

Package ‘IPPMModel’

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Type Package

Title Impact pattern plots and feature interaction networks

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Description This package aims to interpret black box of supervised machine learning models by visualizing the impacts of features on predictal results and feature interaction network.

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LazyData true

imports rpart (>= 4.1-11), R6 (>= 2.2.0), parallel (>= 3.4.0), xlsx (>= 0.5.7), igraph (>= 1.0.1), akmeans (>= 1.1), cluster (>= 2.0.3), fpc (>= 2.1-10)

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VignetteBuilder knitr

R topics documented:

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BuildTree	<i>The method 'BuildTree' in IPPMModel class</i>
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Description

The method builds tree models for each feature based on the clustering results [Clustering.Res](#). The tree size is determined by the columns 'treeSize' and 'minSplit' in the field [ParaTable](#). The method is executed in parallel using package [parallel](#). Each feature corresponds to one core.

Usage

BuildTree()

Value

a list of tree rules of each feature. The result is saved in the field [TreeRules](#).

See Also

[IPPMModel](#)

CheckInitialization	<i>The method 'CheckInitialization' in IPPMModel class</i>
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Description

The method validates the arguments in the method [initialize](#).

Usage

CheckInitialization(XDS, PredType, PredDim, ModelPackage, XB.Size, XB.SamplingMethod)

Arguments

XDS	the dataset of input features.
PredType	the type of prediction.
PredDim	indicating which class is predicted.
ModelPackage	the package name of the interpreted machine learning model.
XB.Size	the size of XB.Sample.
XB.SamplingMethod	the sampling method of XB.Sample.

Value

TRUE, if all arguments are validated. FALSE, if at least one argument is not validated.

See Also

[IPPMModel](#)

CheckParaTable	<i>The method 'CheckParaTable' in IPPMModel class</i>
----------------	---

Description

This method validates the information in [ParaTable](#). For example, if the column 'distMeasure' is 'euclidean' or 'cosine', it is validated.

Usage

```
CheckParaTable()
```

Value

TRUE, if the information in [ParaTable](#) are validated; FALSE, otherwise.

See Also

[IPPMModel](#)

ClusterImpactPlots	<i>The method 'ClusterImpactPlots' in IPPModel class</i>
--------------------	--

Description

Cluster impact curves to generate impact pattern plots.

Usage

```
ClusterImpactPlots()
```

Details

The method clusters the impact curves of each feature based on the predicting results [Pred.Res](#). The parameters of the clustering process are defined in the field [ParaTable](#). The clustering method is defined by the column 'clusteringMethod'; The distance measure is defined by the 'distMeasure'; the column 'centralized' determines if the impact curves are centralized or not before clustering; the 'autoK' tells if the number of clusters is determined automatically by Dunn index or not; the 'numK' determines the maximum number of clusters if autoK = TRUE; otherwise, the 'numK' means the number of clusters. The method is executed in parallel using package [parallel](#). Each feature corresponds to one core.

Value

a list of clustering results of each feature. The result is saved in the field [Clustering.Res](#).

See Also

[IPPModel](#)

Clustering.Res	<i>The field 'Clustering.Res' in IPPModel class</i>
----------------	---

Description

Clustering.Res is the clustering results and is generate by method [ClusterImpactPlots](#). Clustering.Res is a list, each element of which is a data.frame of the clustering results of a feature.

See Also

[IPPModel](#)

ColorList

The field 'ColorList' in [IPPMModel](#) class

Description

ColorList is the list of curve colors used for drawing IPPs. Its default value is c("red", "darkgreen", "blue", "orange", "black", "purple", "pink", "cyan", "cadetblue"). If the default value is not changed and the number of curves in IPPs are greater than the number of colors, 'black' color is used for all of the redundant curves.

See Also

[IPPMModel](#)

DrawFIN

The method 'DrawFIN' in [IPPMModel](#) class

Description

The method draws the feature interaction network (FIN) based on the field [FIN.Data](#).

Usage

```
DrawFIN(threshold = 0, lay.out = igraph::layout.auto)
```

Arguments

threshold	a numeric, the threshold of link weights. Only the links whose weights are greater than the threshold are shown in FIN.
lay.out	the layout defined in the package igraph.

See Also

[IPPMModel](#)

DrawIPP

The method 'DrawIPP' in [IPPMModel](#) class

Description

The method draws the impact pattern plots based on the clustering results [Clustering.Res](#).

Usage

```
DrawIPP(centralized=TRUE, nc=4)
```

Arguments

centralized	a boolean, indicating if the impact pattern plots are centralized.
nc	an integer, the number of subplots that are shown in every row.

See Also

[IPPMModel](#)

ExecuteAll	<i>The method 'ExecuteAll' in IPPMModel class</i>
------------	---

Description

The method executes the methods [SamplingXA](#), [SamplingXB](#), [PredictData](#), [ClusterImpactPlots](#) and [BuildTree](#) in sequence.

Usage

```
ExecuteAll()
```

See Also

[IPPMModel](#)

FIN.Data	<i>The field 'FIN.Data' in IPPMModel class</i>
----------	--

Description

FIN.Data is a data.frame to describe the feature interaction network, and is generated by the method [BuildTree](#). The row names and column names denote the 'from' nodes and 'to' nodes of the network, respectively. The values in FIN.Data denotes the link weights.

See Also

[IPPMModel](#)

GenerateParaTable	<i>The method 'GenerateParaTable' in IPPMModel class</i>
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Description

This method generates the field [ParaTable](#) based on the field [X.Data](#).

Usage

```
GenerateParaTable()
```

Value

a data.frame, which is assigned to the field [ParaTable](#).

Note

The method generates [ParaTable](#) based on the data in [X.Data](#) and some fixed rules, so the result may be wrong. Please check the information in [ParaTable](#) carefully before continuing the other tasks.

See Also

[IPPMModel](#)

initialize	<i>The method 'initialize' in IPPMModel class</i>
------------	---

Description

The method initializes some fields and generate the field [ParaTable](#) by calling the method [GenerateParaTable](#).

Usage

```
initialize(XDS, PredFun, PredType, PredDim=1, ModelPackage, XB.Size=200,
          XB.SamplingMethod="joint")
```

Arguments

XDS	a data.frame, the dataset of input features. It is assigned to the field X.Data .
PredFun	an object, the prediction function. It is assigned to the field Pred.Fun .
PredType	a string, the type of prediction. It is assigned to the field Pred.Type .
PredDim	an integer, indicating which class is predicted. This field is used only for classification model. It is assigned to the field Pred.Dimension .
ModelPackage	a string, the package name of the interpreted machine learning model, such as "nnet" and "randomforest". It is assigned to the field Model.Package .
XB.Size	an integer, the size of XB.Sample . It is assigned to the field XB.Size .
XB.SamplingMethod	a string, the sampling method of XB.Sample , "joint" or "independent". "joint" means that all features are sampled from X.Data jointly. "independent" means that each feature is sampled independently; then all features are combined randomly. It is assigned to the field XB.SamplingMethod .

See Also[IPPMoel](#)

IPPMoel

*Class providing object with methods for drawing IPPs and FIN***Description**

The class provides objects with methods for drawing impact pattern plots (IPPs) and feature interaction network (FIN).

Usage

IPPMoel

Format

R6Class object.

Value

Object of R6Class with methods for drawing IPPs and FIN.

Fields

[X.Data](#) a data.frame, the dataset of input features.

[Pred.Fun](#) an object, the prediction function. It can be any model created by "nnet", "randomforest" and "kernlab" etc.

[Model.Package](#) a string, the package name of the interpreted machine learning model, such as "nnet" and "randomforest".

[Pred.Type](#) a string, the type of prediction.

[Pred.Dimension](#) an integer, indicating which class is predicted. This field is used only for classification model.

[XB.Size](#) an integer, the size of [XB.Sample](#).

[XB.SamplingMethod](#) a string, the sampling method of [XB.Sample](#), "joint" or "independent". "joint" means that all features are sampled from [X.Data](#) jointly. "independent" means that each feature is sampled independently; then all features are combined randomly.

[ParaTable](#) a data.frame, the parameter table. It is generated by method [GenerateParaTable](#).

[XA.Sample](#) a list, the sample of X_A extracted from [X.Data](#). It is generated by method [SamplingXA](#).

[XB.Sample](#) a list, the sample of X_B extracted from [X.Data](#). It is generated by method [SamplingXB](#).

[Pred.Res](#) a list, the prediction results of f(X_A,X_B), which is generated by method [PredictData](#).

[Clustering.Res](#) a list, the clustering results, which is generated by method [ClusterImpactPlots](#).

[TreeRules](#) a list, the decision tree rules, which is generated by method [BuildTree](#).

[FIN.Data](#) a data.frame, the feature interaction network, which is generated by method [BuildTree](#).

[ColorList](#) a list, the curve colors used for drawing IPPs.

[TaskFinishTime](#) a list, the finishing time of tasks.

Methods

initialize initialize some fields of object and excute the method **CheckInitialization** and **GenerateParaTable**.

CheckInitialization validate the initialization information.

GenerateParaTable Generate the parameter table **ParaTable**.

CheckParaTable validate the information in **ParaTable**.

SamplingXA sampling **XA.Sample** from **X.Data**.

SamplingXB sampling **XB.Sample** from **X.Data**.

PredictData predict data using **Pred.Fun** based on **XA.Sample** and **XB.Sample**.

ClusterImpactPlots cluster the impact curves of each feature based on the predicting results **Pred.Res**.

BuildTree build decision tree based on the clustering results **Clustering.Res**.

DrawIPP draw the impact pattern plots.

DrawFIN draw the feature interaction network.

WriteToExcel write the results to an excel file.

ExecuteAll execute the methods **SamplingXA**, **SamplingXB**, **PredictData**, **ClusterImpactPlots** and **BuildTree** in sequence.

References

Xiaohang Zhang, Ji Zhu, SuBang Choe, Yi Lu and Jing Liu. Exploring black box of supervised learning models: Visualizing the impact of features on prediction. Working paper.

Examples

```
library(IPPMoel)
library(igraph)

#----- FIRST EXAMPLE -----
library(nnet)
data("bank")
# build model
bank.NN <- nnet(y ~ ., data = bank, size = 5, maxit = 1000)
# remove the output variable
bank.ds = bank[-17]
# create IPPMoel object
IPPM.bank = IPPMoel$new(XDS=bank.ds, PredFun=bank.NN,
                        ModelPackage="nnet", PredType="raw", PredDim=1,
                        XB.Size=1000, XB.SamplingMethod="joint")
# modify the clustering method to "kmedoids"
IPPM.bank$ParaTable$clusteringMethod = "kmedoids"
# execute all tasks
IPPM.bank$ExecuteAll()
# draw impact pattern plots (IPP)
IPPM.bank$DrawIPP(centralized = TRUE, nc = 4)
# draw feature interaction network (FIN)
IPPM.bank$DrawFIN(threshold = 0.2, lay.out = igraph::layout.auto)
# write the results into an excel file
IPPM.bank$WriteToExcel("output.xlsx")

#----- SECOND EXAMPLE -----
library(randomForest)
```

```

data("whitewine")
# build model
WW.RF <- randomForest(quality ~ ., data = whitewine, mtry = 4, importance=TRUE, na.action=na.omit)
# remove the output variable
WW.ds = whitewine[-12]
# create IPPModel object
IPP.WW = IPPModel$new(XDS=WW.ds, PredFun=WW.RF,
                      ModelPackage="randomForest", PredType="response", PredDim=1,
                      XB.Size=1000, XB.SamplingMethod="joint")
# set the maximum depth of trees to be 5
IPP.WW$ParaTable$treeDepth = 5
# execute all tasks
IPP.WW$ExecuteAll()
# draw impact pattern plots (IPP)
IPP.WW$DrawIPP(centralized = TRUE, nc = 4)
# draw feature interaction network (FIN)
IPP.WW$DrawFIN(threshold = 0.1, lay.out = igraph::layout.circle)

#----- THIRD EXAMPLE -----
library(kernlab)
data("iris")
iris.SVM <- ksvm(Species ~ ., data = iris, kernel="rbfdot", kpar="automatic", C=0.1, prob.model = TRUE)
# remove the output variable
iris.ds = iris[-5]
# create IPPModel object
IPP.iris = IPPModel$new(XDS=iris.ds, PredFun=iris.SVM,
                       ModelPackage="kernlab", PredType="prob", PredDim=1,
                       XB.Size=200, XB.SamplingMethod="independent")
# execute the tasks step by step
IPP.iris$SamplingXA() # sampling XA
IPP.iris$SamplingXB() # sampling XB
IPP.iris$PredictData() # predict
IPP.iris$ClusterImpactPlots() # clustering impact plots
IPP.iris$BuildTree() # build tree
# draw impact pattern plots (IPP)
IPP.iris$DrawIPP(centralized = TRUE, nc = 4)
# draw feature interaction network (FIN)
IPP.iris$DrawFIN(threshold = 0.3, lay.out = igraph::layout.auto)
# write the results into an excel file
IPP.iris$WriteToExcel("output.xlsx")

```

Model.Package

The field 'Model.Package' in *IPPModel* class

Description

Model.Package is the package name of the interpreted machine learning model [Pred.Fun](#), such as "nnet" and "randomforest".

See Also

[IPPModel](#)

ParaTable

*The field 'ParaTable' in [IPPMModel](#) class***Description**

The field 'ParaTable' provides some parameter information for the IPPModel class. It is a data.frame whose rowNames are the names of the input features in [X.Data](#). It includes the following columns.

Columns

dataType string, the data types of input features. It should be "interval", "binary", "ordinal" or "nominal". Interval feature is one for which the mean (or average) makes sense, such as person's height. Binary feature has only two possible levels. Gender is an example. Nominal variable has more than two levels, but the values of the levels have no implied order. Colors are examples. Ordinal feature has more than two levels, and the values of the levels have an implied order. Coffee sizes, such as small, medium, and large, are examples.

uniqueValue integer, the number of unique values of the input features.

X_A boolean, indicating if the feature serves as a target feature to draw impact pattern plots (IPPs) and involves in the feature interaction network (FIN).

L_A integer, the number of levels sampled from [X.Data](#) for the feature.

samplingMethod string, the sampling method of the feature. It should be "equal", "percentile" or "random". "equal" means that all levels are sampled with equal width from the range of the feature. "percentile" means that all levels are sampled based on the percentiles of the feature's distribution. "random" means that all levels are sampled randomly without replacement.

clusteringMethod string, the clustering method. It should be "kmeans" or "kmedoids".

centralized boolean, indicating if the feature's impact plots are centralized before clustering.

distMeasure string, the distance measure used in clustering process. It should be "euclidean" or "cosine".

autoK boolean, indicating if the number of clusters is determined automatically based on the Dunn index.

numK integer, the number of clusters if autoK = FALSE. If autoK = TRUE, numK denotes the maximum number of clusters.

treeDepth integer, the maximum tree depth. It is used to control the size of decision tree.

minSplit integer, the minimum number of observations for tree node splitting. It is used to control the size of decision tree.

Note

The ParaTable can be generated by the method [GenerateParaTable](#) based on the field [X.Data](#). However, the user must check the parameter information carefully before continuing the other tasks.

See Also

[IPPMModel](#)

Pred.Dimension	<i>The field 'Pred.Dimension' in IPPMModel class</i>
----------------	--

Description

Pred.Dimension is an integer, indicating which class is predicted. This field is used only for classification model. For example, the output field is assumed to have three classes, so Pred.Dimension can be 1, 2 or 3. If Pred.Dimension equals 1, then the first class is predicted and analyzed. Note that if Pred.Dimension is larger than 3, then it is reset to 1.

See Also

[IPPMModel](#)

Pred.Fun	<i>The field 'Pred.Fun' in IPPMModel class</i>
----------	--

Description

Pred.fun is the prediction function. It can be any model created by "nnet", "randomforest" and "kernlab" etc. Pred.fun must be consistent with the field [X.Data](#).

See Also

[IPPMModel](#)

Pred.Res	<i>The field 'Pred.Res' in IPPMModel class</i>
----------	--

Description

Pred.Res is the prediction results of the model defined by [Pred.Fun](#) for the combination of [XA.Sample](#) and [XB.Sample](#). Pred.Res is generated by the method [PredictData](#). Pred.Res is a list, each element of which is a data.frame of the prediction results of a feature.

See Also

[IPPMModel](#)

Pred.Type	<i>The description of the field 'Pred.Type' in IPPMModel class</i>
-----------	--

Description

Pred.Type is the type of prediction. The IPP model only supports interpreting the models with numerical outputs, so Pred.Type is used to assure that the output is numeric, not class. The value of Pred.Type depends on what package is used. For example, if "nnet" is used to create [Pred.Fun](#), Pred.Type should be "raw" for both classification and regression. If "randomForest" or "kernlab" is used, Pred.Type should be "prob" for classification, or be "response" for regression. If other package is used, you should reference the predict function of that package.

See Also

[IPPMModel](#)

PredictData	<i>The method 'PredictData' in IPPMModel class</i>
-------------	--

Description

The method predicts data using [Pred.Fun](#) based on [XA.Sample](#) and [XB.Sample](#). The method is executed in parallel using package [parallel](#). Each feature corresponds to one core.

Usage

```
PredictData()
```

Value

a list of predicting results of each feature. The result is saved in the field [Pred.Res](#).

See Also

[IPPMModel](#)

SamplingXA	<i>The method 'SamplingXA' in IPPMModel class</i>
------------	---

Description

The method samples X_A from [X.Data](#) based on the sample size and the sampling method defined by "L_A" and "samplingMethod" in [ParaTable](#), respectively.

Usage

```
SamplingXA()
```

Value

a list of samples of each feature. The result is saved in the field [XA.Sample](#).

See Also

[IPPMModel](#)

SamplingXB

The method 'SamplingXB' in [IPPMModel](#) class

Description

The method samples X_B from [X.Data](#) based on the sample size and sampling method defined by the fields [XB.Size](#) and [XB.SamplingMethod](#), respectively.

Usage

SamplingXB()

Value

a data.frame of sample. It is saved in the field [XB.Sample](#).

See Also

[IPPMModel](#)

TaskFinishTime

The field 'TaskFinishTime' in [IPPMModel](#) class

Description

TaskFinishTime is a list for recording the finishing time of tasks, including initialization, sampling X_A and X_B, prediction, clustering, obtaining tree rules and building FIN.

See Also

[IPPMModel](#)

TreeRules

The field 'TreeRules' in [IPPMModel](#) class

Description

TreeRules are the decision tree rules, which is generated by method [BuildTree](#). It is a list, each element of which is a data.frame of tree rules and the corresponding cluster distribution of a feature.

See Also

[IPPMModel](#)

WriteToExcel	<i>The method 'WriteToExcel' in IPPMModel class</i>
--------------	---

Description

The method writes some results into an excel file, including the impact pattern plots, the tree rules and the feature interaction network.

Usage

```
WriteToExcel(excelName)
```

Arguments

excelName a string, the path and name of the excel file.

See Also

[IPPMModel](#)

X.Data	<i>The field 'X.Data' in IPPMModel class</i>
--------	--

Description

X.Data is a data.frame and is the dataset of input features. X.Data must be consistent with the field [Pred.Fun](#) that is the prediction function. Note that the dataset should not include the output feature (y).

See Also

[IPPMModel](#)

XA.Sample	<i>The field 'XA.Sample' in IPPMModel class</i>
-----------	---

Description

XA.Sample is the sample of X_A extracted from [X.Data](#). It is generated by method [SamplingXA](#). XA.Sample is a list, each element of which is a vector of the sample values of a feature. The included features in XA.Sample are determined by the column 'X_A' in the field [ParaTable](#). The size of XA.Sample is defined by the column 'L_A' in the field [ParaTable](#). The sampling method of XA.Sample is defined by the column 'samplingMethod' in the field [ParaTable](#).

See Also

[IPPMModel](#)

XB.Sample	<i>The field 'XB.Sample' in IPPMModel class</i>
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Description

XB.Sample is the sample of X_B extracted from [X.Data](#). It is generated by method [SamplingXB](#). The size of XB.Sample is defined by the field [XB.Size](#). The sampling method of XB.Sample is defined by the field [XB.SamplingMethod](#). XB.Sample is a data.frame whose columns are the same as [X.Data](#).

See Also

[IPPMModel](#)

XB.SamplingMethod	<i>The field 'XB.SamplingMethod' in IPPMModel class</i>
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Description

XB.SamplingMethod is the sampling method of [XB.Sample](#), "joint" or "independent". "joint" means that all features are sampled from X.Data jointly. "independent" means that each feature is sampled independently; then all features are combined randomly. Note that the "joint" method can keep the features' joint distribution unchanged.

See Also

[IPPMModel](#)

XB.Size	<i>The field 'XB.Size' in IPPMModel class</i>
---------	---

Description

XB.size is the size of [XB.Sample](#). Larger XB.size can bring more robust IPPs and FIN , but higher computational costs.

See Also

[IPPMModel](#)

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