypes, eexprsMat_test = list(wang = eexprsMat_wang_subset), cellTypes_test = list(wang = wang_cellTypes), tree = "HOPACH", algorithm = "WKNN", selectFeatures = c("limma"), similarity = c("pearson"), returnList = FALSE, verbose = FALSE)

scClassifyTrainModel-class

An S4 class to stored training model for scClassify

Description
An S4 class to stored training model for scClassify

Slots

name Name of the training dataset
cellTypeTrain A vector of cell type in training dataset
cellTypeTree A list indicate a cell type tree
features A vector of character indicates the features that are trained for this data
model A list stored the training model, including the features that are selected and the cell expression matrix that are used for training
modelweights A vector of numeric indicates the weights of each model
metaData A DataFrame stored meta data of training model
The `scClassifyTrainModelList` class

**Description**

The `scClassifyTrainModelList` class

**Usage**

`scClassifyTrainModelList(...)`

**Arguments**

`...` scClassifyTrainModel objects

**Value**

A scClassifyTrainModelList object

**Examples**

```r
data("trainClassExample_xin")
data("trainClassExample_wang")
trainClassExampleList <- scClassifyTrainModelList(trainClassExample_xin, trainClassExample_wang)
```

An S4 class to store a list of training models from scClassify
scClassify_example  Example data used in scClassify package

Description
A list includes expression matrix and cell type of subsets of wang et al., xin et al.

Usage
data(scClassify_example, package = 'scClassify')

Format
An object of class list of length 4.

Source

trainClassExample_wang  Subset of pretrained model of Wang et al.

Description
An object of scClassifyTrainModel for Wang et al.

Usage
data(trainClassExample_wang, package = 'scClassify')

Format
An object of class scClassifyTrainModel of length 1.

Source
trainClassExample_xin  Subset of pretrained model of Xin et al.

Description

An object of scClassifyTrainModel for Xin et al.

Usage

data(trainClassExample_xin, package = 'scClassify')

Format

An object of class scClassifyTrainModel of length 1.

Source


train_scClassify  Training scClassify model

Description

Training scClassify model

Usage

train_scClassify(
  exprsMat_train,
  cellTypes_train,
  tree = "HOPACH",
  selectFeatures = "limma",
  topN = 50,
  hopach_kmax = 5,
  pSig = 0.05,
  cellType_tree = NULL,
  weightsCal = FALSE,
  parallel = FALSE,
  BPPARAM = BiocParallel::SerialParam(),
  verbose = TRUE,
  returnList = TRUE,
  ...
)
train_scClassify

Arguments

exprsMat_train  A matrix of log-transformed expression matrix of reference dataset

cellTypes_train  A vector of cell types of reference dataset

tree  A vector indicates the method to build hierarchical tree, set as "HOPACH" by default. This should be one of "HOPACH" and "HC" (using stats::hclust).

selectFeatures  A vector indicates the gene selection method, set as "limma" by default. This should be one or more of "limma", "DV", "DD", "chisq", "BI", "Cepo".

topN  An integer indicates the top number of features that are selected

hopach_kmax  An integer between 1 and 9 specifying the maximum number of children at each node in the HOPACH tree.

pSig  A numeric indicates the cutoff of pvalue for features

getCellType_tree  A list indicates the cell type tree provided by user. (By default, it is NULL)

weightsCal  A logical input indicates whether we need to calculate the weights for the model.

parallel  A logical input indicates whether the algorithms will run in parallel

BPPARAM  A BiocParallelParam class object from the BiocParallel package is used. Default is SerialParam().

verbose  A logical input indicates whether the intermediate steps will be printed

returnList  A logical input indicates whether the output will be class of list

...  Other input for predict_scClassify for the case when weights calculation of the pretrained model is performed

Value

list of results or an object of scClassifyTrainModel

Author(s)

Yingxin Lin

Examples

data("scClassify_example")
xin_cellTypes <- scClassify_example$xin_cellTypes
eleMat_xin_subset <- scClassify_example$eleMat_xin_subset
trainClass <- train_scClassify(exprsMat_train = eleMat_xin_subset,
cellTypes_train = xin_cellTypes,
selectFeatures = c("limma", "BI"),
returnList = FALSE
)
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