Package ‘MSiP’

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**Type** Package

**Title** 'MassSpectrometry' Interaction Prediction

**Version** 1.3.7

**Description** The ‘MSiP’ is a computational approach to predict protein-protein interactions from large-scale affinity purification mass spectrometry (AP-MS) data. This approach includes both spoke and matrix models for interpreting AP-MS data in a network context. The "spoke" model considers only bait-prey interactions, whereas the "matrix" model assumes that each of the identified proteins (baits and prey) in a given AP-MS experiment interacts with each of the others. The spoke model has a high false-negative rate, whereas the matrix model has a high false-positive rate. Although, both statistical models have merits, a combination of both models has shown to increase the performance of machine learning classifiers in terms of their capabilities in discrimination between true and false positive interactions.

**Depends** R (>= 3.6.0)

**Imports** dplyr (>= 1.0.6), tibble (>= 3.1.2), tidyr (>= 1.1.3), magrittr (>= 2.0.1), plyr (>= 1.8.6), PRROC (>= 1.3.1), caret (>= 6.0.88), e1071 (>= 1.7.7), mice (>= 3.13.0), pROC (>= 1.17.0.1), ranger (>= 0.12.1)

**License** GPL-3

**Encoding** UTF-8

**LazyData** true

**RoxygenNote** 7.1.1

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**VignetteBuilder** knitr

**NeedsCompilation** no

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**Repository** CRAN

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Description

This function applies Comparative Proteomic Analysis Software Suite (CompPASS) model to score instances (e.g., bait-prey interactions (BPIs) in the data.frame. The CompPASS is a robust statistical scoring scheme for assigning confidence scores to bait-prey interactions (Sowa et al., 2009). This function was based on the source code. https://github.com/dnusinow/cRomppass

Usage

cPASS(datInput)

Arguments

datInput  Data frame with column names: Experiment.id, Replicate, Bait, Prey, and count (i.e., prey count).

Value

Data frame containing bait-prey pairs with average peptide spectrum match (PSMs), total PSMs, ratio total PSMs,Z-score,S-score,D-score and WD-score.

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References


diceCoefficient

Examples

data(SampleDatInput)
datScoring <- cPASS(SampleDatInput)
head(datScoring)

Description

This function applies Dice coefficient to score instances (e.g., bait-prey interactions (BPIs) in the data.frame). The Dice coefficient was first applied by Zhang et al., 2008 to score interactions between all identified proteins (baits and preys) in a given AP-MS experiment.

Usage

diceCoefficient(datInput)

Arguments

datInput Data frame with column names: Experiment.id, Replicate, Bait, Prey, and count (i.e., prey count).

Value

Data frame containing bait-prey pairs with Dice coefficient score, a number between 0 and 1

Author(s)

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References


Examples

data(SampleDatInput)
datScoring <- diceCoefficient(SampleDatInput)
head(datScoring)
Description

This function computes the Jaccard similarity coefficient scores for instances (e.g., bait-prey interactions (BPIs)) in the data.frame.

Usage

jaccardCoefficient(datInput)

Arguments

datInput: Data frame with column names: Experiment.id, Replicate, Bait, Prey, and count (i.e., prey count).

Value

Data frame containing bait-prey pairs with the Jaccard coefficient score, a number between 0 and 1.

Author(s)

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Examples

data(SampleDatInput)
datScoring <- jaccardCoefficient(SampleDatInput)
head(datScoring)

Description

This function computes the overlap similarity scores for instances (e.g., bait-prey interactions (BPIs)) in the data.frame.

Usage

overlapScore(datInput)

Arguments

datInput: Data frame with column names: Experiment.id, Replicate, Bait, Prey, and count (i.e., prey count).
rfTrain

Value
Data frame containing bait-prey pairs with the overlap score, a number between 0 and 1

Author(s)
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References

Examples
data(SampleDatInput)
datScoring <- overlapScore(SampleDatInput)
head(datScoring)

Description
The labeled feature matrix can be used as input for Random Forest (RF) classifier. The classifier then assigns each bait-prey pair a confidence score, indicating the level of support for that pair of proteins to interact. Hyperparameter optimization can also be performed to select a set of parameters that maximizes the model’s performance. This function also computes the areas under the precision-recall (PR) and ROC curve to evaluate the performance of the classifier.

Usage
rfTrain(
  dtInput,
  impute = TRUE,
  p = 0.3,
  parameterTuning = TRUE,
  mtry = seq(from = 1, to = 10, by = 2),
  min_node_size = seq(from = 1, to = 9, by = 2),
  splitrule = c("gini"),
  metric = "Accuracy",
  resampling.method = "repeatedcv",
  iter = 5,
  repeats = 5,
  pr.plot = TRUE,
  roc.plot = TRUE
)
Arguments

dtInput  Data frame containing instances with class labels
impute  Logical value, indicating whether to impute missing values
p  The percentage of data that goes to training; defaults to 0.3
parameterTuning  Logical value; indicating whether to tune rf hyper parameters
mtry  Number of variables to possibly split at in each node and it is bound by the number of variables in your model
min_node_size  Minimal node size
splitrule  Splitrule rule for classification: 'gini', 'extratrees' or 'hellinger' with default 'gini'
metric  A string that specifies what summary metric will be used to select the optimal model; default to Accuracy
resampling.method  The resampling method: 'boot', 'boot632', 'optimism_boot', 'boot_all', 'cv', 'repeatedcv', 'LOOCV', 'LGOCV'; defaults to repeatedcv
iter  Number of resampling iterations; defaults to 5
repeats  for repeated k-fold cross validation only; defaults to 5
pr.plot  Logical value, indicating whether to plot precision-recall (PR) curve
roc.plot  Logical value, indicating whether to plot ROC curve

Value

Data frame containing a classification results for all instances in the data set, where positive confidence score corresponds to the level of support for the pair of proteins to be true positive, whereas negative score corresponds to the level of support for the pair of proteins to be true negative.

Author(s)

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Examples

data(testdfClassifier)

predicted_RF <-
rfTrain(testdfClassifier,impute = FALSE, p = 0.3, parameterTuning = FALSE,
mtry = seq(from = 1, to = 5, by = 1),
min_node_size = seq(from = 1, to = 5, by = 1),
splitrule =c("gini"),metric = "Accuracy",
resampling.method = "cv",iter = 2,repeats = 2,
pr.plot = TRUE, roc.plot = FALSE)
head(predicted_RF)
SampleDatInput

Test data for scoring

Description

Bait-Prey Interactions (BPIs)

Usage

data(SampleDatInput)

Details

• Experiment ID
• Replicate
• Bait
• Prey
• counts

Author(s)

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simpsonCoefficient

Description

This function computes the Simpson similarity coefficient scores for instances (e.g., bait-prey interactions (BPIs)) in the data.frame.

Usage

simpsonCoefficient(datInput)

Arguments

datInput Data frame with column names: Experiment.id, Replicate, Bait, Prey, and count (i.e., prey count).

Value

Data frame containing bait-prey pairs with Simpson coefficient, a number between 0 and 1
Author(s)

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Examples

data(SampleDatInput)
datScoring <- overlapScore(SampleDatInput)
head(datScoring)

Description

The labeled feature matrix can be used as input for Support Vector Machines (SVM) classifier. The classifier then assigns each bait-prey pair a confidence score, indicating the level of support for that pair of proteins to interact. Hyperparameter optimization can also be performed to select a set of parameters that maximizes the model's performance. This function also computes the areas under the precision-recall (PR) and ROC curve to evaluate the performance of the classifier.

Usage

svmTrain(
dtInput,
impute = TRUE,
p = 0.3,
parameterTuning = TRUE,
cost = seq(from = 2, to = 10, by = 2),
gamma = seq(from = 0.01, to = 0.1, by = 0.02),
kernels = "radial",
ncross = 10,
pr.plot = TRUE,
roc.plot = TRUE
)

Arguments

dtInput Data frame containing instances with class labels
impute Logical value, indicating whether to impute missing values
p The percentage of data that goes to training; defaults to 0.3
parameterTuning Logical value; indicating whether to tune SVM hyper parameters
cost Cost of constraints violation
gamma Parameter needed for all kernels except linear
kernels Kernel type: 'linear', 'polynomial', 'sigmoid', or 'radial'; defaults to 'radial'
K-fold cross validation on the training data is performed to assess the quality of the model; defaults to 10

Logical value, indicating whether to plot precision-recall (PR) curve

Logical value, indicating whether to plot ROC curve

Data frame containing a classification results for all instances in the data set, where positive confidence score corresponds to the level of support for the pair of proteins to be true positive, whereas negative score corresponds to the level of support for the pair of proteins to be true negative.

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```r
data(testdfClassifier)
predicted_SVM <-
svmTrain(testdfClassifier, impute = FALSE, p = 0.3, parameterTuning = FALSE,
         cost = seq(from = 2, to = 10, by = 2),
         gamma = seq(from = 0.01, to = 0.10, by = 0.02),
         kernel = "radial", ncross = 10,
         pr.plot = FALSE, roc.plot = TRUE)
head(predicted_SVM)
```
Description

This function computes the weighted matrix model for instances (e.g., bait-prey interactions (BPIs)) in the data.frame. The output of the weighted matrix model includes the number of experiments for which the pair of proteins is co-purified (i.e., k) and -1*log(P-value) of the hypergeometric test (i.e., logHG) given the experimental overlap value, each protein’s total number of observed experiments, and the total number of experiments (Drew et al., 2017).

Usage

Weighted.matrixModel(datInput)

Arguments

datInput  Data frame with column names: Experiment.id, Replicate, Bait, Prey, and count (i.e., prey count).

Value

Data frame containing bait-prey pairs with k (i.e., number of co-purifications) & logHG (i.e., -$1^*$log(P-val) of the hypergeometric test)

Author(s)

Matineh Rahmatbakhsh, <matinerb.94@gmail.com>

References


Examples

data(SampleDatInput)
datScoring <- Weighted.matrixModel(SampleDatInput)
head(datScoring)
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