Package 'BioM2'

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Version 1.1.0		
Description F	iologically Explainable Machine Learning Framework for Phenotype Prediction 1	15

ing omics data described in Chen and Schwarz (2017) <doi:10.48550/arXiv.1712.00336>.Identifying reproducible and interpretable biological patterns from high-dimensional omics data is a critical factor in understanding the risk mechanism of complex disease. As such, explainable machine learning can offer biological insight in addition to personalized risk scoring. In this process, a feature space of biological pathways will be generated, and the feature space can also be subsequently analyzed using WGCNA (Described in Horvath and Zhang (2005) <doi:10.2202/1544-6115.1128> and Langfelder and Horvath (2008) <doi:10.1186/1471-2105-9-559>) methods.

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Title Biologically Explainable Machine Learning Framework

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AddUnmapped

Add unmapped probe

Description

Add unmapped probe

Usage

```
AddUnmapped(
  train = NULL,
  test = NULL,
  Unmapped_num = NULL,
  Add_FeartureSelection_Method = "wilcox.test",
  anno = NULL,
  len = NULL,
  verbose = TRUE,
  cores = 1
)
```

Arguments

train
The input training dataset. The first column is the label or the output. For binary classes, 0 and 1 are used to indicate the class member.

test
The input test dataset. The first column is the label or the output. For binary classes, 0 and 1 are used to indicate the class member.

Unmapped_num
The number of unmapped probes.

baseModel 3

Add_FeartureSelection_Method

Feature selection methods. Available options are c('cor', 'wilcox.test').

anno The annotation data stored in a data frame for probe mapping. It must have at

least two columns named 'ID' and 'entrezID'. (For details, please refer to data(

data("MethylAnno"))

len The number of unmapped probes

verbose Whether to print running process information to the console

cores The number of cores used for computation.

Value

Matrix of unmapped probes

baseModel

Prediction by Machine Learning

Description

Prediction by Machine Learning with different learners (From 'mlr3')

Usage

```
baseModel(
  trainData,
  testData,
  predMode = "probability",
  classifier,
  paramlist = NULL,
  inner_folds = 10
)
```

Arguments

trainData The input training dataset. The first column is the label or the output. For binary

classes, 0 and 1 are used to indicate the class member.

testData The input test dataset. The first column is the label or the output. For binary

classes, 0 and 1 are used to indicate the class member.

predMode The prediction mode. Currently only supports 'probability' for binary classifica-

tion tasks.

classifier Learners in mlr3
paramlist Learner parameters

inner_folds k-fold cross validation (Only supported when testData = NULL)

Value

The predicted output for the test data.

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Author(s)

Shunjie Zhang

Examples

BioM2

Biologically Explainable Machine Learning Framework

Description

Biologically Explainable Machine Learning Framework

Usage

```
BioM2(
  TrainData = NULL,
  TestData = NULL,
  pathlistDB = NULL,
  FeatureAnno = NULL,
  resampling = NULL,
  nfolds = 5,
  classifier = "liblinear",
  predMode = "probability",
  PathwaySizeUp = 200,
  PathwaySizeDown = 20,
 MinfeatureNum_pathways = 10,
  Add_UnMapped = TRUE,
  Unmapped_num = 300,
  Add_FeartureSelection_Method = "wilcox.test",
  Inner_CV = TRUE,
  inner_folds = 10,
  Stage1_FeartureSelection_Method = "cor",
  cutoff = 0.3,
  Stage2_FeartureSelection_Method = "RemoveHighcor",
  cutoff2 = 0.95,
  classifier2 = NULL,
```

BioM2 5

```
target = "predict",
p.adjust.method = "fdr",
save_pathways_matrix = FALSE,
cores = 1,
verbose = TRUE
)
```

Arguments

TrainData The input training dataset. The first column is the label or the output. For binary

classes, 0 and 1 are used to indicate the class member.

TestData The input test dataset. The first column is the label or the output. For binary

classes, 0 and 1 are used to indicate the class member.

pathlistDB A list of pathways with pathway IDs and their corresponding genes ('entrezID'

is used). For details, please refer to (data("GO2ALLEGS_BP"))

FeatureAnno The annotation data stored in a data frame for probe mapping. It must have at

least two columns named 'ID' and 'entrezID'. (For details, please refer to data(

data("MethylAnno"))

resampling Resampling in mlr3verse.

nfolds k-fold cross validation (Only supported when TestData = NULL)

classifier Learners in mlr3

predMode The prediction mode. Currently only supports 'probability' for binary classifi-

cation tasks.

PathwaySizeUp The upper-bound of the number of genes in each biological pathways.

PathwaySizeDown

The lower-bound of the number of genes in each biological pathways.

MinfeatureNum_pathways

The minimal defined pathway size after mapping your own data to pathlistDB(KEGG

database/GO database).

Add_UnMapped Whether to add unmapped probes for prediction

Add_FeartureSelection_Method

Feature selection methods.

Inner_CV Whether to perform a k-fold verification on the training set.

inner_folds k-fold verification on the training set.

 $Stage1_FeartureSelection_Method$

Feature selection methods.

cutoff The cutoff used for feature selection threshold. It can be any value between 0

and 1.

Stage2_FeartureSelection_Method

Feature selection methods.

cutoff2 The cutoff used for feature selection threshold. It can be any value between 0

and 1.

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classifier2 Learner for stage 2 prediction(if classifier2==NULL,then it is the same as the

learner in stage 1.)

target Is it used to predict or explore potential biological mechanisms? Available op-

tions are c('predict', 'pathways').

p.adjust.method

p-value adjustment method.(holm", "hochberg", "hommel", "bonferroni", "BH",

"BY",

save_pathways_matrix

Whether to output the path matrix file

cores The number of cores used for computation.

verbose Whether to print running process information to the console

Value

A list containing prediction results and prediction result evaluation

Examples

```
library(mlr3verse)
library(caret)
library(parallel)
library(BioM2)
data=MethylData_Test
set.seed(1)
part=unlist(createDataPartition(data$label,p=0.8))
Train=data[part,]
Test=data[-part,]
pathlistDB=G02ALLEGS_BP
FeatureAnno=MethylAnno
pred=BioM2(TrainData = Train,TestData = Test,
           pathlistDB=pathlistDB,FeatureAnno=FeatureAnno,
           classifier='svm',nfolds=5,
           PathwaySizeUp=25, PathwaySizeDown=20, MinfeatureNum_pathways=10,
           Add_UnMapped='Yes',Unmapped_num=300,
           Inner_CV='None',inner_folds=5,
           Stage1_FeartureSelection_Method='cor',cutoff=0.3,
           Stage2_FeartureSelection_Method='None',
           target='predict',cores=1
)#(To explore biological mechanisms, set target='pathways')
```

FindParaModule 7

FindParaModule	Find suitable parameters for partitioning pathways modules

Description

Find suitable parameters for partitioning pathways modules

Usage

```
FindParaModule(
  pathways_matrix = NULL,
  control_label = 0,
  minModuleSize = seq(10, 20, 5),
  mergeCutHeight = seq(0, 0.3, 0.1),
  minModuleNum = 5,
  power = NULL,
  exact = TRUE,
  ancestor_anno = NULL
)
```

Arguments

```
pathways_matrix
                 A pathway matrix generated by the BioM2( target='pathways') function.
control_label
                 The label of the control group ( A single number, factor, or character )
                 minimum module size for module detection. Detail for WGCNA::blockwiseModules()
minModuleSize
                 dendrogram cut height for module merging. Detail for WGCNA::blockwiseModules()
mergeCutHeight
minModuleNum
                 Minimum total number of modules detected
power
                 soft-thresholding power for network construction. Detail for WGCNA::blockwiseModules()
exact
                 Whether to divide GO pathways more accurately (work when ancestor_anno=NULL)
                 Annotations for ancestral relationships (like data('GO_Ancestor'))
ancestor_anno
```

Value

A list containing recommended parameters

8 GO_Ancestor

GO2ALLEGS_BP

An example about pathlistDB

Description

An example about pathlistDB

Format

A list:

..

Details

A list of pathways with pathway IDs and their corresponding genes ('entrezID' is used).

GO_Ancestor

Pathways in the GO database and their Ancestor

Description

Inclusion relationships between pathways

Format

A data frame:

•••

Details

In the GO database, each pathway will have its own ancestor pathway. Map pathways in GO database to about 20 common ancestor pathways.

Source

From GO.db

GO_Ancestor_exact 9

GO_Ancestor_exact

Pathways in the GO database and their Ancestor

Description

Inclusion relationships between pathways

Format

```
A data frame:
```

...

Details

In the GO database, each pathway will have its own ancestor pathway. Map pathways in GO database to about 400 common ancestor pathways.

Source

From GO.db

HyBioM2

BioM2 Hyperparametric Combination

Description

BioM2 Hyperparametric Combination

Usage

```
HyBioM2(
  TrainData = NULL,
  pathlistDB = NULL,
  FeatureAnno = NULL,
  resampling = NULL,
  nfolds = 5,
  classifier = "liblinear",
  predMode = "probability",
  PathwaySizeUp = 200,
  PathwaySizeDown = 20,
  MinfeatureNum_pathways = 10,
  Add_UnMapped = TRUE,
  Add_FeartureSelection_Method = "wilcox.test",
  Unmapped_num = 300,
  Inner_CV = TRUE,
```

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```
inner_folds = 10,
Stage1_FeartureSelection_Method = "cor",
stage1_cutoff = 0.3,
Stage2_FeartureSelection_Method = "RemoveHighcor",
stage2_cutoff = 0.8,
classifier2 = NULL,
cores = 1,
verbose = TRUE
)
```

Arguments

TrainData The input training dataset. The first column is the label or the output. For binary

classes, 0 and 1 are used to indicate the class member.

pathlistDB A list of pathways with pathway IDs and their corresponding genes ('entrezID'

is used). For details, please refer to (data("GO2ALLEGS_BP"))

FeatureAnno The annotation data stored in a data.frame for probe mapping. It must have at

least two columns named 'ID' and 'entrezID'. (For details, please refer to data(

data("MethylAnno"))

resampling Resampling in mlr3verse.

nfolds k-fold cross validation (Only supported when TestData = NULL)

classifier Learners in mlr3

predMode The prediction mode. Currently only supports 'probability' for binary classifi-

cation tasks.

PathwaySizeUp The upper-bound of the number of genes in each biological pathways.

PathwaySizeDown

The lower-bound of the number of genes in each biological pathways.

MinfeatureNum_pathways

The minimal defined pathway size after mapping your own data to pathlistDB(KEGG

database/GO database).

Add_UnMapped Whether to add unmapped probes for prediction

Add_FeartureSelection_Method

Feature selection methods.

Inner_CV Whether to perform a k-fold verification on the training set.

inner_folds k-fold verification on the training set.

Stage1_FeartureSelection_Method

Feature selection methods.

stage1_cutoff The cutoff used for feature selection threshold. It can be any value between 0

and 1.

Stage2_FeartureSelection_Method

Feature selection methods.

stage2_cutoff The cutoff used for feature selection threshold. It can be any value between 0

and 1.

MethylAnno 11

classifier2 Learner for stage 2 prediction(if classifier2==NULL,then it is the same as the

learner in stage 1.)

cores The number of cores used for computation.

verbose Whether to print running process information to the console

Value

A data frame contains hyperparameter results

MethylAnno An example about FeatureAnno for methylation data

Description

An example about FeatureAnno for methylation data

Format

A data frame:

...

Details

The annotation data stored in a data.frame for probe mapping. It must have at least two columns named 'ID' and 'entrezID'.

MethylData_Test

An example about TrainData/TestData for methylation data

Description

An example about TrainData/TestData for methylation data MethylData_Test.

Format

A data frame:

•••

Details

The first column is the label or the output. For binary classes, 0 and 1 are used to indicate the class member.

12 PathwaysModule

PathwaysModule	Delineate differential pathway modules with high biological interpretability

Description

Delineate differential pathway modules with high biological interpretability

Usage

```
PathwaysModule(
  pathways_matrix = NULL,
  control_label = NULL,
  power = NULL,
  minModuleSize = NULL,
  mergeCutHeight = NULL,
  cutoff = 70,
  MinNumPathways = 5,
  p.adjust.method = "fdr",
  exact = TRUE,
  ancestor_anno = NULL
)
```

Arguments

```
pathways_matrix
                  A pathway matrix generated by the BioM2( target='pathways') function.
control_label
                 The label of the control group ( A single number, factor, or character )
                  soft-thresholding power for network construction. Detail for WGCNA::blockwiseModules()
power
                 minimum module size for module detection. Detail for WGCNA::blockwiseModules()
minModuleSize
mergeCutHeight dendrogram cut height for module merging. Detail for WGCNA::blockwiseModules()
cutoff
                 Thresholds for Biological Interpretability Difference Modules
MinNumPathways Minimum number of pathways included in the biologically interpretable differ-
                 ence module
p.adjust.method
                  p-value adjustment method.(holm", "hochberg", "hommel", "bonferroni", "BH",
                  Whether to divide GO pathways more accurately (work when ancestor_anno=NULL)
exact
ancestor_anno
                 Annotations for ancestral relationships (like data('GO_Ancestor'))
```

Value

A list containing differential module results that are highly biologically interpretable

PlotCorModule 13

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	$\Gamma \perp$. U	L	U	u	П	I۲I	()	u	u	1	H

Correlatogram for Biological Differences Modules

Description

Correlalogram for Biological Differences Modules

Usage

```
PlotCorModule(
   PathwaysModule_obj = NULL,
   alpha = 0.7,
   begin = 0.2,
   end = 0.9,
   option = "C",
   family = "serif"
)
```

Arguments

PathwaysModule_obj

Results produced by PathwaysModule()

alpha The alpha transparency, a number in (0,1). Detail for scale_fill_viridis()

begin The (corrected) hue in (0,1) at which the color map begins. Detail for scale_fill_viridis(). end The (corrected) hue in (0,1) at which the color map ends. Detail for scale_fill_viridis()

option A character string indicating the color map option to use. Detail for scale_fill_viridis()

family calligraphic style

Value

a ggplot object

 ${\tt PlotPathFearture}$

Visualisation of significant pathway-level features

Description

Visualisation of significant pathway-level features

14 PlotPathInner

Usage

```
PlotPathFearture(
   BioM2_pathways_obj = NULL,
   pathlistDB = NULL,
   top = 10,
   p.adjust.method = "none",
   begin = 0.1,
   end = 0.9,
   alpha = 0.9,
   option = "C",
   seq = 1
)
```

Arguments

BioM2_pathways_obj

Results produced by BioM2(,target='pathways')

pathlistDB A list of pathways with pathway IDs and their corresponding genes ('entrezID'

is used). For details, please refer to (data("GO2ALLEGS_BP"))

top Number of significant pathway-level features visualised

p.adjust.method

p-value adjustment method.(holm", "hochberg", "hommel", "bonferroni", "BH",

"BY","fdr","none")

begin The (corrected) hue in (0,1) at which the color map begins. Detail for scale_fill_viridis().

end The (corrected) hue in (0,1) at which the color map ends. Detail for scale_fill_viridis()

alpha The alpha transparency, a number in (0,1). Detail for scale_fill_viridis()

option A character string indicating the color map option to use. Detail for scale_fill_viridis()

seq Interval of x-coordinate

Value

a ggplot2 object

PlotPathInner

Visualisation Original features that make up the pathway

Description

Visualisation Original features that make up the pathway

PlotPathNet 15

Usage

```
PlotPathInner(
  data = NULL,
  pathlistDB = NULL,
  FeatureAnno = NULL,
  PathNames = NULL,
  p.adjust.method = "none",
  save_pdf = FALSE,
  alpha = 1,
  cols = NULL
)
```

Arguments

data The input omics data

pathlistDB A list of pathways with pathway IDs and their corresponding genes ('entrezID'

is used). For details, please refer to (data("GO2ALLEGS_BP"))

FeatureAnno The annotation data stored in a data.frame for probe mapping. It must have at

least two columns named 'ID' and 'entrezID'. (For details, please refer to data(

data("MethylAnno"))

PathNames A vector. A vector containing the names of pathways

p.adjust.method

p-value adjustment method.(holm", "hochberg", "hommel", "bonferroni", "BH",

"BY","fdr","none")

save_pdf Whether to save images in PDF format

alpha The alpha transparency, a number in (0,1).

cols palette (vector of colour names)

Value

a plot object

PlotPathNet

Network diagram of pathways-level features

Description

Network diagram of pathways-level features

16 ShowModule

Usage

```
PlotPathNet(
  data = NULL,
  BioM2_pathways_obj = NULL,
  FeatureAnno = NULL,
  pathlistDB = NULL,
  PathNames = NULL,
  cutoff = 0.2,
  num = 10
)
```

Arguments

data The input omics data

BioM2_pathways_obj

Results produced by BioM2()

FeatureAnno The annotation data stored in a data.frame for probe mapping. It must have at

least two columns named 'ID' and 'entrezID'. (For details, please refer to data(

data("MethylAnno"))

pathlistDB A list of pathways with pathway IDs and their corresponding genes ('entrezID'

is used). For details, please refer to (data("GO2ALLEGS_BP"))

PathNames A vector. A vector containing the names of pathways

cutoff Threshold for correlation between features within a pathway

num The first few internal features of each pathway that are most relevant to the

phenotype

Value

a ggplot object

ShowModule Display biological information within each pathway module

Description

Display biological information within each pathway module

Usage

```
ShowModule(obj = NULL, ID_Module = NULL, exact = TRUE, ancestor_anno = NULL)
```

Arguments

obj Results produced by PathwaysModule()

ID_Module ID of the diff module

exact Whether to divide GO pathways more accurately (work when ancestor_anno=NULL)

ancestor_anno Annotations for ancestral relationships (like data('GO_Ancestor'))

Value

List containing biologically specific information within the module

```
Stage1_FeartureSelection
```

Stage 1 Fearture Selection

Description

Stage 1 Fearture Selection

Usage

```
Stage1_FeartureSelection(
   Stage1_FeartureSelection_Method = "cor",
   data = NULL,
   cutoff = NULL,
   featureAnno = NULL,
   pathlistDB_sub = NULL,
   MinfeatureNum_pathways = 10,
   cores = 1,
   verbose = TRUE
)
```

Arguments

Stage1_FeartureSelection_Method

Feature selection methods. Available options are c(NULL, 'cor', 'wilcox.test',

'cor_rank', 'wilcox.test_rank').

data The input training dataset. The first column is the label.

cutoff The cutoff used for feature selection threshold. It can be any value between 0

and 1. Commonly used cutoffs are c(0.5, 0.1, 0.05, 0.01, etc.).

featureAnno The annotation data stored in a data.frame for probe mapping. It must have at

least two columns named 'ID' and 'entrezID'. (For details, please refer to data(

data("MethylAnno"))

pathlistDB_sub A list of pathways with pathway IDs and their corresponding genes ('entrezID'

is used). For details, please refer to (data("GO2ALLEGS_BP"))

MinfeatureNum_pathways

The minimal defined pathway size after mapping your own data to pathlistDB(KEGG

database/GO database).

cores The number of cores used for computation.

verbose Whether to print running process information to the console

Value

A list of matrices with pathway IDs as the associated list member names.

Author(s)

Shunjie Zhang

Examples

Stage2_FeartureSelection

Stage 2 Fearture Selection

Description

Stage 2 Fearture Selection

Usage

```
Stage2_FeartureSelection(
   Stage2_FeartureSelection_Method = "RemoveHighcor",
   data = NULL,
   label = NULL,
   cutoff = NULL,
   preMode = NULL,
   classifier = NULL,
   verbose = TRUE,
   cores = 1
)
```

Arguments

Stage2_FeartureSelection_Method

Feature selection methods. Available options are c(NULL, 'cor', 'wilcox.test', 'cor_rank', 'wilcox.test_ran

'RemoveLinear').

data The input training dataset. The first column is the label.

label The label of dataset

cutoff The cutoff used for feature selection threshold. It can be any value between 0

and 1.

preMode The prediction mode. "Currently only supports 'probability' for binary classifi-

cation tasks."

classifier Learners in mlr3

verbose Whether to print running process information to the console

cores The number of cores used for computation.

TransAnno 19

Value

Column index of feature

Author(s)

Shunjie Zhang

TransAnno

An example about FeatureAnno for gene expression

Description

An example about FeatureAnno for gene expression

Format

A data frame:

...

Details

The annotation data stored in a data.frame for probe mapping. It must have at least two columns named 'ID' and 'entrezID'.

TransData_Test

An example about TrainData/TestData for gene expression

Description

An example about TrainData/TestData for gene expression MethylData_Test.

Format

A data frame:

..

Details

The first column is the label or the output. For binary classes, 0 and 1 are used to indicate the class member.

20 VisMultiModule

VisMultiModule

Visualisation of the results of the analysis of the pathway modules

Description

Visualisation of the results of the analysis of the pathway modules

Usage

```
VisMultiModule(
     BioM2_pathways_obj = NULL,
      FindParaModule_obj = NULL,
      ShowModule_obj = NULL,
     PathwaysModule_obj = NULL,
      exact = TRUE,
      ancestor_anno = NULL,
      type_text_table = FALSE,
      text_table_theme = ttheme("mOrange"),
      volin = FALSE,
      control_label = 0,
     module = NULL,
     cols = NULL,
     n_neighbors = 8,
      spread = 1,
     min_dist = 2,
     target_weight = 0.5,
      size = 1.5,
     alpha = 1,
      ellipse = TRUE,
     ellipse.alpha = 0.2,
      theme = ggthemes::theme_base(base_family = "serif"),
      save_pdf = FALSE,
     width = 7,
     height = 7
   )
Arguments
   BioM2_pathways_obj
                    Results produced by BioM2(,target='pathways')
   FindParaModule_obj
                    Results produced by FindParaModule()
   ShowModule_obj Results produced by ShowModule()
```

PathwaysModule_obj

Results produced by PathwaysModule()

Whether to divide GO pathways more accurately (work when ancestor_anno=NULL) exact

VisMultiModule 21

ancestor_anno Annotations for ancestral relationships (like data('GO_Ancestor')) type_text_table

Whether to display it in a table

text_table_theme

The topic of this table. Detail for ggtexttable()

volin Can only be used when PathwaysModule_obj exists. (Violin diagram)

control_label Can only be used when PathwaysModule_obj exists. (Control group label)

module Can only be used when PathwaysModule_obj exists. (PathwaysModule ID)

cols palette (vector of colour names)

n_neighbors The size of local neighborhood (in terms of number of neighboring sample

points) used for manifold approximation. Larger values result in more global views of the manifold, while smaller values result in more local data being pre-

served. In general values should be in the range 2 to 100.

spread The effective scale of embedded points. In combination with min_dist, this

determines how clustered/clumped the embedded points are.

min_dist The effective minimum distance between embedded points. Smaller values will

result in a more clustered/clumped embedding where nearby points on the manifold are drawn closer together, while larger values will result on a more even dispersal of points. The value should be set relative to the spread value, which

determines the scale at which embedded points will be spread out.

target_weight Weighting factor between data topology and target topology. A value of 0.0

weights entirely on data, a value of 1.0 weights entirely on target. The default of 0.5 balances the weighting equally between data and target. Only applies if y

is non-NULL.

size Scatter plot point size

alpha Alpha for ellipse specifying the transparency level of fill color. Use alpha = 0

for no fill color.

ellipse logical value. If TRUE, draws ellipses around points.

ellipse.alpha Alpha for ellipse specifying the transparency level of fill color. Use alpha = 0

for no fill color.

theme Default:theme_base(base_family = "serif")
save_pdf Whether to save images in PDF format

width image width height image height

Value

a ggplot2 object

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