

Package ‘rSAFE’

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Title Surrogate-Assisted Feature Extraction

Version 0.1.4

Description

Provides a model agnostic tool for white-box model trained on features extracted from a black-box model. For more information see: Gosiewska et al. (2020) <[doi:10.1016/j.dss.2021.113556](https://doi.org/10.1016/j.dss.2021.113556)>.

Depends R (>= 3.5.0)

License GPL-3

Encoding UTF-8

LazyData true

RoxygenNote 7.2.1

Imports DALEX, dendextend, ggplot2, ggpubr, grDevices, ingredients, sets, stats

Suggests gbm, knitr, pander, randomForest, rmarkdown, spelling, testthat, vdiff

VignetteBuilder knitr

URL <https://github.com/ModelOriented/rSAFE>

BugReports <https://github.com/ModelOriented/rSAFE/issues>

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NeedsCompilation no

Author Alicja Gosiewska [aut, cre],
Anna Gierlak [aut],
Przemyslaw Biecek [aut, ths],
Michal Burdukiewicz [ctb] (<<https://orcid.org/0000-0001-8926-582X>>)

Maintainer Alicja Gosiewska <alicjagosiewska@gmail.com>

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apartments	<i>Apartments data</i>
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Description

Datasets apartments and apartmentsTest are artificial, generated from the same model. Structure of the dataset is copied from real dataset from PBImisc package, but they were generated in a way to mimic effect of Anscombe quartet for complex black box models.

Usage

```
data(apartments)
```

Format

a data frame with 1000 rows and 6 columns

Details

- m2.price - price per square meter
- surface - apartment area in square meters
- no.rooms - number of rooms (correlated with surface)
- district - district in which apartment is located, factor with 10 levels (Bemowo, Bielany, Mokotow, Ochota, Praga, Srodmiescie, Ursus, Ursynow, Wola, Zoliborz)
- floor - floor
- construction.year - construction year

HR_data	<i>Why are our best and most experienced employees leaving prematurely?</i>
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Description

A dataset from Kaggle competition Human Resources Analytics. <https://www.kaggle.com/>

Format

A data frame with 14999 rows and 10 variables

Details

- satisfaction_level Level of satisfaction (0-1)
- last_evaluation Time since last performance evaluation (in Years)
- number_project Number of projects completed while at work
- average_monthly_hours Average monthly hours at workplace
- time_spend_company Number of years spent in the company
- work_accident Whether the employee had a workplace accident
- left Whether the employee left the workplace or not (1 or 0) Factor
- promotion_last_5years Whether the employee was promoted in the last five years
- sales Department in which they work for
- salary Relative level of salary (high)

Source

Dataset HR-analytics from <https://www.kaggle.com>

plot.safe_extractor	<i>Plotting Transformations of the SAFE Extractor Object</i>
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Description

Plotting Transformations of the SAFE Extractor Object

Usage

```
## S3 method for class 'safe_extractor'  
plot(x, ..., variable = NULL)
```

Arguments

x	safe_extractor object containing information about variables transformations created with safe_extraction() function
...	other parameters
variable	character, name of the variable to be plotted

Value

a plot object

`print.safe_extractor` *Printing Summary of the SAFE Extractor Object*

Description

Printing Summary of the SAFE Extractor Object

Usage

```
## S3 method for class 'safe_extractor'
print(x, ..., variable = NULL)
```

Arguments

x	safe_extractor object containing information about variables transformations created with safe_extraction() function
...	other parameters
variable	character, name of the variable to be plotted. If this argument is not specified then transformations for all variables are printed

Value

No return value, prints the structure of the object

`safely_detect_changepoints`*Identifying Changes in a Series Using PELT Algorithm*

Description

The `safely_detect_changepoints()` function calculates the optimal positioning and number of change-points for given data and penalty. It uses a PELT algorithm with a nonparametric cost function based on the empirical distribution. The implementation is inspired by the code available on <https://github.com/rkillick/changepoint>.

Usage

```
safely_detect_changepoints(data, penalty = "MBIC", nquantiles = 10)
```

Arguments

<code>data</code>	a vector within which you wish to find changepoints
<code>penalty</code>	penalty for introducing another changepoint, one of "AIC", "BIC", "SIC", "MBIC", "Hannan-Quinn" or numeric non-negative value
<code>nquantiles</code>	the number of quantiles used in integral approximation

Value

a vector of optimal changepoint positions (last observations of each segment)

See Also

[safely_transform_continuous](#)

Examples

```
library(rSAFE)

data <- rep(c(2,7), each=4)
safely_detect_changepoints(data)

set.seed(123)
data <- c(rnorm(15, 0), rnorm(20, 2), rnorm(30, 8))
safely_detect_changepoints(data)
safely_detect_changepoints(data, penalty = 25)
```

`safely_detect_interactions`*Detecting Interactions via Permutation Approach*

Description

The `safely_detect_interactions()` function detects second-order interactions based on predictions made by a surrogate model. For each pair of features it performs values permutation in order to evaluate their non_additive effect.

Usage

```
safely_detect_interactions(  
  explainer,  
  inter_param = 0.5,  
  inter_threshold = 0.5,  
  verbose = TRUE  
)
```

Arguments

<code>explainer</code>	DALEX explainer created with <code>explain()</code> function
<code>inter_param</code>	numeric, a positive value indicating which of single observation non-additive effects are to be regarded as significant, the higher value the higher non-additive effect has to be taken into account
<code>inter_threshold</code>	numeric, a value from $[0, 1]$ interval indicating which interactions should be returned as significant. It corresponds to the percentage of observations for which interaction measure is greater than <code>inter_param</code> - if this percentage is less than <code>inter_threshold</code> then interaction effect is ignored.
<code>verbose</code>	logical, if progress bar is to be printed

Value

dataframe object containing interactions effects greater than or equal to the specified `inter_threshold`

See Also

[safe_extraction](#)

Examples

```
library(DALEX)  
library(randomForest)  
library(rSAFE)
```

```

data <- apartments[1:500,]
set.seed(111)
model_rf <- randomForest(m2.price ~ construction.year + surface + floor +
                        no.rooms + district, data = data)
explainer_rf <- explain(model_rf, data = data[,2:6], y = data[,1])
safely_detect_interactions(explainer_rf, inter_param = 0.25,
                          inter_threshold = 0.2, verbose = TRUE)

```

safely_select_variables

Performing Feature Selection on the Dataset with Transformed Variables

Description

The `safely_select_variables()` function selects variables from dataset returned by `safely_transform_data()` function. For each original variable exactly one variable is chosen

- either original one or transformed one. The choice is based on the AIC value for linear model (regression) or logistic regression (classification).

Usage

```

safely_select_variables(
  safe_extractor,
  data,
  y = NULL,
  which_y = NULL,
  class_pred = NULL,
  verbose = TRUE
)

```

Arguments

<code>safe_extractor</code>	object containing information about variables transformations created with <code>safe_extraction()</code> function
<code>data</code>	data, original dataset or the one returned by <code>safely_transform_data()</code> function. If data do not contain transformed variables then transformation is done inside this function using 'safe_extractor' argument. Data may contain response variable or not - if it does then 'which_y' argument must be given, otherwise 'y' argument should be provided.
<code>y</code>	vector of responses, must be given if data does not contain it
<code>which_y</code>	numeric or character (optional), must be given if data contains response values
<code>class_pred</code>	numeric or character, used only in multi-classification problems. If response vector has more than two levels, then 'class_pred' should indicate the class of interest which will denote failure - all other classes will stand for success.
<code>verbose</code>	logical, if progress bar is to be printed

Value

vector of variables names, selected based on AIC values

See Also

[safely_transform_data](#)

Examples

```
library(DALEX)
library(randomForest)
library(rSAFE)

data <- apartments[1:500,]
set.seed(111)
model_rf <- randomForest(m2.price ~ construction.year + surface + floor +
                        no.rooms + district, data = data)
explainer_rf <- explain(model_rf, data = data[,2:6], y = data[,1])
safe_extractor <- safe_extraction(explainer_rf, verbose = FALSE)
safely_select_variables(safe_extractor, data, which_y = "m2.price", verbose = FALSE)
```

safely_transform_categorical

Calculating a Transformation of Categorical Feature Using Hierarchical Clustering

Description

The `safely_transform_categorical()` function calculates a transformation function for the categorical variable using predictions obtained from black box model and hierarchical clustering. The gap statistic criterion is used to determine the optimal number of clusters.

Usage

```
safely_transform_categorical(
  explainer,
  variable,
  method = "complete",
  B = 500,
  collapse = "_"
)
```


Arguments

explainer	DALEX explainer created with explain() function
variable	a feature for which the transformation function is to be computed
method	the agglomeration method to be used in hierarchical clustering, one of: "ward.D", "ward.D2", "single", "complete", "average", "mcquitty", "median", "centroid"
B	number of reference datasets used to calculate gap statistics
collapse	a character string to separate original levels while combining them to the new one

Value

list of information on the transformation of given variable

See Also

[safe_extraction](#)

Examples

```
library(DALEX)
library(randomForest)
library(rSAFE)

data <- apartments[1:500,]
set.seed(111)
model_rf <- randomForest(m2.price ~ construction.year + surface + floor +
                        no.rooms + district, data = data)
explainer_rf <- explain(model_rf, data = data[,2:6], y = data[,1])
safely_transform_categorical(explainer_rf, "district")
```

safely_transform_continuous

*Calculating a Transformation of a Continuous Feature Using
PDP/ALE Plot*

Description

The `safely_transform_continuous()` function calculates a transformation function for the continuous variable using a PD/ALE plot obtained from black box model.

Usage

```
safely_transform_continuous(
  explainer,
  variable,
  response_type = "ale",
  grid_points = 50,
  N = 200,
  penalty = "MBIC",
  nquantiles = 10,
  no_segments = 2
)
```

Arguments

explainer	DALEX explainer created with explain() function
variable	a feature for which the transformation function is to be computed
response_type	character, type of response to be calculated, one of: "pdp", "ale". If features are uncorrelated, one can use "pdp" type - otherwise "ale" is strongly recommended.
grid_points	number of points on x-axis used for creating the PD/ALE plot, default 50
N	number of observations from the dataset used for creating the PD/ALE plot, default 200
penalty	penalty for introducing another changepoint, one of "AIC", "BIC", "SIC", "MBIC", "Hannan-Quinn" or numeric non-negative value
nquantiles	the number of quantiles used in integral approximation
no_segments	numeric, a number of segments variable is to be divided into in case of founding no breakpoints

Value

list of information on the transformation of given variable

See Also

[safe_extraction](#), [safely_detect_changepoints](#)

Examples

```
library(DALEX)
library(randomForest)
library(rSAFE)

data <- apartments[1:500,]
set.seed(111)
model_rf <- randomForest(m2.price ~ construction.year + surface + floor +
  no.rooms + district, data = data)
explainer_rf <- explain(model_rf, data = data[,2:6], y = data[,1])
safely_transform_continuous(explainer_rf, "construction.year")
```

safely_transform_data *Performing Transformations on All Features in the Dataset*

Description

The `safely_transform_data()` function creates new variables in dataset using `safe_extractor` object.

Usage

```
safely_transform_data(safe_extractor, data, verbose = TRUE)
```

Arguments

<code>safe_extractor</code>	object containing information about variables transformations created with <code>safe_extraction()</code> function
<code>data</code>	data for which features are to be transformed
<code>verbose</code>	logical, if progress bar is to be printed

Value

data with extra columns containing newly created variables

See Also

[safe_extraction](#), [safely_select_variables](#)

Examples

```
library(DALEX)
library(randomForest)
library(rSAFE)

data <- apartments[1:500,]
set.seed(111)
model_rf <- randomForest(m2.price ~ construction.year + surface + floor +
                        no.rooms + district, data = data)
explainer_rf <- explain(model_rf, data = data[,2:6], y = data[,1])
safe_extractor <- safe_extraction(explainer_rf, verbose = FALSE)
safely_transform_data(safe_extractor, data, verbose = FALSE)
```

safe_extraction	<i>Creating SAFE Extractor - an Object Used for Surrogate-Assisted Feature Extraction</i>
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Description

The `safe_extraction()` function creates a SAFE-extractor object which may be used later for surrogate feature extraction.

Usage

```
safe_extraction(
  explainer,
  response_type = "ale",
  grid_points = 50,
  N = 200,
  penalty = "MBIC",
  nquantiles = 10,
  no_segments = 2,
  method = "complete",
  B = 500,
  collapse = "_",
  interactions = FALSE,
  inter_param = 0.25,
  inter_threshold = 0.25,
  verbose = TRUE
)
```

Arguments

<code>explainer</code>	DALEX explainer created with <code>explain()</code> function
<code>response_type</code>	character, type of response to be calculated, one of: "pdp", "ale". If features are uncorrelated, one can use "pdp" type - otherwise "ale" is strongly recommended.
<code>grid_points</code>	number of points on x-axis used for creating the PD/ALE plot, default 50
<code>N</code>	number of observations from the dataset used for creating the PD/ALE plot, default 200
<code>penalty</code>	penalty for introducing another changepoint, one of "AIC", "BIC", "SIC", "MBIC", "Hannan-Quinn" or numeric non-negative value
<code>nquantiles</code>	the number of quantiles used in integral approximation
<code>no_segments</code>	numeric, a number of segments variable is to be divided into in case of founding no breakpoints
<code>method</code>	the agglomeration method to be used in hierarchical clustering, one of: "ward.D", "ward.D2", "single", "complete", "average", "mcquitty", "median", "centroid"
<code>B</code>	number of reference datasets used to calculate gap statistics

collapse	a character string to separate original levels while combining them to the new one
interactions	logical, if interactions between variables are to be taken into account
inter_param	numeric, a positive value indicating which of single observation non-additive effects are to be regarded as significant, the higher value the higher non-additive effect has to be taken into account
inter_threshold	numeric, a value from $[0, 1]$ interval indicating which interactions should be returned as significant. It corresponds to the percentage of observations for which interaction measure is greater than <code>inter_param</code> - if this percentage is less than <code>inter_threshold</code> then interaction effect is ignored.
verbose	logical, if progress bar is to be printed

Value

safe_extractor object containing information about variables transformation

See Also

[safely_transform_categorical](#), [safely_transform_continuous](#), [safely_detect_interactions](#), [safely_transform_data](#)

Examples

```
library(DALEX)
library(randomForest)
library(rSAFE)

data <- apartments[1:500,]
set.seed(111)
model_rf <- randomForest(m2.price ~ construction.year + surface + floor +
                        no.rooms + district, data = data)
explainer_rf <- explain(model_rf, data = data[,2:6], y = data[,1], verbose = FALSE)
safe_extractor <- safe_extraction(explainer_rf, grid_points = 30, N = 100, verbose = FALSE)
print(safe_extractor)
plot(safe_extractor, variable = "construction.year")
```

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