Package ‘UBayFS’

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**Type** Package

**Title** A User-Guided Bayesian Framework for Ensemble Feature Selection

**Version** 1.0

**Description** The framework proposed in Jenul et al., (2022) [doi:10.1007/s10994-022-06221-9], together with an interactive Shiny dashboard. 'UBayFS' is an ensemble feature selection technique embedded in a Bayesian statistical framework. The method combines data and user knowledge, where the first is extracted via data-driven ensemble feature selection. The user can control the feature selection by assigning prior weights to features and penalizing specific feature combinations. 'UBayFS' can be used for common feature selection as well as block feature selection.

**License** GPL-3


**BugReports** [https://github.com/annajenul/UBayFS/issues](https://github.com/annajenul/UBayFS/issues)

**Depends** R (>= 3.5.0)

**Imports** DirichletReg, GA, ggplot2, gridExtra, hyper2, matrixStats, methods, mRMRe, Rdimtools, shiny, utils

**Suggests** caret, dplyr, DT, glmnet, GSelection, knitr, plyr, RColorBrewer, rmarkdown, rpart, shinyalert, shinyBS, shinyjs, shinyWidgets, testthat (>= 3.0.0)

**VignetteBuilder** knitr

**Config/testthat/edition** 3

**Encoding** UTF-8

**LazyData** true

**RoxygenNote** 7.2.1

**NeedsCompilation** no

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**bcw**

**Breast Cancer Wisconsin dataset**

**Description**

A dataset containing features computed from digitized images of a fine needle aspirate (FNA) of a breast mass. The target function contains two classes representing patient diagnoses (M...malignant and B...benign). The dataset has been taken from the UCI Repository of Machine Learning Databases and was created by W. H. Wolberg, W. N. Street and O. L. Mangasarian in 1995. For details, see UCI documentation or literature:

- doi:10.1117/12.148698

Feature blocks were added to the original dataset according to the dataset description (10 blocks corresponding to different image characteristics).

**Usage**

bcw
build.UBayconstraint

**Format**

A list containing:

- a matrix ‘data’ with 569 rows and 30 columns representing features,
- a vector ‘labels’ of factor type with 569 entries representing the binary target variable, and
- a list of feature indices representing feature blocks.

**Source**


---

**build.UBayconstraint**  
*Build a customized constraint for UBayFS*

**Description**

Builds a constraint using a left side ‘A’, a right side ‘b’, a relaxation parameter ‘rho’, and a block matrix ‘block_matrix’.

**Usage**

build.UBayconstraint(A, b, rho, block_matrix = NULL)

**Arguments**

- **A**  
  matrix containing the left side of the linear inequality system
- **b**  
  vector containing the right side of the linear inequality system
- **rho**  
  vector containing the relaxation parameters for each constraint
- **block_matrix**  
  a matrix indicating the membership of features in feature blocks

**Value**

a ‘UBayconstraint’ object
build.UBaymodel  

Build an ensemble for UBayFS

Description

Build a data structure for UBayFS and train an ensemble of elementary feature selectors.

Usage

build.UBaymodel(
  data,
  target,
  M = 100,
  tt_split = 0.75,
  nr_features = "auto",
  method = "mRMR",
  prior_model = "dirichlet",
  weights = 1,
  constraints = NULL,
  lambda = 1,
  optim_method = "GA",
  popsize = 50,
  maxiter = 100,
  shiny = FALSE,
  ...
)

Arguments

data  a matrix of input data

target  a vector of input labels; for binary problems a factor variable should be used

M  the number of elementary models to be trained in the ensemble

tt_split  the ratio of samples drawn for building an elementary model (train-test-split)

nr_features  number of features to select in each elementary model; if 'auto' a randomized number of features is used in each elementary model

method  a vector denoting the method(s) used as elementary models; options: 'mRMR', 'laplace' (Laplacian score) Also self-defined functions are possible methods; they must have the arguments X (data), y (target), n (number of features) and name (name of the function). For more details see examples.

prior_model  a string denoting the prior model to use; options: 'dirichlet', 'wong', 'hankin'; 'hankin' is the most general prior model, but also the most time consuming

weights  the vector of user-defined prior weights for each feature

constraints  a list containing a relaxed system ‘Ax<=b’ of user constraints, given as matrix ‘A’, vector ‘b’ and vector or scalar ‘rho’ (relaxation parameter). At least one max-size constraint must be contained. For details, see buildConstraints.
build.UBaymodel

lambda: a positive scalar denoting the overall strength of the constraints
optim_method: the method to evaluate the posterior distribution. Currently, only the option 'GA' (genetic algorithm) is supported.
popsize: size of the initial population of the genetic algorithm for model optimization
maxiter: maximum number of iterations of the genetic algorithm for model optimization
shiny: TRUE indicates that the function is called from Shiny dashboard

Details
The function aggregates input parameters for UBayFS - including data, parameters defining ensemble and user knowledge and parameters specifying the optimization procedure - and trains the ensemble model.

Value
a 'UBaymodel' object containing the following list elements:
• 'data' - the input dataset
• 'target' - the input target
• 'lambda' - the input lambda value (constraint strength)
• 'prior_model' - the chosen prior model
• 'ensemble.params' - information about input and output of ensemble feature selection
• 'constraint.params' - parameters representing the constraints
• 'user.params' - parameters representing the user’s prior knowledge
• 'optim.params' - optimization parameters

Examples
# build a UBayFS model using Breast Cancer Wisconsin dataset
data(bcw)  # dataset
c <- buildConstraints(constraint_types = 'max_size',
constraint_vars = list(10),
num_elements = ncol(bcw$data),
rho = 1)  # prior constraints
w <- rep(1, ncol(bcw$data))  # weights
model <- build.UBaymodel(
  data = bcw$data,
  target = bcw$labels,
  M = 20,
  constraints = c,
  weights = w
)

# use a function computing a decision tree as input
library('rpart')
decision_tree <- function(X, y, n, name = 'tree'){


rf_data = as.data.frame(cbind(y, X))
colnames(rf_data) <- make.names(colnames(rf_data))
tree = rpart::rpart(y~., data = rf_data)
return(list(ranks = which(colnames(X) %in% names(tree$variable.importance)[1:n]),
            name = name))
}

model <- build.UBaymodel(
  data = bcw$data,
  target = bcw$labels,
  constraints = c,
  weights = w,
  method = decision_tree
)

# include block-constraints
c_block <- buildConstraints(constraint_types = 'max_size',
                             constraint_vars = list(2),
                             num_elements = length(bcw$blocks),
                             rho = 10,
                             block_list = bcw$blocks)

model <- setConstraints(model, c_block)

---

buildConstraints  Build a constraint system

Description

Build an inequation system from constraints provided by the user.

Usage

buildConstraints(
  constraint_types,
  constraint_vars,
  num_elements,
  rho = 1,
  block_list = NULL,
  block_matrix = NULL
)

Arguments

constraint_types
  a vector of strings denoting the type of constraint to be added; options: ‘max_size’,
  ‘must_link’, ‘cannot_link’
**buildDecorrConstraints**

**constraint_vars**  
a list of parameters defining the constraints; in case of max-size constraints, the list element must contain an integer denoting the maximum size of the feature set, in case of max-link or cannot link, the list element must be a vector of feature indices to be linked

**num_elements**  
the total number of features (feature-wise constraints) or blocks (block-wise constraints) in the dataset

**rho**  
a positive parameter denoting the level of relaxation; ‘Inf’ denotes a hard constraint, i.e. no relaxation

**block_list**  
the list of feature indices for each block; only required, if block-wise constraints are built and ‘block_matrix’ is ‘NULL’

**block_matrix**  
the matrix containing affiliations of features to each block; only required, if block-wise constraints are built and ‘block_list’ is ‘NULL’

**Details**

The function transforms user information about relations between features (must-link or cannot-link constraints) and maximum feature set size (max-size) into a linear inequation system. In addition, the relaxation parameter ‘rho’ can be specified to achieve soft constraints.

**Value**

a ‘UBayconstraint’ containing a matrix ‘A’ and a vector ‘b’ representing the inequality system ‘Ax<=b’, and a vector ‘rho’ representing the penalty shape

**Examples**

```r
# given a dataset with 10 features, we create a max-size constraint limiting
# the set to 5 features and a cannot-link constraint between features 1 and 2
buildConstraints(constraint_types = c("max_size", "cannot_link"),
                 constraint_vars = list(5, c(1,2)),
                 num_elements = 10,
                 rho = 1)
```

---

**buildDecorrConstraints**

**Build decorrelation constraints**

**Description**

Build a cannot link constraint between highly correlated features. The user defines the correlation threshold.

**Usage**

```r
buildDecorrConstraints(data, level = 0.5, method = "spearman")
```
### Arguments

- **data** the dataset in the 'UBaymodel' object
- **level** the threshold correlation-level
- **method** the method used to compute correlation; must be one of 'pearson', 'spearman' or 'kendall'

### Value

A list containing a matrix ‘A’ and a vector ‘b’ representing the inequality system ‘Ax\leq b’, a vector ‘rho’ and a block matrix

---

### Description

**build_train_set**

Perform stratified data partition.

**Usage**

```r
build_train_set(y, tt_split)
```

**Arguments**

- **y** a column, often the target, by which the data shall be partitioned.
- **tt_split** the percentage of data used for training in each ensemble model.

**Value**

data indices for training ensembles

---

### Description

**evaluateFS**

Evaluate a feature set

**Usage**

```r
evaluateFS(state, model, method = "spearman", log = FALSE)
evaluateMultiple(state, model, method = "spearman", log = TRUE)
```
Arguments

state a binary membership vector describing a feature set
model a 'UBaymodel' object created using build.UBaymodel
method type of correlation ('pearson', 'kendall', or 'spearman')
log whether the admissibility should be returned on log scale

Value

a posterior probability value

Functions

• evaluateMultiple(): Evaluate multiple feature sets

Description

Evaluate the value of the admissibility function 'kappa'.

Usage

group_admissibility(state, constraints, log = TRUE)
admissibility(state, constraint_list, log = TRUE)

Arguments

state a binary membership vector describing a feature set
constraints group of constraints with common block matrix
log whether the admissibility should be returned on log scale
constraint_list a list of constraint groups, each containing a matrix ‘A’ and a vector ‘b’ representing the inequality system ‘Ax<=b’, a vector ‘rho’, and a matrix ‘block_matrix’

Value

an admissibility value

Functions

• group_admissibility(): computes admissibility for a group of constraints (with a common block).
is.UBayconstraint  Checks whether a list object implements proper UBayFS user constraints

Description
Checks whether a list object implements proper UBayFS user constraints

Usage
is.UBayconstraint(x)

Arguments
x  a ‘UBayconstraint’ object

Value
boolean value

is.UBaymodel  Check whether an object is a UBaymodel

Description
Perform consistency checks of a UBaymodel.

Usage
is.UBaymodel(x)

Arguments
x  an object to be checked for class consistency

Value
returns a single scalar (TRUE or FALSE) indicating whether the object fulfills the consistency requirements of the UBayFS model
posteriorExpectation

Posterior expectation of features

**Description**

compute the posterior score for each feature.

**Usage**

```r
posteriorExpectation(model)
```

**Arguments**

- `model`: a ‘UBaymodel’ object

print.UBayconstraint

Prints the ‘UBayconstraint’ object

**Description**

Prints the ‘UBayconstraint’ object

**Usage**

```r
## S3 method for class 'UBayconstraint'
print(x, ...)

## S3 method for class 'UBayconstraint'
summary(object, ...)
```

**Arguments**

- `x`: a ‘UBayconstraint’ object
- `object`: a ‘UBayconstraint’ object
- `...`: additional print parameters

**Value**

prints model summary to the console, no return value

**Functions**

- `summary(UBayconstraint)`: Prints a summary of the ‘UBayconstraint’ object
print.UBaymodel  

Print a UBayFS model

Description

Print details of a ‘UBaymodel’

Usage

```r
## S3 method for class 'UBaymodel'
print(x, ...)
printResults(model)
## S3 method for class 'UBaymodel'
summary(object, ...)
## S3 method for class 'UBaymodel'
plot(x, ...)
```

Arguments

- `x`  
  a ‘UBaymodel’ object created using `build.UBaymodel`
- `...`  
  additional print parameters
- `model`  
  a ‘UBaymodel’ object created using `build.UBaymodel` after training
- `object`  
  a ‘UBaymodel’ object created using `build.UBaymodel`

Value

prints model summary to the console, no return value

Functions

- `printResults()`: Display and summarize the results of UBayFS after feature selection.
- `summary(UBaymodel)`: A summary of a ‘UBaymodel’
- `plot(UBaymodel)`: A barplot of a ‘UBaymodel’ containing prior weights, ensemble counts and the selected features.
runInteractive

**Run an interactive Shiny app for demonstration**

**Description**
Starts an interactive R Shiny application in the browser.

**Usage**
```r
runInteractive()
```

**Value**
calls Shiny app, no return value

---

sampleInitial

**Initial feature set sampling using probabilistic Greedy algorithm**

**Description**
Sample initial solutions using a probabilistic version of Greedy algorithm.

**Usage**
```r
sampleInitial(post_scores, constraints, size)
```

**Arguments**
- `post_scores`: a vector of posterior scores (prior scores + likelihood) for each feature
- `constraints`: a list containing feature-wise constraints
- `size`: initial number of samples to be created. The output sample size can be lower, since duplicates are removed.

**Value**
a matrix containing initial feature sets as rows
setConstraints  

Set constraints in UBaymodel object

**Description**

Set the constraints in a ‘UBaymodel’ object.

**Usage**

`setConstraints(model, constraints, append = FALSE)`

**Arguments**

- `model`: a ‘UBaymodel’ object created using `build.UBaymodel`
- `constraints`: a ‘UBayconstraint’ object created using `build.UBayconstraint`
- `append`: if ‘TRUE’, constraints are appended to the existing constraint system

**Value**

a ‘UBaymodel’ object with updated constraint parameters

**See Also**

`build.UBaymodel`

---

setOptim  

Set optimization parameters in a UBaymodel object

**Description**

Set the optimization parameters in a UBaymodel object.

**Usage**

`setOptim(model, method = "GA", popsize, maxiter)`

**Arguments**

- `model`: a UBaymodel object created using `build.UBaymodel`
- `method`: the method to evaluate the posterior distribution; currently only ‘GA’ (genetic algorithm) is supported
- `popsize`: size of the initial population of the genetic algorithm for model optimization
- `maxiter`: maximum number of iterations of the genetic algorithm for model optimization
**setWeights**

**Value**

a UBaymodel object with updated optimization parameters

**See Also**

build.UBaymodel

---

**setWeights** *Set weights in UBaymodel object*

**Description**

Set the prior weights in a UBaymodel object.

**Usage**

```r
setWeights(model, weights, block_list = NULL, block_matrix = NULL)
```

**Arguments**

- `model` a UBaymodel object created using build.UBaymodel
- `weights` the vector of user-defined prior weights for each feature
- `block_list` the list of feature indices for each block; only required, if block-wise weights are specified and block_matrix is NULL
- `block_matrix` the matrix containing affiliations of features to each block; only required, if block-wise weights are specified and block_list is NULL

**Value**

a UBaymodel object with updated prior weights

**See Also**

build.UBaymodel
train

UBayFS feature selection

Description

Genetic algorithm to train UBayFS feature selection model.

Usage

train(x, verbose = FALSE)

Arguments

  x   a ‘UBaymodel‘ created by build.UBaymodel
  verbose   if TRUE: GA optimization output is printed to the console

Value

a ‘UBaymodel‘ with an additional list element output containing the optimized solution, see build.UBaymodel
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