

Package ‘SHAPforxgboost’

May 29, 2023

Title SHAP Plots for 'XGBoost'

Version 0.1.3

Date 2023-05-18

Description Aid in visual data investigations
using SHAP (SHapley Additive exPlanation) visualization plots for 'XGBoost' and 'LightGBM'.
It provides summary plot, dependence plot, interaction plot, and force plot and relies on
the SHAP implementation provided by 'XGBoost' and 'LightGBM'.
Please refer to 'slundberg/shap' for the original implementation of SHAP in 'Python'.

License MIT + file LICENSE

URL <https://github.com/liuyanguu/SHAPforxgboost>

BugReports <https://github.com/liuyanguu/SHAPforxgboost/issues>

Encoding UTF-8

LazyData true

Depends R (>= 3.5.0)

VignetteBuilder knitr

Imports stats, ggplot2 (>= 3.0.0), xgboost (>= 0.81.0.0), data.table
(>= 1.12.0), ggforce (>= 0.2.1.9000), ggExtra (>= 0.8),
RColorBrewer (>= 1.1.2), ggpubr, BBmisc

Suggests knitr, rmarkdown, gridExtra (>= 2.3), here, parallel,
lightgbm (>= 2.1)

RoxygenNote 7.2.1

NeedsCompilation no

Author Yang Liu [aut, cre] (<<https://orcid.org/0000-0001-6557-6439>>),
Allan Just [aut, ctb] (<<https://orcid.org/0000-0003-4312-5957>>),
Michael Mayer [ctb]

Maintainer Yang Liu <lyhello@gmail.com>

Repository CRAN

Date/Publication 2023-05-29 17:20:07 UTC

R topics documented:

dataXY_df	2
label.feature	3
labels_within_package	3
new_labels	4
plot.label	4
scatter.plot.diagonal	5
scatter.plot.simple	6
shap.importance	7
shap.plot.dependence	7
shap.plot.force_plot	10
shap.plot.force_plot_bygroup	11
shap.plot.summary	11
shap.plot.summary.wrap1	13
shap.plot.summary.wrap2	14
shap.prep	15
shap.prep.interaction	17
shap.prep.stack.data	18
shap.values	19
shap_int_iris	20
shap_long_iris	21
shap_score	21
shap_values_iris	21
Index	22

dataXY_df	<i>Terra satellite data (X,Y) for running the xgboost model .</i>
-----------	---

Description

Data.table, contains 9 features, and about 10,000 observations

Usage

```
dataXY_df
```

Format

An object of class `data.table` (inherits from `data.frame`) with 10148 rows and 10 columns.

References

[doi:10.5281/zenodo.3568449](https://doi.org/10.5281/zenodo.3568449)

label.feature	<i>Modify labels for features under plotting</i>
---------------	--

Description

label.feature helps to modify labels. If a list is created in the global environment named **new_labels** (!is.null(new_labels)), the plots will use that list to replace default list of labels [labels_within_package](#).

Usage

```
label.feature(x)
```

Arguments

x variable names

Value

a character, e.g. "date", "Time Trend", etc.

labels_within_package	<i>labels_within_package: Some labels package auther defined to make his plot, mainly serve the paper publication.</i>
-----------------------	--

Description

It contains a list that match each feature to its labels. It is used in the function [label.feature](#).

Usage

```
labels_within_package
```

Format

An object of class list of length 20.

Details

```
labels_within_package <- list( dayint = "Time trend", diffcwv = "delta CWV (cm)", date = "",
Column_WV = "MAIAC CWV (cm)", AOT_Uncertainty = "Blue band uncertainty", elev = "El-
evation (m)", aod = "Aerosol optical depth", RelAZ = "Relative azimuth angle", DevAll_P1km
= expression(paste("Proportion developed area in 1",km^2)), dist_water_km = "Distance to water
(km)", forestProp_1km = expression(paste("Proportion of forest in 1",km^2)), Aer_optical_depth
= "DSCOVR EPIC MAIAC AOD400nm", aer_aod440 = "AERONET AOD440nm", aer_aod500 =
"AERONET AOD500nm", diff440 = "DSCOVR MAIAC - AERONET AOD", diff440_pred = "Pre-
dicted Error", aer_aod440_hat = "Predicted AERONET AOD440nm", AOD_470nm = "AERONET
AOD470nm", Optical_Depth_047_t = "MAIAC AOD470nm (Terra)", Optical_Depth_047_a = "MA-
IAC AOD470nm (Aqua)" )
```

References

[doi:10.5281/zenodo.3568449](https://doi.org/10.5281/zenodo.3568449)

new_labels	<i>new_labels: a place holder default to NULL.</i>
------------	--

Description

if supplied as a list, it offers user to rename labels

Usage

```
new_labels
```

Format

An object of class NULL of length 0.

plot.label	<i>Internal-function to revise axis label for each feature</i>
------------	--

Description

This function further fine-tune the format of each feature

Usage

```
## S3 method for class 'label'
plot(plot1, show_feature)
```

Arguments

plot1	ggplot2 object
show_feature	feature to plot

Value

returns ggplot2 object with further modified layers based on the feature

scatter.plot.diagonal *Make customized scatter plot with diagonal line and R2 printed.*

Description

Make customized scatter plot with diagonal line and R2 printed.

Usage

```
scatter.plot.diagonal(
  data,
  x,
  y,
  size0 = 0.2,
  alpha0 = 0.3,
  dilute = FALSE,
  add_abline = FALSE,
  add_hist = TRUE,
  add_stat_cor = TRUE
)
```

Arguments

data	dataset
x	x
y	y
size0	point size, default to 1 of nobs<1000, 0.4 if nobs>1000
alpha0	alpha of point
dilute	a number or logical, default to TRUE, will plot nrow(data_long)/dilute data. For example, if dilute = 5 will plot 1/5 of the data. if dilute = TRUE will plot half of the data.
add_abline	default to FALSE, add a diagonal line ggExtra::ggMarginal but notice if add histogram, what is returned is no longer a ggplot2 object
add_hist	optional to add marginal histogram using ggExtra::ggMarginal but notice if add histogram, what is returned is no longer a ggplot2 object
add_stat_cor	add correlation and p-value from ggpubr::stat_cor

Value

ggplot2 object if add_hist = FALSE

Examples

```
scatter.plot.diagonal(data = iris, x = "Sepal.Length", y = "Petal.Length")
```

`scatter.plot.simple` *Simple scatter plot, adding marginal histogram by default.*

Description

Simple scatter plot, adding marginal histogram by default.

Usage

```
scatter.plot.simple(
  data,
  x,
  y,
  size0 = 0.2,
  alpha0 = 0.3,
  dilute = FALSE,
  add_hist = TRUE,
  add_stat_cor = FALSE
)
```

Arguments

<code>data</code>	dataset
<code>x</code>	x
<code>y</code>	y
<code>size0</code>	point size, default to 1 of nobs<1000, 0.4 if nobs>1000
<code>alpha0</code>	alpha of point
<code>dilute</code>	a number or logical, default to TRUE, will plot <code>nrow(data_long)/dilute</code> data. For example, if <code>dilute = 5</code> will plot 1/5 of the data. if <code>dilute = TRUE</code> will plot half of the data.
<code>add_hist</code>	optional to add marginal histogram using <code>ggExtra::ggMarginal</code> but notice if add histogram, what is returned is no longer a <code>ggplot2</code> object
<code>add_stat_cor</code>	add correlation and p-value from <code>ggpubr::stat_cor</code>

Value

`ggplot2` object if `add_hist = FALSE`

Examples

```
scatter.plot.simple(data = iris, x = "Sepal.Length", y = "Petal.Length")
```

shap.importance	<i>Variable importance as measured by mean absolute SHAP value.</i>
-----------------	---

Description

Variable importance as measured by mean absolute SHAP value.

Usage

```
shap.importance(data_long, names_only = FALSE, top_n = Inf)
```

Arguments

data_long	a long format data of SHAP values from shap.prep
names_only	If TRUE, returns variable names only.
top_n	How many variables to be returned?

Value

returns `data.table` with average absolute SHAP values per variable, sorted in decreasing order of importance.

Examples

```
shap.importance(shap_long_iris)

shap.importance(shap_long_iris, names_only = 1)
```

shap.plot.dependence	<i>SHAP dependence plot and interaction plot, optional to be colored by a selected feature</i>
----------------------	--

Description

This function by default makes a simple dependence plot with feature values on the x-axis and SHAP values on the y-axis, optional to color by another feature. It is optional to use a different variable for SHAP values on the y-axis, and color the points by the feature value of a designated variable. Not colored if `color_feature` is not supplied. If `data_int` (the SHAP interaction values dataset) is supplied, it will plot the interaction effect between y and x on the y-axis. Dependence plot is easy to make if you have the SHAP values dataset from `predict.xgb.Booster` or `predict.lgb.Booster`. It is not necessary to start with the long format data, but since that is used for the summary plot, we just continue to use it here.

Usage

```
shap.plot.dependence(
  data_long,
  x,
  y = NULL,
  color_feature = NULL,
  data_int = NULL,
  dilute = FALSE,
  smooth = TRUE,
  size0 = NULL,
  add_hist = FALSE,
  add_stat_cor = FALSE,
  alpha = NULL,
  jitter_height = 0,
  jitter_width = 0,
  ...
)
```

Arguments

<code>data_long</code>	the long format SHAP values from shap.prep
<code>x</code>	which feature to show on x-axis, it will plot the feature value
<code>y</code>	which shap values to show on y-axis, it will plot the SHAP value of that feature. y is default to x, if y is not provided, just plot the SHAP values of x on the y-axis
<code>color_feature</code>	which feature value to use for coloring, color by the feature value. If "auto", will select the feature "c" minimizing the variance of the shap value given x and c, which can be viewed as a heuristic for the strongest interaction.
<code>data_int</code>	the 3-dimension SHAP interaction values array. if <code>data_int</code> is supplied, y-axis will plot the interaction values of y (vs. x). <code>data_int</code> is obtained from either <code>predict.xgb.Booster</code> or shap.prep.interaction
<code>dilute</code>	a number or logical, default to TRUE, will plot <code>nrow(data_long)/dilute</code> data. For example, if <code>dilute = 5</code> will plot 20% of the data. As long as <code>dilute != FALSE</code> , will plot at most half the data
<code>smooth</code>	optional to add a <i>loess</i> smooth line, default to TRUE.
<code>size0</code>	point size, default to 1 if <code>nobs < 1000</code> , 0.4 if <code>nobs > 1000</code>
<code>add_hist</code>	whether to add histogram using <code>ggMarginal</code> , default to TRUE. But notice the plot after adding histogram is a <code>ggExtraPlot</code> object instead of <code>ggplot2</code> so cannot add geom to that anymore. Turn the histogram off if you wish to add more <code>ggplot2</code> geoms
<code>add_stat_cor</code>	add correlation and p-value from <code>ggpubr::stat_cor</code>
<code>alpha</code>	point transparency, default to 1 if <code>nobs < 1000</code> else 0.6
<code>jitter_height</code>	amount of vertical jitter (see <code>height</code> in <code>geom_jitter</code>)
<code>jitter_width</code>	amount of horizontal jitter (see <code>width</code> in <code>geom_jitter</code>). Use values close to 0, e.g. 0.02
<code>...</code>	additional parameters passed to <code>geom_jitter</code>

Value

be default a ggplot2 object, based on which you could add more geom layers.

Examples

```
# **SHAP dependence plot**

# 1. simple dependence plot with SHAP values of x on the y axis
shap.plot.dependence(data_long = shap_long_iris, x="Petal.Length",
  add_hist = TRUE, add_stat_cor = TRUE)

# 2. can choose a different SHAP values on the y axis
shap.plot.dependence(data_long = shap_long_iris, x="Petal.Length",
  y = "Petal.Width")

# 3. color by another feature's feature values
shap.plot.dependence(data_long = shap_long_iris, x="Petal.Length",
  color_feature = "Petal.Width")

# 4. choose 3 different variables for x, y, and color
shap.plot.dependence(data_long = shap_long_iris, x="Petal.Length",
  y = "Petal.Width", color_feature = "Petal.Width")

# Optional to add hist or remove smooth line, optional to plot fewer data (make plot quicker)
shap.plot.dependence(data_long = shap_long_iris, x="Petal.Length",
  y = "Petal.Width", color_feature = "Petal.Width",
  add_hist = TRUE, smooth = FALSE, dilute = 3)

# to make a list of plot
plot_list <- lapply(names(iris)[2:3], shap.plot.dependence, data_long = shap_long_iris)

# **SHAP interaction effect plot **

# To get the interaction SHAP dataset for plotting, need to get `shap_int` first:
mod1 = xgboost::xgboost(
  data = as.matrix(iris[,-5]), label = iris$Species,
  gamma = 0, eta = 1, lambda = 0, nrounds = 1, verbose = FALSE, nthread = 1)
# Use either:
data_int <- shap.prep.interaction(xgb_mod = mod1,
  X_train = as.matrix(iris[,-5]))
# or:
shap_int <- predict(mod1, as.matrix(iris[,-5]),
  predinteraction = TRUE)

# if data_int is supplied, y axis will plot the interaction values of y (vs. x)
shap.plot.dependence(data_long = shap_long_iris,
  data_int = shap_int_iris,
  x="Petal.Length",
  y = "Petal.Width",
  color_feature = "Petal.Width")
```

shap.plot.force_plot *Make the SHAP force plot*

Description

The force/stack plot, optional to zoom in at certain x-axis location or zoom in a specific cluster of observations.

Usage

```
shap.plot.force_plot(  
  shapobs,  
  id = "sorted_id",  
  zoom_in_location = NULL,  
  y_parent_limit = NULL,  
  y_zoomin_limit = NULL,  
  zoom_in = TRUE,  
  zoom_in_group = NULL  
)
```

Arguments

shapobs The dataset obtained by shap.prep.stack.data.
id the id variable.
zoom_in_location where to zoom in, default at place of 60 percent of the data.
y_parent_limit set y-axis limits.
y_zoomin_limit c(a,b) to limit the y-axis in zoom-in.
zoom_in default to TRUE, zoom in by ggforce::facet_zoom.
zoom_in_group optional to zoom in certain cluster.

Examples

```
# **SHAP force plot**  
plot_data <- shap.prep.stack.data(shap_contrib = shap_values_iris,  
                                n_groups = 4)  
shap.plot.force_plot(plot_data)  
shap.plot.force_plot(plot_data, zoom_in_group = 2)  
  
# plot all the clusters:  
shap.plot.force_plot_bygroup(plot_data)
```

```
shap.plot.force_plot_bygroup
```

Make the stack plot, optional to zoom in at certain x or certain cluster

Description

A collective display of zoom-in plots: one plot for every group of the clustered observations.

Usage

```
shap.plot.force_plot_bygroup(shapobs, id = "sorted_id", y_parent_limit = NULL)
```

Arguments

shapobs The dataset obtained by shap.prep.stack.data.
id the id variable.
y_parent_limit set y-axis limits.

Examples

```
# **SHAP force plot**
plot_data <- shap.prep.stack.data(shap_contrib = shap_values_iris,
                                n_groups = 4)
shap.plot.force_plot(plot_data)
shap.plot.force_plot(plot_data, zoom_in_group = 2)

# plot all the clusters:
shap.plot.force_plot_bygroup(plot_data)
```

```
shap.plot.summary
```

SHAP summary plot core function using the long format SHAP values

Description

The summary plot (a sina plot) uses a long format data of SHAP values. The SHAP values could be obtained from either a XGBoost/LightGBM model or a SHAP value matrix using [shap.values](#). So this summary plot function normally follows the long format dataset obtained using [shap.values](#). If you want to start with a model and data_X, use [shap.plot.summary.wrap1](#). If you want to use a self-derived dataset of SHAP values, use [shap.plot.summary.wrap2](#). If a list named **new_labels** is provided in the global environment (new_labels is pre-loaded by the package as NULL), the plots will use that list to label the variables, here is an example of such a list (the default labels): [labels_within_package](#).

Usage

```
shap.plot.summary(
  data_long,
  x_bound = NULL,
  dilute = FALSE,
  scientific = FALSE,
  my_format = NULL,
  min_color_bound = "#FFCC33",
  max_color_bound = "#6600CC",
  kind = c("sina", "bar")
)
```

Arguments

<code>data_long</code>	a long format data of SHAP values from shap.prep
<code>x_bound</code>	use to set horizontal axis limit in the plot
<code>dilute</code>	being numeric or logical (TRUE/FALSE), it aims to help make the test plot for large amount of data faster. If <code>dilute = 5</code> will plot 1/5 of the data. If <code>dilute = TRUE</code> or a number, will plot at most half points per feature, so the plotting won't be too slow. If you put <code>dilute</code> too high, at least 10 points per feature would be kept. If the dataset is too small after dilution, will just plot all the data
<code>scientific</code>	show the mean SHAP in scientific format. If TRUE, label format is 0.0E-0, default to FALSE, and the format will be 0.000
<code>my_format</code>	supply your own number format if you really want
<code>min_color_bound</code>	min color hex code for colormap. Color gradient is scaled between <code>min_color_bound</code> and <code>max_color_bound</code> . Default is "#FFCC33".
<code>max_color_bound</code>	max color hex code for colormap. Color gradient is scaled between <code>min_color_bound</code> and <code>max_color_bound</code> . Default is "#6600CC".
<code>kind</code>	By default, a "sina" plot is shown. As an alternative, set <code>kind = "bar"</code> to visualize mean absolute SHAP values as a barplot. Its color is controlled by <code>max_color_bound</code> . Other arguments are ignored for this kind of plot.

Value

returns a ggplot2 object, could add further layers.

Examples

```
data("iris")
X1 = as.matrix(iris[,-5])
mod1 = xgboost::xgboost(
  data = X1, label = iris$Species, gamma = 0, eta = 1,
  lambda = 0, nrounds = 1, verbose = FALSE, nthread = 1)

# shap.values(model, X_dataset) returns the SHAP
```

```

# data matrix and ranked features by mean|SHAP|
shap_values <- shap.values(xgb_model = mod1, X_train = X1)
shap_values$mean_shap_score
shap_values_iris <- shap_values$shap_score

# shap.prep() returns the long-format SHAP data from either model or
shap_long_iris <- shap.prep(xgb_model = mod1, X_train = X1)
# is the same as: using given shap_contrib
shap_long_iris <- shap.prep(shap_contrib = shap_values_iris, X_train = X1)

# **SHAP summary plot**
shap.plot.summary(shap_long_iris, scientific = TRUE)
shap.plot.summary(shap_long_iris, x_bound = 1.5, dilute = 10)

# Alternatives options to make the same plot:
# option 1: from the xgboost model
shap.plot.summary.wrap1(mod1, X = as.matrix(iris[,-5]), top_n = 3)

# option 2: supply a self-made SHAP values dataset
# (e.g. sometimes as output from cross-validation)
shap.plot.summary.wrap2(shap_score = shap_values_iris, X = X1, top_n = 3)

```

```
shap.plot.summary.wrap1
```

A wrapped function to make summary plot from model object and predictors

Description

shap.plot.summary.wrap1 wraps up function [shap.prep](#) and [shap.plot.summary](#)

Usage

```
shap.plot.summary.wrap1(model, X, top_n, dilute = FALSE)
```

Arguments

model	the model
X	the dataset of predictors used for calculating SHAP
top_n	how many predictors you want to show in the plot (ranked)
dilute	being numeric or logical (TRUE/FALSE), it aims to help make the test plot for large amount of data faster. If dilute = 5 will plot 1/5 of the data. If dilute = TRUE or a number, will plot at most half points per feature, so the plotting won't be too slow. If you put dilute too high, at least 10 points per feature would be kept. If the dataset is too small after dilution, will just plot all the data

Examples

```

data("iris")
X1 = as.matrix(iris[,-5])
mod1 = xgboost::xgboost(
  data = X1, label = iris$Species, gamma = 0, eta = 1,
  lambda = 0, nrounds = 1, verbose = FALSE, nthread = 1)

# shap.values(model, X_dataset) returns the SHAP
# data matrix and ranked features by mean|SHAP|
shap_values <- shap.values(xgb_model = mod1, X_train = X1)
shap_values$mean_shap_score
shap_values_iris <- shap_values$shap_score

# shap.prep() returns the long-format SHAP data from either model or
shap_long_iris <- shap.prep(xgb_model = mod1, X_train = X1)
# is the same as: using given shap_contrib
shap_long_iris <- shap.prep(shap_contrib = shap_values_iris, X_train = X1)

# **SHAP summary plot**
shap.plot.summary(shap_long_iris, scientific = TRUE)
shap.plot.summary(shap_long_iris, x_bound = 1.5, dilute = 10)

# Alternatives options to make the same plot:
# option 1: from the xgboost model
shap.plot.summary.wrap1(mod1, X = as.matrix(iris[,-5]), top_n = 3)

# option 2: supply a self-made SHAP values dataset
# (e.g. sometimes as output from cross-validation)
shap.plot.summary.wrap2(shap_score = shap_values_iris, X = X1, top_n = 3)

```

```
shap.plot.summary.wrap2
```

A wrapped function to make summary plot from given SHAP values matrix

Description

`shap.plot.summary.wrap2` wraps up function `shap.prep` and `shap.plot.summary`. Since SHAP matrix could be returned from cross-validation instead of only one model, here the wrapped `shap.prep` takes the SHAP score matrix `shap_score` as input

Usage

```
shap.plot.summary.wrap2(shap_score, X, top_n, dilute = FALSE)
```

Arguments

<code>shap_score</code>	the SHAP values dataset, could be obtained by <code>shap.prep</code>
<code>X</code>	the dataset of predictors used for calculating SHAP values

`top_n` how many predictors you want to show in the plot (ranked)

`dilute` being numeric or logical (TRUE/FALSE), it aims to help make the test plot for large amount of data faster. If `dilute = 5` will plot 1/5 of the data. If `dilute = TRUE` or a number, will plot at most half points per feature, so the plotting won't be too slow. If you put `dilute` too high, at least 10 points per feature would be kept. If the dataset is too small after dilution, will just plot all the data

Examples

```
data("iris")
X1 = as.matrix(iris[,-5])
mod1 = xgboost::xgboost(
  data = X1, label = iris$Species, gamma = 0, eta = 1,
  lambda = 0, nrounds = 1, verbose = FALSE, nthread = 1)

# shap.values(model, X_dataset) returns the SHAP
# data matrix and ranked features by mean|SHAP|
shap_values <- shap.values(xgb_model = mod1, X_train = X1)
shap_values$mean_shap_score
shap_values_iris <- shap_values$shap_score

# shap.prep() returns the long-format SHAP data from either model or
shap_long_iris <- shap.prep(xgb_model = mod1, X_train = X1)
# is the same as: using given shap_contrib
shap_long_iris <- shap.prep(shap_contrib = shap_values_iris, X_train = X1)

# **SHAP summary plot**
shap.plot.summary(shap_long_iris, scientific = TRUE)
shap.plot.summary(shap_long_iris, x_bound = 1.5, dilute = 10)

# Alternatives options to make the same plot:
# option 1: from the xgboost model
shap.plot.summary.wrap1(mod1, X = as.matrix(iris[,-5]), top_n = 3)

# option 2: supply a self-made SHAP values dataset
# (e.g. sometimes as output from cross-validation)
shap.plot.summary.wrap2(shap_score = shap_values_iris, X = X1, top_n = 3)
```

shap.prep

Prepare SHAP values into long format for plotting

Description

Produce a dataset of 6 columns: ID of each observation, variable name, SHAP value, variable values (feature value), deviation of the feature value for each observation (for coloring the point), and the mean SHAP values for each variable. You can view this example dataset included in the package: [shap_long_iris](#)

Usage

```
shap.prep(
  xgb_model = NULL,
  shap_contrib = NULL,
  X_train,
  top_n = NULL,
  var_cat = NULL
)
```

Arguments

<code>xgb_model</code>	an XGBoost (or LightGBM) model object, will derive the SHAP values from it
<code>shap_contrib</code>	optional to directly supply a SHAP values dataset. If supplied, it will overwrite the <code>xgb_model</code> if <code>xgb_model</code> is also supplied
<code>X_train</code>	the dataset of predictors used to calculate SHAP values, it provides feature values to the plot, must be supplied
<code>top_n</code>	to choose <code>top_n</code> variables ranked by <code>mean SHAP </code> if needed
<code>var_cat</code>	if supplied, will provide long format data, grouped by this categorical variable

Details

The ID variable is added for each observation in the `shap_contrib` dataset for better tracking, it is created as `1:nrow(shap_contrib)` before melting `shap_contrib` into long format.

Value

a long-format `data.table`, named as `shap_long`

Examples

```
data("iris")
X1 = as.matrix(iris[,-5])
mod1 = xgboost::xgboost(
  data = X1, label = iris$Species, gamma = 0, eta = 1,
  lambda = 0, nrounds = 1, verbose = FALSE, nthread = 1)

# shap.values(model, X_dataset) returns the SHAP
# data matrix and ranked features by mean|SHAP|
shap_values <- shap.values(xgb_model = mod1, X_train = X1)
shap_values$mean_shap_score
shap_values_iris <- shap_values$shap_score

# shap.prep() returns the long-format SHAP data from either model or
shap_long_iris <- shap.prep(xgb_model = mod1, X_train = X1)
# is the same as: using given shap_contrib
shap_long_iris <- shap.prep(shap_contrib = shap_values_iris, X_train = X1)

# **SHAP summary plot**
shap.plot.summary(shap_long_iris, scientific = TRUE)
```



```

shap.plot.summary(shap_long_iris, x_bound = 1.5, dilute = 10)

# Alternatives options to make the same plot:
# option 1: from the xgboost model
shap.plot.summary.wrap1(mod1, X = as.matrix(iris[,-5]), top_n = 3)

# option 2: supply a self-made SHAP values dataset
# (e.g. sometimes as output from cross-validation)
shap.plot.summary.wrap2(shap_score = shap_values_iris, X = X1, top_n = 3)
####
#
# use `var_cat` to add a categorical variable, output the long-format data differently:
library("data.table")
data("iris")
set.seed(123)
iris$Group <- 0
iris[sample(1:nrow(iris), nrow(iris)/2), "Group"] <- 1

data.table::setDT(iris)
X_train = as.matrix(iris[,c(colnames(iris)[1:4], "Group"), with = FALSE])
mod1 = xgboost::xgboost(
  data = X_train, label = iris$Species, gamma = 0, eta = 1,
  lambda = 0, nrounds = 1, verbose = FALSE, nthread = 1)

shap_long2 <- shap.prep(xgb_model = mod1, X_train = X_train, var_cat = "Group")
# **SHAP summary plot**
shap.plot.summary(shap_long2, scientific = TRUE) +
  ggplot2::facet_wrap(~ Group)

```

shap.prep.interaction *Prepare the interaction SHAP values from predict.xgb.Booster*

Description

shap.prep.interaction just runs `shap_int <- predict(xgb_mod, (X_train), predinteraction = TRUE)`, thus it may not be necessary. Read more about the xgboost predict function at `xgboost::predict.xgb.Booster`. Note that this functionality is unavailable for LightGBM models.

Usage

```
shap.prep.interaction(xgb_model, X_train)
```

Arguments

xgb_model	a xgboost model object
X_train	the dataset of predictors used for the xgboost model

Value

a 3-dimension array: #obs x #features x #features

Examples

```

# To get the interaction SHAP dataset for plotting:
# fit the xgboost model

# options("Ncup" = 1)
mod1 = xgboost::xgboost(
  data = as.matrix(iris[,-5]), label = iris$Species,
  gamma = 0, eta = 1, lambda = 0, nrounds = 1, verbose = FALSE, nthread = 1)
# Use either:
data_int <- shap.prep.interaction(xgb_mod = mod1,
                                X_train = as.matrix(iris[,-5]))
# or:
shap_int <- predict(mod1, as.matrix(iris[,-5]),
                   predinteraction = TRUE)

# **SHAP interaction effect plot **
shap.plot.dependence(data_long = shap_long_iris,
                    data_int = shap_int_iris,
                    x="Petal.Length",
                    y = "Petal.Width",
                    color_feature = "Petal.Width")

```

shap.prep.stack.data *Prepare data for SHAP force plot (stack plot)*

Description

Make force plot for top_n features, optional to randomly plot certain portion of the data in case the dataset is large.

Usage

```

shap.prep.stack.data(
  shap_contrib,
  top_n = NULL,
  data_percent = 1,
  cluster_method = "ward.D",
  n_groups = 10L
)

```

Arguments

shap_contrib	shap_contrib is the SHAP value data returned from predict, here an ID variable is added for each observation in the shap_contrib dataset for better tracking, it is created in the beginning as 1:nrow(shap_contrib). The ID matches the output from shap.prep
top_n	integer, optional to show only top_n features, combine the rest

data_percent what percent of data to plot (to speed up the testing plot). The accepted input range is (0,1], if observations left is too few, there will be an error from the clustering function
cluster_method default to ward.D, please refer to `stats::hclust` for details
n_groups a integer, how many groups to plot in [shap.plot.force_plot_bygroup](#)

Value

a dataset for stack plot

Examples

```

# **SHAP force plot**
plot_data <- shap.prep.stack.data(shap_contrib = shap_values_iris,
                                n_groups = 4)
shap.plot.force_plot(plot_data)
shap.plot.force_plot(plot_data, zoom_in_group = 2)

# plot all the clusters:
shap.plot.force_plot_bygroup(plot_data)

```

shap.values

Get SHAP scores from a trained XGBoost or LightGBM model

Description

shap.values returns a list of three objects from XGBoost or LightGBM model: 1. a dataset (data.table) of SHAP scores. It has the same dimension as the X_train; 2. the ranked variable vector by each variable's mean absolute SHAP value, it ranks the predictors by their importance in the model; and 3. The BIAS, which is like an intercept. The rowsum of SHAP values including the BIAS would equal to the predicted value (y_hat) generally speaking.

Usage

```
shap.values(xgb_model, X_train)
```

Arguments

xgb_model an XGBoost or LightGBM model object
X_train the data supplied to the predict function to get the prediction. It should be a matrix. Notice that coercing the matrix to a dense matrix by using `as.matrix` might lead to wrong behaviors in some cases. See discussion in issues on this topic.

Value

a list of three elements: the SHAP values as data.table, ranked mean|SHAP|, and BIAS

Examples

```

data("iris")
X1 = as.matrix(iris[,-5])
mod1 = xgboost::xgboost(
  data = X1, label = iris$Species, gamma = 0, eta = 1,
  lambda = 0, nrounds = 1, verbose = FALSE, nthread = 1)

# shap.values(model, X_dataset) returns the SHAP
# data matrix and ranked features by mean|SHAP|
shap_values <- shap.values(xgb_model = mod1, X_train = X1)
shap_values$mean_shap_score
shap_values_iris <- shap_values$shap_score

# shap.prep() returns the long-format SHAP data from either model or
shap_long_iris <- shap.prep(xgb_model = mod1, X_train = X1)
# is the same as: using given shap_contrib
shap_long_iris <- shap.prep(shap_contrib = shap_values_iris, X_train = X1)

# **SHAP summary plot**
shap.plot.summary(shap_long_iris, scientific = TRUE)
shap.plot.summary(shap_long_iris, x_bound = 1.5, dilute = 10)

# Alternatives options to make the same plot:
# option 1: from the xgboost model
shap.plot.summary.wrap1(mod1, X = as.matrix(iris[,-5]), top_n = 3)

# option 2: supply a self-made SHAP values dataset
# (e.g. sometimes as output from cross-validation)
shap.plot.summary.wrap2(shap_score = shap_values_iris, X = X1, top_n = 3)

```

shap_int_iris

The interaction effect SHAP values example using iris dataset.

Description

The interaction effect SHAP values example using iris dataset.

Usage

```
shap_int_iris
```

Format

An object of class array of dimension 150 x 5 x 5.

shap_long_iris	<i>The long-format SHAP values example using iris dataset.</i>
----------------	--

Description

The long-format SHAP values example using iris dataset.

Usage

```
shap_long_iris
```

Format

An object of class `data.table` (inherits from `data.frame`) with 600 rows and 6 columns.

shap_score	<i>SHAP values example from dataXY_df.</i>
------------	--

Description

SHAP values example from `dataXY_df`.

Usage

```
shap_score
```

Format

An object of class `data.table` (inherits from `data.frame`) with 10148 rows and 9 columns.

References

[doi:10.5281/zenodo.3568449](https://doi.org/10.5281/zenodo.3568449)

shap_values_iris	<i>SHAP values example using iris dataset.</i>
------------------	--

Description

SHAP values example using iris dataset.

Usage

```
shap_values_iris
```

Format

An object of class `data.table` (inherits from `data.frame`) with 150 rows and 4 columns.

Index

* Labels

labels_within_package, 3
new_labels, 4

* Terra

dataXY_df, 2
shap_score, 21

* iris

shap_int_iris, 20
shap_long_iris, 21
shap_values_iris, 21

dataXY_df, 2

label.feature, 3, 3

labels_within_package, 3, 3, 11

new_labels, 4

plot.label, 4

scatter.plot.diagonal, 5

scatter.plot.simple, 6

shap.importance, 7

shap.plot.dependence, 7

shap.plot.force_plot, 10

shap.plot.force_plot_bygroup, 11, 19

shap.plot.summary, 11, 13, 14

shap.plot.summary.wrap1, 11, 13

shap.plot.summary.wrap2, 11, 14

shap.prep, 7, 8, 12–14, 15, 18

shap.prep.interaction, 8, 17

shap.prep.stack.data, 18

shap.values, 11, 19

shap_int_iris, 20

shap_long_iris, 15, 21

shap_score, 21

shap_values_iris, 21