

Package ‘XAItest’

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Title XAItest: Enhancing Feature Discovery with eXplainable AI

Version 1.0.1

Description XAItest is an R Package that identifies features using eXplainable AI (XAI) methods such as SHAP or LIME. This package allows users to compare these methods with traditional statistical tests like t-tests, empirical Bayes, and Fisher's test. Additionally, it includes a system that enables the comparison of feature importance with p-values by incorporating calibrated simulated data.

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getFeatImpThresholds	<i>The getFeatImpThresholds function identifies the minimum level of feature importance required to exceed a specified significance threshold, which is determined by the p-value.</i>
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Description

The getFeatImpThresholds function identifies the minimum level of feature importance required to exceed a specified significance threshold, which is determined by the p-value.

Usage

```
getFeatImpThresholds(  
  df,  
  refPvalColumn = "adjpval",  
  featImpColumns = "feat",  
  refPval = 0.05  
)
```

Arguments

df	A dataframe containing p-value columns and feature importance columns.
refPvalColumn	Optional; the name of the column containing the reference p-values. If not provided, the function will search for a column name containing "adjpval", if not existing a column name containing "pval" (case insensitive).
featImpColumns	Optional; a vector of column names containing the feature importance values. If not provided, the function will search for column names containing "feat" (case insensitive).
refPval	The reference p-value threshold for filtering features. Defaults to 0.05.

Details

The reference p-value column can be given by the refPvalColumn argument. If not provided, the function will search for the first df column name containing "pval". The feature importance columns can be given by the featImpColumns argument. If not provided, the function will search for all df column names containing "feat".

It then selects feature importance values of features with p-values under the specified threshold and returns the lowest.

This is useful for identifying the most significant features in a dataset based on statistical testing, aiding in the interpretation of machine learning models and exploratory data analysis.

Value

A named vector of minimum feature importance values for each feature passing the p-value filter. The names of the vector elements correspond to the feature importance columns in df.

Examples

```
# Assuming `df` is a dataframe with columns `feature1_pval`,
# `feature2_pval`, `feature1_imp`, `feature2_imp`
df <- data.frame(pval = c(0.04, 0.02, 0.06, 0.8),
                 adjPval = c(0.01, 0.03, 0.05, 0.9),
                 feat_imp_1 = c(0.2, 0.3, 0.1, 0.6),
                 feat_imp_2 = c(0.4, 0.5, 0.3, 0.6))
thresholds <- getFeatImpThresholds(df)
print(thresholds)
```

getMetricsTable

Get the Metrics Table

Description

This method retrieves the metrics table from an ObjXAI object.

Usage

```
getMetricsTable(object)
```

Arguments

object An ObjXAI object.

Value

A data frame containing the metrics.

Examples

```
obj <- new("ObjXAI",
  data = data.frame(),
  dataSim = data.frame(),
  metricsTable = data.frame(Metric = c("Accuracy", "Precision"),
                             Value = c(0.95, 0.89)),
  map = list(),
  models = list(),
  modelPredictions = list(),
  args = list())
getMetricsTable(obj)
```

mapPvalImportance	<i>The mapPvalImportance function displays a datatable with color-coded cells based on significance thresholds for feature importance and p-value columns.</i>
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Description

The mapPvalImportance function displays a datatable with color-coded cells based on significance thresholds for feature importance and p-value columns.

Usage

```
mapPvalImportance(
  objXAI,
  refPvalColumn = "adjpval",
  featImpColumns = "feat",
  pvalColumns = NULL,
  refPval = 0.05
)
```

Arguments

objXAI	An object of class ObjXAI.
refPvalColumn	Optional; the name of the column containing reference p-values for feature importance. If not provided, the function will attempt to auto-detect.
featImpColumns	Optional; a vector of column names containing feature importance values. If not provided, the function will attempt to auto-detect.
pvalColumns	Optional; a vector of column names containing p-values. If not provided, the function searches for columns containing "pval" (case insensitive).
refPval	The reference p-value threshold used for filtering. Defaults to 0.05.

Details

The function first identifies the relevant p-value columns and feature importance columns, if not explicitly provided. It then calculates feature importance thresholds based on the specified p-value threshold. Then the dataframe is displayed with color-coded cells based on significance thresholds for feature importance and p-value columns.

Value

A dataframe and a datatable object with color-coded cells based on significance thresholds for feature importance and p-value columns.

Examples

```
df <- data.frame(
  feature1 = rnorm(10),
  feature2 = rnorm(10, mean = 5),
  feature3 = runif(10, min = 0, max = 10),
  feature4 = c(rnorm(5), rnorm(5, mean = 5)),
  categ = c(rep("Cat1", 5), rep("Cat2", 5))
)

results <- XAI.test(df, y = "categ", simData = TRUE)

my_map <- mapPvalImportance(results)
my_map$df
my_map$dt
```

modelsOverview

Models Overview

Description

Returns **mse**, **rmse**, **mae** and **r2** of regression models or **accuracy**, **precision**, **recall** and **f1_score** of classification models.

Usage

```
modelsOverview(objXAI, verbose = FALSE)
```

Arguments

objXAI	An object of class ObjXAI.
verbose	Logical; if TRUE, prints the models names.

Value

Returns **mse**, **rmse**, **mae** and **r2** of regression models or **accuracy**, **precision**, **recall** and **f1_score** of classification models.

Examples

```
# Example with SummarizedExperiment object with a regression dataset.

library(S4Vectors)
library(SummarizedExperiment)

df <- data.frame(
  feature1 = rnorm(100),
  feature2 = rnorm(100, mean = 5),
  feature3 = runif(100, min = 0, max = 10),
  feature4 = c(rnorm(50), rnorm(50, mean = 5)),
  y = 1:100
)

assays <- SimpleList(counts = as.matrix(t(df[, 1:4])))
colData <- DataFrame(y = df[, "y"])
se <- SummarizedExperiment(assays = assays,
                           colData = colData)

resultsRegr <- XAI.test(se, y = "y", verbose = TRUE)

modelsOverview(resultsRegr)

# Example with a dataframe with a classification dataset.
df <- data.frame(
  feature1 = rnorm(100),
  feature2 = rnorm(100, mean = 5),
  feature3 = runif(100, min = 0, max = 10),
  feature4 = c(rnorm(50), rnorm(50, mean = 5)),
  y = c(rep("Cat1", 50), rep("Cat2", 50))
)
resultsClassif <- XAI.test(df, y = "y", verbose = TRUE)

modelsOverview(resultsClassif)
```

ObjXAI-class

ObjXAI class

Description

ObjXAI is a class used to store the output values of the `XAI.test` function.

Value

A ObjXAI object

Examples

```
obj <- new("ObjXAI",
  data = data.frame(),
  dataSim = data.frame(),
  metricsTable = data.frame(Metric = c("Accuracy", "Precision"),
                             Value = c(0.95, 0.89)),
  map = list(),
  models = list(),
  modelPredictions = list(),
  args = list())
```

plotModel

Plot the model

Description

This function plots the model.

Usage

```
plotModel(objXAI, modelName, xFeature, yFeature = "")
```

Arguments

objXAI	The ObjXAI object created with the XAItest function
modelName	The name of the model, can be found in 'names(objXAI@models)'
xFeature	The x feature
yFeature	The y feature

Value

A plot

Examples

```
data(iris)
iris = subset(iris, Species == "setosa" | Species == "versicolor")
iris$Species = as.character(iris$Species)
objXAI <- XAI.test(iris, y = "Species")
plotModel(objXAI, "RF_feat_imp", "Sepal.Length", "Sepal.Width")
```

setMetricsTable	<i>Set the Metrics Table</i>
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Description

This method sets the metrics table for an ObjXAI object.

Usage

```
setMetricsTable(object, value)
```

Arguments

object	An ObjXAI object.
value	A data frame to set as the metrics table.

Value

The modified ObjXAI object.

Examples

```
obj <- new("ObjXAI",
  data = data.frame(),
  dataSim = data.frame(),
  metricsTable = data.frame(Metric = c("Accuracy", "Precision"),
    Value = c(0.95, 0.89)),
  map = list(),
  models = list(),
  modelPredictions = list(),
  args = list())

setMetricsTable(obj, data.frame(Metric = c("Accuracy", "Precision", "Recall"),
  Value = c(0.95, 0.89, 0.91)))
```

show,ObjXAI-method	<i>Show Method for ObjXAI</i>
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Description

Prints the first 5 rows of the metrics table from an ObjXAI object.

Usage

```
## S4 method for signature 'ObjXAI'
show(object)
```

Arguments

object An ObjXAI object.

Value

The first 5 rows of the metrics table.

XAI.test	<i>The XAI.test function complements t-test and correlation analyses in feature discovery by integrating eXplainable AI techniques such as feature importance, SHAP, LIME, or custom functions. It provides the option of automatic integration of simulated data to facilitate matching significance between p-values and feature importance.</i>
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Description

The XAI.test function complements t-test and correlation analyses in feature discovery by integrating eXplainable AI techniques such as feature importance, SHAP, LIME, or custom functions. It provides the option of automatic integration of simulated data to facilitate matching significance between p-values and feature importance.

Usage

```
XAI.test(
  data,
  y = "y",
  featImpAgr = "mean",
  simData = FALSE,
  simMethod = "regnorm",
  simPvalTarget = 0.045,
  adjMethod = "bonferroni",
  customPVals = NULL,
  customFeatImps = NULL,
  modelType = "default",
  corMethod = "pearson",
  defaultMethods = c("ttest", "ebayes", "cor", "lm", "rf", "shap", "lime"),
  caretMethod = "rf",
  caretTrainArgs = NULL,
  verbose = FALSE
)
```

Arguments

data SummarizedExperiment or dataframe containing the data. If dataframe rows are samples and columns are features.

y Name of the SummarizedExperiment metadata or column of the dataframe containing the target variable. Default to "y".

featImpAgr	Can be "mean" or "max_abs". It defines how the feature importance is aggregated.
simData	If TRUE, a simulated feature column is added to the dataframe to target a defined p-value that will serve as a benchmark for determining the significance thresholds of feature importances.
simMethod	Method used to generate the simulated data. Can be "regnorm" or "rnorm", "regnorm" by default. "regnorm" creates simulated data points that match specific percentiles within a normal distribution, defined by a given mean and standard deviation. "rnorm" creates simulated data points that follow a normal distribution. "regnorm" is more accurate in targeting the specified p-value.
simPvalTarget	Target p-value for the simulated data. It is used to determine the significance thresholds of feature importances.
adjMethod	Method used to adjust the p-values. "bonferroni" by default, can be any other method available in the p.adjust function.
customPVals	List of custom functions that compute p-values. The functions must take the dataframe and the target variable as arguments and return a names list with: • 'pvals' => a dataframe with the p-values. • 'adjPVal' => a dataframe with the adjusted p-values. Optional. • 'model' => the prediction model object. Optional.
customFeatImps	List of custom functions that compute feature importances. The functions must take the dataframe and the target variable as arguments and return a names list with: • 'featImps' => a dataframe with the feature importances. The names of the functions will be used as the column names in the output dataframe. Mandatory. • 'model' => the predictionmodel object. Optional.
modelType	Type of the model. Can be "classification", "regression" or "default". If "default", the function will try to infer the model type from the target variable. If the target variable is a character, the model type will be "classification". If the target variable is numeric, the model type will be "regression".
corMethod	Method used to compute the correlation between the features and the target variable. "pearson" by default, can be any other method available in the cor.test function.
defaultMethods	List of default p-values and feature importances methods to compute. By default "ttest", "ebayes", "cor", "lm", "rf", "shap" and "lime".
caretMethod	Method used by the caret package to train the model. "rf" by default.
caretTrainArgs	List of arguments to pass to the caret::train function. Optional.
verbose	If TRUE, the function will print messages to the console.

Details

The XAI.test function is designed to extend the capabilities of conventional statistical analysis methods for feature discovery, such as t-tests and correlation, by incorporating techniques from explainable AI (XAI), such as feature importance, SHAP, LIME, or custom functions. This function aims

at identifying significant features that influence a given target variable in a dataset, supporting both categorical and numerical target values. A key feature of XAI.test is its ability to automatically incorporate simulated data into the analysis. This simulated data is specifically designed to establish significance thresholds for feature importance values based on the p-values. This capability is useful for reinforcing the reliability of the feature importance metrics derived from machine learning models, by directly comparing them with established statistical significance metrics.

Value

A dataframe containing the pvalues and the feature importances of each features computed by the different methods.

Examples

```
library(S4Vectors)
library(SummarizedExperiment)

# With a dataframe
data <- data.frame(
  feature1 = rnorm(100),
  feature2 = rnorm(100, mean = 5),
  feature3 = runif(100, min = 0, max = 10),
  feature4 = c(rnorm(50), rnorm(50, mean = 5)),
  y = c(rep("Cat1", 50), rep("Cat2", 50))
)

results <- XAI.test(data, y = "y", verbose = TRUE)
results

# With a SummarizedExperiment
assays <- SimpleList(counts = as.matrix(t(data[, 1:4])))
colData <- DataFrame(y = data[, "y"])
se <- SummarizedExperiment(assays = assays,
                           colData = colData)
results <- XAI.test(se, y = "y", verbose = TRUE)
results
```

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