Package 'shapley'

October 23, 2024

Type Package

Title Weighted Mean SHAP for Feature Selection in ML Grid and Ensemble

Version 0.4

Depends R $(>= 3.5.0)$

Description This R package introduces Weighted Mean SHapley Additive exPlanations (WMSHAP), an innovative method for calculating SHAP values for a grid of fine-tuned base-learner machine learning models as well as stacked ensembles, a method not previously available due to the common reliance on single best-performing models. By integrating the weighted mean SHAP values from individual base-learners comprising the ensemble or individual base-learners in a tuning grid search, the package weights SHAP contributions according to each model's performance, assessed by multiple either R squared (for both regression and classification models). alternatively, this software also offers weighting SHAP values based on the area under the precision-recall curve (AUCPR), the area under the curve (AUC), and F2 measures for binary classifiers. It further extends this framework to implement weighted confidence intervals for weighted mean SHAP values, offering a more comprehensive and robust feature importance evaluation over a grid of machine learning models, instead of solely computing SHAP values for the best model. This methodology is particularly beneficial for addressing the severe class imbalance (class rarity) problem by providing a transparent, generalized measure of feature importance that mitigates the risk of reporting SHAP values for an overfitted or biased model and maintains robustness under severe class imbalance, where there is no universal criteria of identifying the absolute best model. Furthermore, the package implements hypothesis testing to ascertain the statistical significance of SHAP values for individual features, as well as comparative significance testing of SHAP contributions between features. Additionally, it tackles a critical gap in feature selection literature by presenting criteria for the automatic feature selection of the most important features across a grid of models or stacked ensembles, eliminating the need for arbitrary determination of the number of top features to be extracted. This utility is invaluable for researchers analyzing feature significance, particularly within severely imbalanced outcomes where conventional methods fall short. Moreover, it is also expected to report democratic feature importance across a grid of models, resulting in a more comprehensive and generalizable feature selection. The package further implements a novel method for visualizing SHAP values both at subject level and feature level as well as a plot for feature selection based on the weighted mean SHAP ratios.

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Encoding UTF-8

Imports ggplot2 ($> = 3.4.2$), h2o ($> = 3.34.0.0$), curl ($> = 4.3.0$), waffle $(>= 1.0.2)$

RoxygenNote 7.3.1

URL <https://github.com/haghish/shapley>,

<https://www.sv.uio.no/psi/english/people/academic/haghish/>

BugReports <https://github.com/haghish/shapley/issues>

NeedsCompilation no

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Repository CRAN

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Contents

h2o.get_ids *h2o.get_ids*

Description

extracts the model IDs from H2O AutoML object or H2O grid

Usage

h2o.get_ids(automl)

Arguments

automl a h2o "AutoML" grid object

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Value

a character vector of trained models' names (IDs)

Author(s)

E. F. Haghish

Examples

```
## Not run:
library(h2o)
h2o.init(ignore_config = TRUE, nthreads = 2, bind_to_localhost = FALSE, insecure = TRUE)
prostate_path <- system.file("extdata", "prostate.csv", package = "h2o")
prostate <- h2o.importFile(path = prostate_path, header = TRUE)
y <- "CAPSULE"
prostate[,y] <- as.factor(prostate[,y]) #convert to factor for classification
aml \leq h2o.automl(y = y, training_frame = prostate, max_runtime_secs = 30)
# get the model IDs
ids \le h2o.ids(aml)
## End(Not run)
```
normalize *Normalize a vector based on specified minimum and maximum values*

Description

This function normalizes a vector based on specified minimum and maximum values. If the minimum and maximum values are not specified, the function will use the minimum and maximum values of the vector.

Usage

 $normalize(x, min = NULL, max = NULL)$

Arguments

Value

normalized numeric vector

Author(s)

E. F. Haghish

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shapley *Weighted average of SHAP values and weighted SHAP confidence intervals for a grid of fine-tuned models or base-learners of a stacked ensemble model*

Description

Weighted average of SHAP values and weighted SHAP confidence intervals provide a measure of feature importance for a grid of fine-tuned models or base-learners of a stacked ensemble model. Instead of reporting relative SHAP contributions for a single model, this function takes the variability in feature importance of multiple models into account and computes weighted mean and confidence intervals for each feature, taking the performance metric of each model as the weight. The function also provides a plot of the weighted SHAP values and confidence intervals. Currently only models trained by h2o machine learning software or autoEnsemble package are supported.

Usage

```
shapley(
 models,
 newdata,
 plot = TRUE,
  performance_metric = "r2",
  standardize_performance_metric = FALSE,
  performance_type = "xval",
 minimum\_performance = 0,method = c("lowerCI"),
  cutoff = 0,
  top_n_features = NULL,
 n_models = 10
)
```
Arguments

Value

a list including the GGPLOT2 object, the data frame of SHAP values, and performance metric of all models, as well as the model IDs.

Author(s)

E. F. Haghish

Examples

```
## Not run:
# load the required libraries for building the base-learners and the ensemble models
library(h2o) #shapley supports h2o models
library(shapley)
# initiate the h2o server
h2o.init(ignore_config = TRUE, nthreads = 2, bind_to_localhost = FALSE, insecure = TRUE)
# upload data to h2o cloud
prostate_path <- system.file("extdata", "prostate.csv", package = "h2o")
prostate <- h2o.importFile(path = prostate_path, header = TRUE)
set.seed(10)
### H2O provides 2 types of grid search for tuning the models, which are
### AutoML and Grid. Below, I demonstrate how weighted mean shapley values
### can be computed for both types.
#######################################################
### PREPARE AutoML Grid (takes a couple of minutes)
#######################################################
# run AutoML to tune various models (GBM) for 60 seconds
y <- "CAPSULE"
prostate[,y] <- as.factor(prostate[,y]) #convert to factor for classification
aml \leq h2o.automl(y = y, training_frame = prostate, max_runtime_secs = 120,
                 include_algos=c("GBM"),
              # this setting ensures the models are comparable for building a meta learner
                 seed = 2023, nfolds = 10,
                 keep_cross_validation_predictions = TRUE)
### call 'shapley' function to compute the weighted mean and weighted confidence intervals
### of SHAP values across all trained models.
### Note that the 'newdata' should be the testing dataset!
result <- shapley(models = aml, newdata = prostate, performance_metric = "aucpr", plot = TRUE)
#######################################################
### PREPARE H2O Grid (takes a couple of minutes)
#######################################################
# make sure equal number of "nfolds" is specified for different grids
grid \leq h2o.grid(algorithm = "gbm", y = y, training_frame = prostate,
                 hyper_params = list(ntrees = seq(1, 50, 1)),grid_id = "ensemble_grid",
              # this setting ensures the models are comparable for building a meta learner
                 seed = 2023, fold_assignment = "Modulo", nfolds = 10,
                 keep_cross_validation_predictions = TRUE)
result2 <- shapley(models = grid, newdata = prostate, performance_metric = "aucpr", plot = TRUE)
#######################################################
```
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```
### PREPARE autoEnsemble STACKED ENSEMBLE MODEL
#######################################################
### get the models' IDs from the AutoML and grid searches.
### this is all that is needed before building the ensemble,
### i.e., to specify the model IDs that should be evaluated.
library(autoEnsemble)
ids <- c(h2o.get_ids(aml), h2o.get_ids(grid))
autoSearch <- ensemble(models = ids, training_frame = prostate, strategy = "search")
result3 <- shapley(models = autoSearch, newdata = prostate,
                  performance_metric = "aucpr", plot = TRUE)
```
End(Not run)

shapley.domain *compute and plot weighted mean SHAP contributions at group level (factors or domains)*

Description

This function applies different criteria to visualize SHAP contributions

Usage

```
shapley.domain(
  shapley,
  domains,
 plot = "bar",
 method = "AUTO",
  legendstyle = "continuous",
  scale_colour_gradient = NULL,
 print = FALSE
)
```
Arguments

Value

ggplot object

Author(s)

E. F. Haghish

Examples

```
## Not run:
# load the required libraries for building the base-learners and the ensemble models
library(h2o) #shapley supports h2o models
library(shapley)
```

```
# initiate the h2o server
h2o.init(ignore_config = TRUE, nthreads = 2, bind_to_localhost = FALSE, insecure = TRUE)
```

```
# upload data to h2o cloud
prostate_path <- system.file("extdata", "prostate.csv", package = "h2o")
prostate <- h2o.importFile(path = prostate_path, header = TRUE)
```

```
### H2O provides 2 types of grid search for tuning the models, which are
### AutoML and Grid. Below, I demonstrate how weighted mean shapley values
### can be computed for both types.
```
set.seed(10)

```
#######################################################
### PREPARE AutoML Grid (takes a couple of minutes)
```

```
#######################################################
# run AutoML to tune various models (GBM) for 60 seconds
y <- "CAPSULE"
prostate[,y] <- as.factor(prostate[,y]) #convert to factor for classification
aml \le h2o.automl(y = y, training_frame = prostate, max_runtime_secs = 120,
                 include_algos=c("GBM"),
              # this setting ensures the models are comparable for building a meta learner
                 seed = 2023, nfolds = 10,
                 keep_cross_validation_predictions = TRUE)
### call 'shapley' function to compute the weighted mean and weighted confidence intervals
### of SHAP values across all trained models.
### Note that the 'newdata' should be the testing dataset!
result <- shapley(models = aml, newdata = prostate, plot = TRUE)
#######################################################
### PLOT THE WEIGHTED MEAN SHAP VALUES
#######################################################
shapley.plot(result, plot = "bar")
shapley.plot(result, plot = "waffle")
## End(Not run)
```

```
shapley.feature.selection
```
Selects the top features with highest weighted mean shap values based on the specified criteria

Description

This function specifies the top features and prepares the data for plotting SHAP contributions for each row, or summary of absolute SHAP contributions for each feature.

Usage

```
shapley.feature.selection(
  shapley,
 method = "lowerCI",
 cutoff = 0,
  top_n_features = NULL,
  features = NULL
)
```
Arguments

shapley shapley object

Value

normalized numeric vector

Author(s)

E. F. Haghish

shapley.plot *Plot weighted SHAP contributions*

Description

This function applies different criteria to visualize SHAP contributions

Usage

```
shapley.plot(
  shapley,
 plot = "bar",
 method = "lowerCI",
 cutoff = 0,
  top_n_features = NULL,
  features = NULL,
 legendstyle = "continuous",
  scale_colour_gradient = NULL
\mathcal{E}
```
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Arguments

character vector for specifying the color gradients for the plot.

Value

ggplot object

Author(s)

E. F. Haghish

Examples

```
## Not run:
# load the required libraries for building the base-learners and the ensemble models
library(h2o) #shapley supports h2o models
library(shapley)
```

```
# initiate the h2o server
h2o.init(ignore_config = TRUE, nthreads = 2, bind_to_localhost = FALSE, insecure = TRUE)
# upload data to h2o cloud
prostate_path <- system.file("extdata", "prostate.csv", package = "h2o")
prostate <- h2o.importFile(path = prostate_path, header = TRUE)
```
H2O provides 2 types of grid search for tuning the models, which are

```
### AutoML and Grid. Below, I demonstrate how weighted mean shapley values
### can be computed for both types.
set.seed(10)
#######################################################
### PREPARE AutoML Grid (takes a couple of minutes)
#######################################################
# run AutoML to tune various models (GBM) for 60 seconds
y <- "CAPSULE"
prostate[,y] <- as.factor(prostate[,y]) #convert to factor for classification
aml \leq h2o.automl(y = y, training_frame = prostate, max_runtime_secs = 120,
                 include_algos=c("GBM"),
              # this setting ensures the models are comparable for building a meta learner
                 seed = 2023, nfolds = 10,
                 keep_cross_validation_predictions = TRUE)
### call 'shapley' function to compute the weighted mean and weighted confidence intervals
### of SHAP values across all trained models.
### Note that the 'newdata' should be the testing dataset!
result <- shapley(models = aml, newdata = prostate, plot = TRUE)
#######################################################
### PLOT THE WEIGHTED MEAN SHAP VALUES
#######################################################
shapley.plot(result, plot = "bar")
shapley.plot(result, plot = "waffle")
## End(Not run)
```
shapley.row.plot *Weighted mean SHAP values computed at subject level*

Description

Weighted mean of SHAP values and weighted SHAP confidence intervals provide a measure of feature importance for a grid of fine-tuned models or base-learners of a stacked ensemble model at subject level, showing that how each feature influences the prediction made for a row in the dataset and to what extend different models agree on that effect. If the 95 vertical line at 0.00, then it can be concluded that the feature does not significantly influences the subject, when variability across models is taken into consideration.

Usage

```
shapley.row.plot(
  shapley,
  row_index,
```
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```
features = NULL,
  plot = TRUE,
  print = FALSE
\lambda
```
Arguments

Value

a list including the GGPLOT2 object, the data frame of SHAP values, and performance metric of all models, as well as the model IDs.

Author(s)

E. F. Haghish

Examples

```
## Not run:
# load the required libraries for building the base-learners and the ensemble models
library(h2o) #shapley supports h2o models
library(shapley)
```

```
# initiate the h2o server
h2o.init(ignore_config = TRUE, nthreads = 2, bind_to_localhost = FALSE,
         insecure = TRUE)
```

```
# upload data to h2o cloud
prostate_path <- system.file("extdata", "prostate.csv", package = "h2o")
prostate <- h2o.importFile(path = prostate_path, header = TRUE)
```
set.seed(10)

```
### H2O provides 2 types of grid search for tuning the models, which are
### AutoML and Grid. Below, I demonstrate how weighted mean shapley values
### can be computed for both types.
```

```
#######################################################
### PREPARE AutoML Grid (takes a couple of minutes)
#######################################################
# run AutoML to tune various models (GBM) for 60 seconds
y <- "CAPSULE"
prostate[,y] <- as.factor(prostate[,y]) #convert to factor for classification
aml \le h2o.automl(y = y, training_frame = prostate, max_runtime_secs = 120,
```

```
include_algos=c("GBM"),
                 seed = 2023, nfolds = 10,
                 keep_cross_validation_predictions = TRUE)
### call 'shapley' function to compute the weighted mean and weighted confidence intervals
### of SHAP values across all trained models.
### Note that the 'newdata' should be the testing dataset!
result <- shapley(models = aml, newdata = prostate,
                  performance_metric = "aucpr", plot = TRUE)
#######################################################
### PREPARE H2O Grid (takes a couple of minutes)
#######################################################
# make sure equal number of "nfolds" is specified for different grids
grid \le h2o.grid(algorithm = "gbm", y = y, training_frame = prostate,
                 hyper_params = list(ntrees = seq(1, 50, 1)),grid_id = "ensemble_grid",
              # this setting ensures the models are comparable for building a meta learner
                 seed = 2023, fold_assignment = "Modulo", nfolds = 10,
                 keep_cross_validation_predictions = TRUE)
result2 <- shapley(models = grid, newdata = prostate,
                   performance_metric = "aucpr", plot = TRUE)
#######################################################
### PREPARE autoEnsemble STACKED ENSEMBLE MODEL
#######################################################
### get the models' IDs from the AutoML and grid searches.
### this is all that is needed before building the ensemble,
### i.e., to specify the model IDs that should be evaluated.
library(autoEnsemble)
ids <- c(h2o.get_ids(aml), h2o.get_ids(grid))
autoSearch <- ensemble(models = ids, training_frame = prostate, strategy = "search")
result3 <- shapley(models = autoSearch, newdata = prostate,
                   performance_metric = "aucpr", plot = TRUE)
#plot all important features
shapley.row.plot(shapley, row_index = 11)
#plot only the given features
shapPlot <- shapley.row.plot(shapley, row_index = 11, features = c("PSA", "AGE"))
# inspect the computed data for the row 11
ptint(shapPlot$rowSummarySHAP)
## End(Not run)
```
shapley.test *Normalize a vector based on specified minimum and maximum values*

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Description

This function normalizes a vector based on specified minimum and maximum values. If the minimum and maximum values are not specified, the function will use the minimum and maximum values of the vector.

Usage

```
shapley.test(shapley, features, n = 5000)
```
Arguments

Value

normalized numeric vector

Author(s)

E. F. Haghish

Examples

```
## Not run:
# load the required libraries for building the base-learners and the ensemble models
library(h2o) #shapley supports h2o models
library(autoEnsemble) #autoEnsemble models, particularly useful under severe class imbalance
library(shapley)
```

```
# initiate the h2o server
h2o.init(ignore_config = TRUE, nthreads = 2, bind_to_localhost = FALSE, insecure = TRUE)
```

```
# upload data to h2o cloud
prostate_path <- system.file("extdata", "prostate.csv", package = "h2o")
prostate <- h2o.importFile(path = prostate_path, header = TRUE)
```
H2O provides 2 types of grid search for tuning the models, which are ### AutoML and Grid. Below, I demonstrate how weighted mean shapley values ### can be computed for both types.

```
set.seed(10)
```

```
#######################################################
### PREPARE AutoML Grid (takes a couple of minutes)
#######################################################
# run AutoML to tune various models (GBM) for 60 seconds
y <- "CAPSULE"
prostate[,y] <- as.factor(prostate[,y]) #convert to factor for classification
aml \le h2o.automl(y = y, training_frame = prostate, max_runtime_secs = 120,
```

```
include_algos=c("GBM"),
             # this setting ensures the models are comparable for building a meta learner
                 seed = 2023, nfolds = 10,
                 keep_cross_validation_predictions = TRUE)
### call 'shapley' function to compute the weighted mean and weighted confidence intervals
### of SHAP values across all trained models.
### Note that the 'newdata' should be the testing dataset!
result <- shapley(models = aml, newdata = prostate, plot = TRUE)
#######################################################
### Significance testing of contributions of two features
#######################################################
shapley.test(result, features = c("GLEASON", "PSA"), n=5000)
## End(Not run)
```
shapley.top *Select top features in a model*

Description

This function applies different criteria simultaniously to identify the most important features in a model. The criteria include: 1) minimum limit of lower weighted confidence intervals of SHAP values relative to the feature with highest SHAP value. 2) minimum limit of percentage of weighted mean SHAP values relative to over all SHAP values of all features. These are specified with two different cutoff values.

Usage

```
shapley.top(shapley, lowerci = 0.01, shapratio = 0.005)
```
Arguments

Value

data.frame of selected features

Author(s)

E. F. Haghish

Examples

```
## Not run:
# load the required libraries for building the base-learners and the ensemble models
library(h2o) #shapley supports h2o models
library(shapley)
# initiate the h2o server
h2o.init(ignore_config = TRUE, nthreads = 2, bind_to_localhost = FALSE, insecure = TRUE)
# upload data to h2o cloud
prostate_path <- system.file("extdata", "prostate.csv", package = "h2o")
prostate <- h2o.importFile(path = prostate_path, header = TRUE)
### H2O provides 2 types of grid search for tuning the models, which are
### AutoML and Grid. Below, I demonstrate how weighted mean shapley values
### can be computed for both types.
set.seed(10)
#######################################################
### PREPARE AutoML Grid (takes a couple of minutes)
#######################################################
# run AutoML to tune various models (GBM) for 60 seconds
y <- "CAPSULE"
prostate[,y] <- as.factor(prostate[,y]) #convert to factor for classification
aml \le h2o.automl(y = y, training_frame = prostate, max_runtime_secs = 120,
                 include_algos=c("GBM"),
              # this setting ensures the models are comparable for building a meta learner
                 seed = 2023, nfolds = 10,
                 keep_cross_validation_predictions = TRUE)
### call 'shapley' function to compute the weighted mean and weighted confidence intervals
### of SHAP values across all trained models.
### Note that the 'newdata' should be the testing dataset!
result <- shapley(models = aml, newdata = prostate, plot = TRUE)
#######################################################
### Significance testing of contributions of two features
#######################################################
shapley.top(result, lowerci = 0.01, shapratio = 0.005)
## End(Not run)
```
test *Weighted Permutation Test for Difference of Means*

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Description

This function performs a weighted permutation test to determine if there is a significant difference between the means of two weighted numeric vectors. It tests the null hypothesis that the difference in means is zero against the alternative that it is not zero.

Usage

test(var1, var2, weights, n = 2000)

Arguments

Value

A list containing the observed difference in means and the p-value of the test.

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