## Package 'LedPred'

December 12, 2025

Title Learning from DNA to Predict Enhancers

**Description** This package aims at creating a predictive model of regulatory sequences used to score unknown sequences based on the content of DNA motifs, next-generation sequencing (NGS) peaks and signals and other numerical scores of the sequences using supervised classification. The package contains a workflow based on the support vector machine (SVM) algorithm that maps features to sequences, optimize SVM parameters and feature number and creates a model that can be stored and used to score the regulatory potential of unknown sequences.

```
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Author Elodie Darbo, Denis Seyres, Aitor Gonzalez

Maintainer Aitor Gonzalez <aitor.gonzalez@univ-amu.fr>

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```

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## **Description**

createModel function creates a SVM model from the training data set with the selected features.

## Usage

```
createModel(data, cl = 1, kernel = "radial", cost = 1, gamma = 1,
  valid.times = 10, feature.ranking = NULL, feature.nb = NULL,
  file.prefix = NULL)
```

data	data.frame containing the training set
cl	integer indicating the column number corresponding to the response vector that classify positive and negative regions (default = 1)
kernel	SVM kernel, a character string: "linear" or "radial". (default = "radial")
cost	The SVM cost parameter for both linear and radial kernels. If NULL (default), the function mcTune is run.
gamma	The SVM gamma parameter for radial kernel. If radial kernel and NULL (default), the function mcTune is run.
valid.times	Integer indicating how many times the training set will be split for the cross validation step (default = 10). This number must be smaller than positive and negative sets sizes.
feature.ranking	g
	List of ordered features.
feature.nb	the optimal number of feature to use from the list of ordered features.
file.prefix	A character string that will be used as a prefix followed by "_model.RData" for the resulting model file, if it is NULL (default), no model is saved

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#### Value

the best SVM model

### **Examples**

```
data(crm.features)
  cost <- 1
  gamma <- 1
  data(feature.ranking)
  feature.nb <- 70
#svm.model <- createModel(data.granges=crm.features, cost=cost, gamma=gamma,
# feature.ranking=feature.ranking, feature.nb=feature.nb)
#feature.weights <- as.data.frame(t(t(svm.model$coefs) %*% svm.model$SV))</pre>
```

crm.features

This is data to be included in my package

## **Description**

This is data to be included in my package

evaluateModelPerformance

Evaluate model performances

#### **Description**

evaluateModelPerformance function computes the precision and recall measures to evaluate the model through cross validation steps using ROCR package.

## Usage

```
evaluateModelPerformance(data, cl = 1, valid.times = 10,
  feature.ranking = NULL, feature.nb = NULL,
  numcores = ifelse(.Platform$0S.type == "windows", 1, parallel::detectCores()
  - 1), file.prefix = NULL, kernel = "linear", cost = NULL,
  gamma = NULL)
```

data	data.frame containing the training set
cl	integer indicating the column number corresponding to the response vector that classify positive and negative regions (default $= 1$ )
valid.times	Integer indicating how many times the training set will be split for the cross validation step (default = 10). This number must be smaller than positive and negative sets sizes.

4 feature.ranking

feature.ranking

List of ordered features.

feature.nb the optimal number of feature to use from the list of ordered features.

numcores Number of cores to use for parallel computing (default: the number of available

cores in the machine - 1)

file.prefix A character string that will be used as a prefix followed by "\_ROCR\_perf.png"

for the result plot file, if it is NULL (default), no plot is returned

kernel SVM kernel, a character string: "linear" or "radial". (default = "radial")

cost The SVM cost parameter for both linear and radial kernels. If NULL (default),

the function mcTune is run.

gamma The SVM gamma parameter for radial kernel. If radial kernel and NULL (de-

fault), the function mcTune is run.

#### Value

A list with two objects.

probs The predictions computed by the model for each subset during the cross-validation

labels The actual class for each subset

## **Examples**

feature.ranking

This is data to be included in my package

## **Description**

This is data to be included in my package

LedPred 5

LedPred	Creates an SVM model given a feature matrix
	g

## **Description**

The LedPred function computes the best SVM parameters, defines the optimal features for creating the SVM model by running sequentially mcTune, rankFeatures, tuneFeatureNb and createModel. The performances of this model are then computed usong evaluateModelPerformance.

## Usage

```
LedPred(data = NULL, cl = 1, ranges = list(gamma = c(1, 10), cost = c(1, 10)), cost = NULL, gamma = NULL, kernel = "linear", valid.times = 10, file.prefix = NULL, numcores = ifelse(.Platform$0S.type == "windows", 1, parallel::detectCores() - 1), step.nb = 10, halve.above = 100)
```

data	data.frame containing the training set
cl	integer indicating the column number corresponding to the response vector that classify positive and negative regions (default = $1$ )
ranges	list object containing one (linear kernel) or two (radial kernel) vectors of integers corresponding to SVM cost and SVM gamma parameters to test.
cost	The SVM cost parameter for both linear and radial kernels. If NULL (default), the function $mcTune$ is run.
gamma	The SVM gamma parameter for radial kernel. If radial kernel and NULL (default), the function mcTune is run.
kernel	SVM kernel, a character string: "linear" or "radial". (default = "radial")
valid.times	Integer indicating how many times the training set will be split for the cross validation step (default = 10). This number must be smaller than positive and negative sets sizes.
file.prefix	A character string that will be used as a prefix for the result files. If it is NULL (default), no plot is returned
numcores	Number of cores to use for parallel computing (default: the number of available cores in the machine - 1)
step.nb	Number of features to add at each step (default = 10)
halve.above	During RFE, all the features are ranked at the first round and the half lowest ranked features (that contribute the least in the model) are removed for the next round. When the number of feature is lower or equal to halve above, the features are removed one by one. (default=100)

#### Value

A list of the object produced at each step

best.params A list of the parameters giving the lowest misclassification error

feature.ranking

List of ordered features from rankFeatures

feature.nb he optimal number of feature to use from the list of ordered features from

tuneFeatureNb

model.svm The best SVM model createModel

probs.label.list

The cross-validation results from evaluateModelPerformance

## **Examples**

```
data(crm.features)
#cost_vector <- c(1,3,10)
#gamma_vector <- c(1,3,10)
#ledpred.list=LedPred(data.granges=crm.features, cl=1, ranges = list(cost=cost_vector,
# gamma=gamma_vector), kernel="linear", halve.above=50)
#names(ledpred.list)</pre>
```

mapFeaturesToCRMs

R interface to bed\_to\_matrix REST in server

## Description

The mapFeaturesToCRMs function allows the user to create a training set matrix to build a predictive model. The training set is composed of positive regions (known to be involved in the pathway of interest) and negative regions (randomly picked or known to not be involved in the pathway of interest) that will be described (scored) by features. Three types of features file format are accepted: Position specific scoring matrices modeling motifs recognised by transcription factors, bed files containing region coordinates for any discrete feature (NGS peaks, conservation blocks) and wig/bigWig files containing signal data. This script has been tested with version 0.99 of the online server. Go here to see current version of the server http://ifbprod.aitorgonzalezlab.org/map\_features\_to\_crms.php

#### Usage

```
mapFeaturesToCRMs(URL = "http://ifbprod.aitorgonzalezlab.org/map_features_to_crms.php",
positive.bed = NULL, genome = NULL, negative.bed = NULL,
shuffling = NULL, background.seqs = NULL, genome.info = NULL,
pssm = NULL, background.freqs = NULL, ngs = NULL, bed.overlap = NULL,
my.values = NULL, feature.ranking = NULL, feature.nb = NULL,
crm.feature.file = NULL, stderr.log.file = NULL, stdout.log.file = NULL)
```

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#### **Arguments**

URL URL of the server REST target

positive.bed Positive bed file path. Compulsory

genome Genome code, eg. dm3 for Drosophila Melanogaster. Compulsory

negative.bed Negative bed file path.

shuffling Integer with number of time shuffle background sequences (background.seqs).

If negative.bed is NULL and shuffling is set at 0, the feature matrix does not

contain negative sequences. It is useful to produce a test set matrix.

background.seqs

Background sequences used for shuffling. If shuffling = 0, set this parameter at

0.

genome.info File require for shuffling bed. If shuffling = 0, set this parameter at 0.

pssm Position specific scoring matrices

background.freqs

Background frequencies of nucleotides in genome

ngs NGS (bed and wig) files

bed.overlap Minimal overlap as a fraction of query sequence with NGS bed peak. Equivalent

with intersectBed -f argument. Default 1bp.

my.values Bed file where fourth column are values to append to the SVM matrix

feature.ranking

File with ranked features (Output of rankFeatures). It is used for scoring a query

bed file

feature.nb Integer with feature.nb

crm.feature.file

Path to feature matrix file

stderr.log.file

Path to error log

stdout.log.file

Path to standard output log

### Value

A list

feature.matrix a data frame where each row is a region and each column a feature, each cell

carry a score, the first column is the response vector

stdout.log Standard output log of mapFeaturesToCRMs script in server

stderr.log Standard error log of mapFeaturesToCRMs script in server

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#### **Examples**

```
## Not run:
dirPath <- system.file("extdata", package="LedPred")</pre>
 file.list <- list.files(dirPath, full.names=TRUE)</pre>
 background.freqs <- file.list[grep("freq", file.list)]</pre>
 positive.regions <- file.list[grep("positive", file.list)]</pre>
 negative.regions <- file.list[grep("negative", file.list)]</pre>
 TF.matrices <- file.list[grep("tf", file.list)]</pre>
 ngs.path <- system.file("extdata/ngs", package="LedPred")</pre>
 ngs.files=list.files(ngs.path, full.names=TRUE)
 crm.features.list <- mapFeaturesToCRMs(positive.bed=positive.regions,</pre>
     negative.bed=negative.regions, background.freqs=background.freqs,
     pssm=TF.matrices, genome="dm3", ngs=ngs.files,
     crm.feature.file = "crm.features.tab",
     stderr.log.file = "stderr.log", stdout.log.file = "stdout.log")
 names(crm.features.list)
 class(crm.features.list$crm.features)
 crm.features.list$stdout.log
 crm.features.list$stderr.log
## End(Not run)
```

mcTune

Tuning the SVM parameters

## Description

The mcTune function is a modified version of the function tune from package e1071 [6]. It tests the different combinations of C and gamma parameters given as vectors in a list and will return the prediction error computed during the cross-validation step.

## Usage

```
mcTune(data, cl = 1, ranges = list(gamma = c(1, 10), cost = c(1, 10)),
   kernel = "linear", valid.times = 10, file.prefix = NULL,
   numcores = ifelse(.Platform$OS.type == "windows", 1, parallel::detectCores()
   - 1))
```

data	data.frame containing the training set
cl	integer indicating the column number corresponding to the response vector that classify positive and negative regions (default = 1)
ranges	list object containing one (linear kernel) or two (radial kernel) vectors of integers corresponding to SVM cost and SVM gamma parameters to test.
kernel	SVM kernel, a character string: "linear" or "radial". (default = "radial")

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valid.times Integer indicating how many times the training set will be split for the cross

validation step (default = 10). This number must be smaller than positive and

negative sets sizes.

file.prefix A character string that will be used as a prefix followed by "\_c\_g\_eval.png" for

result plot files, if it is NULL (default), no plot is returned

numcores Number of cores to use for parallel computing (default: the number of available

cores in the machine - 1)

#### Value

A list of class tune

best.parameters

A list of the parameters giving the lowest misclassification error

best.performance

The lowest misclassification error

method The method used

nparcomb the number of tested parameter combinations

train.ind The indexes used to produce subsets during the cross validation step

sampling The cross-validation fold number

performances A matrix summarizing the cross-validation step with the error for each tested

parameter at each round and the dispersion of these errors (regarding to the

average error)

best.model The model produced by the best parameters

## **Examples**

```
data(crm.features)
cost.vector <- c(1,3,10,30)
gamma.vector <- c(1,3,10,30)
#c.g.obj <- mcTune(data.granges= crm.features, ranges = list(cost=cost.vector,
# gamma=gamma.vector), kernel='linear', file.prefix = "test")
#names(c.g.obj)
# cost <- c.g.obj$best.parameters$cost
# gamma <- c.g.obj$best.parameters$gamma</pre>
```

rankFeatures

Ranking the features according to their importance

#### **Description**

The rankFeatures function performs a Recursive Feature Elimination (RFE) on subsets of the feature matrix. For each subset the features are ranked according to the weight attributed by SVM at each round of elimination and the average rank of each feature over the subsets is returned. We recommand to save the object containing the ranked features for the following steps.

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## Usage

```
rankFeatures(data, cl = 1, halve.above = 100, valid.times = 10,
  kernel = "linear", cost = 1, gamma = 1,
  numcores = ifelse(.Platform$OS.type == "windows", 1, parallel::detectCores()
  - 1), file.prefix = NULL)
```

## **Arguments**

data	data.frame containing the training set
cl	integer indicating the column number corresponding to the response vector that classify positive and negative regions (default = $1$ )
halve.above	During RFE, all the features are ranked at the first round and the half lowest ranked features (that contribute the least in the model) are removed for the next round. When the number of feature is lower or equal to halve above, the features are removed one by one. (default=100)
valid.times	Integer indicating how many times the training set will be split (default = 10). This number must be smaller than positive and negative sets sizes.
kernel	SVM kernel, a character string: "linear" or "radial". (default = "radial")
cost	The SVM cost parameter for both linear and radial kernels. If NULL (default), the function $mcTune$ is run.
gamma	The SVM gamma parameter for radial kernel. If radial kernel and NULL (default), the function $mcTune$ is run.
numcores	Number of cores to use for parallel computing (default: the number of available cores in the machine - 1)
file.prefix	A character string that will be used as a prefix for output file, if it is NULL (default), no file is writen.

## Value

A 3-columns data frame with ranked features. First column contains the feature names, the second the original position of the feature in the feature.matrix and the third the average rank over the subsets.

## **Examples**

scoreData 11

scoreData	Predicting new regulatory regions

## **Description**

scoreData function predict new regulatory regions using SVM model from a test data set

#### Usage

```
scoreData(data, ledpred = NULL, model = NULL, score.file = NULL)
```

## **Arguments**

data frame containing the test set. This test set must have the same descriptive

features as the one that were used to build the model.

ledpred Returned object from the LedPred function model Returned object of the createModel function

score.file A character string that will be used as the file name for the output file, if it is

NULL (default), no file is writen. The output file takes the form of two columns

with object names and scores.

#### Value

A 2-columns dataframe. First column containg the SVM model prediction probabilities and the second containing the corresponding regions

#### **Examples**

```
data(crm.features)
data(svm.model)
#pred.test <- scoreData(data.granges=crm.features, model=svm.model,
# score.file="test_prediction.tab")</pre>
```

tuneFeatureNb

Selecting the optimal number of features

## **Description**

tuneFeatureNb iterates through increasing feature numbers to calculate kappa values which represents the performance of the model computed with the given features. We recommand to save the object containing the optimal number of features for the following steps.

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## Usage

```
tuneFeatureNb(data, cl = 1, feature.ranking, step.nb = 10,
  valid.times = 10, cost = NULL, gamma = NULL, kernel = "linear",
  numcores = ifelse(.Platform$OS.type == "windows", 1, parallel::detectCores()
  - 1), file.prefix = NULL)
```

### **Arguments**

data data.frame containing the training set

cl integer indicating the column number corresponding to the response vector that

classify positive and negative regions (default = 1)

feature.ranking

List of ordered features.

step.nb Number of features to add at each step (default = 10)

valid.times Integer indicating how many times the training set will be split for the cross

validation step (default = 10). This number must be smaller than positive and

negative sets sizes.

cost The SVM cost parameter for both linear and radial kernels. If NULL (default),

the function mcTune is run.

gamma The SVM gamma parameter for radial kernel. If radial kernel and NULL (de-

fault), the function mcTune is run.

kernel SVM kernel, a character string: "linear" or "radial". (default = "radial")

numcores Number of cores to use for parallel computing (default: the number of available

cores in the machine - 1)

file.prefix A character string that will be used as a prefix followed by "\_kappa\_measures.png"

for the result plot file. If it is NULL (default), no plot is returned

## Value

A list with two objects.

performance 2-columns data frame. first column correspond to the number of tested features,

second column contains the corresponding kappa value

best.feature.nb

Integer corresponding to the number of features producing the model with the

highest kappa value

#### **Examples**

```
data(crm.features)
data(feature.ranking)
cost <- 1
gamma <- 1
#feature.nb.obj <- tuneFeatureNb(data.granges=crm.features,
# feature.ranking=feature.ranking, kernel='linear', cost=cost,gamma=gamma,
# file.prefix = "test")
#names(feature.nb.obj)</pre>
```

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