Package ‘iml’

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BugReports https://github.com/christophM/iml/issues

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### Description

The iml package provides tools to analyze machine learning models and predictions.

### Author(s)

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**extract.glmnet.effects**

*Extract glmnet effects*

**Description**

Extract glmnet effects

**Usage**

```r
extract.glmnet.effects(betas, best.index, x.recoded, x.original)
```

**Arguments**

- `betas`: `glmnet$beta`
- `best.index`: index k
- `x.recoded`: the recoded version of x
- `x.original`: the original x Assuming that the first row is the x.interest

---

**FeatureEffect**

*Effect of a feature on predictions*

**Description**

FeatureEffect computes and plots (individual) feature effects of prediction models.

**Details**

The FeatureEffect class compute the effect a feature has on the prediction. Different methods are implemented:

- Accumulated Local Effect (ALE) plots
- Partial Dependence Plots (PDPs)
- Individual Conditional Expectation (ICE) curves

Accumulated local effects and partial dependence plots both show the average model prediction over the feature. The difference is that ALE are computed as accumulated differences over the conditional distribution and partial dependence plots over the marginal distribution. ALE plots preferable to PDPs, because they are faster and unbiased when features are correlated.
ALE plots for categorical features are automatically ordered by the similarity of the categories based on the distribution of the other features for instances in a category. When the feature is an ordered factor, the ALE plot leaves the order as is.

Individual conditional expectation curves describe how, for a single observation, the prediction changes when the feature changes and can be combined with partial dependence plots.

To learn more about accumulated local effects, read the Interpretable Machine Learning book.

For the partial dependence plots: https://christophm.github.io/interpretable-ml-book/pdp.html

For individual conditional expectation: https://christophm.github.io/interpretable-ml-book/ice.html

Super class

iml::InterpretationMethod -> FeatureEffect

Public fields

grid.size (numeric(1)|numeric(2))
  The size of the grid.

feature.name (character(1)|character(2))
  The names of the features for which the partial dependence was computed.

n.features (numeric(1))
  The number of features (either 1 or 2).

feature.type (character(1)|character(2))
  The detected types of the features, either "categorical" or "numerical".

method (character(1))

Active bindings

center.at numeric
  Value at which the plot was centered. Ignored in the case of two features.

Methods

Public methods:

• FeatureEffect$new()
• FeatureEffect$set.feature()
• FeatureEffect$center()
• FeatureEffect$s predict()
• FeatureEffect$clone()

Method new(): Create a FeatureEffect object

Usage:
FeatureEffect$new(
  predictor,
  feature,
  method = "ale",
  center.at = NULL,
  grid.size = 20
)

**Arguments:**

- **predictor** *Predictor*
  - The object (created with Predictor$new()) holding the machine learning model and the data.

- **feature** *(character(1) | character(2) | numeric(1) | numeric(2))*
  - The feature name or index for which to compute the effects.

- **method** *(character(1))*
  - 'ale' for accumulated local effects,
  - 'pdp' for partial dependence plot,
  - 'ice' for individual conditional expectation curves,
  - 'pdp + ice' for partial dependence plot and ice curves within the same plot.

- **center.at** *(numeric(1))*
  - Value at which the plot should be centered. Ignored in the case of two features.

- **grid.size** *(numeric(1) | numeric(2))*
  - The size of the grid for evaluating the predictions.

**Method** `set.feature()`: Get/set feature(s) (by index) for which to compute PDP.

**Usage:**
`FeatureEffect$set.feature(feature)`

**Arguments:**

- **feature** *(character(1))*
  - Feature name.

**Method** `center()`: Set the value at which the ice computations are centered.

**Usage:**
`FeatureEffect$center(center.at)`

**Arguments:**

- **center.at** *(numeric(1))*
  - Value at which the plot should be centered. Ignored in the case of two features.

**Method** `predict()`: Predict the marginal outcome given a feature.

**Usage:**
`FeatureEffect$predict(data, extrapolate = FALSE)`

**Arguments:**

- **data** *data.frame*
  - Data.frame with the feature or a vector.
extrapolate (character(1))

If TRUE, predict returns NA for x values outside of observed range. If FALSE, predict returns the closest PDP value for x values outside the range. Ignored for categorical features

Returns: Values of the effect curves at the given values.

Method clone(): The objects of this class are cloneable with this method.

Usage:
FeatureEffect$clone(deep = FALSE)

Arguments:
dep Whether to make a deep clone.

References


See Also

plot.FeatureEffect

Examples

# We train a random forest on the Boston dataset:
data("Boston", package = "MASS")
library("randomForest")
rf <- randomForest(medv ~ ., data = Boston, ntree = 50)
mod <= Predictor$new(rf, data = Boston)

# Compute the accumulated local effects for the first feature
eff <= FeatureEffect$new(mod, feature = "rm", grid.size = 30)
eff$plot()

# Again, but this time with a partial dependence plot and ice curves
eff <= FeatureEffect$new(mod,
  feature = "rm", method = "pdp+ice",
  grid.size = 30
)
plot(eff)

# Since the result is a ggplot object, you can extend it:
library("ggplot2")
plot(eff) +
  # Adds a title
  ggtitle("Partial dependence") +
  # Adds original predictions
geom_point(
  data = Boston, aes(y = mod$predict(Boston)[[1]], x = rm),
  color = "pink", size = 0.5
)

# If you want to do your own thing, just extract the data:
eff.dat <- eff$results
head(eff.dat)

# You can also use the object to "predict" the marginal values.
eff$predict(Boston[1:3,])
# Instead of the entire data.frame, you can also use feature values:
eff$predict(c(5, 6, 7))

# You can reuse the pdp object for other features:
eff$set.feature("lstat")
plot(eff)

# Only plotting the aggregated partial dependence:
eff <- FeatureEffect$new(mod, feature = "crim", method = "pdp")
eff$plot()

# Only plotting the individual conditional expectation:
eff <- FeatureEffect$new(mod, feature = "crim", method = "ice")
eff$plot()

# Accumulated local effects and partial dependence plots support up to two
# features:
eff <- FeatureEffect$new(mod, feature = c("crim", "lstat"))
plot(eff)

# FeatureEffect plots also works with multiclass classification
rf <- randomForest(Species ~ ., data = iris, ntree = 50)
mod <- Predictor$new(rf, data = iris, type = "prob")

# For some models we have to specify additional arguments for the predict
# function
plot(FeatureEffect$new(mod, feature = "Petal.Width"))

# FeatureEffect plots support up to two features:
eff <- FeatureEffect$new(mod, feature = c("Sepal.Length", "Petal.Length"))
eff$plot()

# show where the actual data lies
eff$plot(show.data = TRUE)

# For multiclass classification models, you can choose to only show one class:
mod <- Predictor$new(rf, data = iris, type = "prob", class = 1)
plot(FeatureEffect$new(mod, feature = "Sepal.Length"))
FeatureEffects

---

**Effect of a feature on predictions**

**Description**

FeatureEffects computes and plots feature effects of multiple features at once.

**Details**

FeatureEffects computes the effects for all given features on the model prediction. FeatureEffects is a convenience class that calls FeatureEffect multiple times. See ?FeatureEffect for details what’s actually computed.

Only first-order effects can be computed with the FeatureEffects interface. If you are interested in the visualization of interactions between two features, directly use FeatureEffect.

**Parallelization**

Parallelization is supported via package future. To initialize future-based parallelization, select an appropriate backend and specify the amount of workers. For example, to use a PSOCK based cluster backend do:

```r
future::plan(multisession, workers = 2)
<iml function here>
```

Consult the resources of the future package for more parallel backend options.

**Super class**

iml::InterpretationMethod -> FeatureEffects

**Public fields**

- grid.size (numeric(1) | numeric(2))
  The size of the grid.
- method (character(1))
  - "ale" for accumulated local effects,
  - "pdp" for partial dependence plot,
  - "ice" for individual conditional expectation curves,
  - "pdp+ ice" for partial dependence plot and ice curves within the same plot.
- effects (list)
  Named list of FeatureEffects.
- features (character())
  The names of the features for which the effects were computed.
- center.at numeric
  Value at which the plot was centered. Ignored in the case of two features.
Methods

Public methods:
• FeatureEffects$new()
• FeatureEffects$clone()

Method new(): Create a FeatureEffects object

Usage:
FeatureEffects$new(
  predictor,
  features = NULL,
  method = "ale",
  center.at = NULL,
  grid.size = 20
)

Arguments:
predictor  Predictor
  The object (created with Predictor$new()) holding the machine learning model and the
data.
features  (character())
  The names of the features for which to compute the feature effects.
method  (character(1))
  • 'ale' for accumulated local effects,
  • 'pdp' for partial dependence plot,
  • 'ice' for individual conditional expectation curves,
  • 'pdp+ice' for partial dependence plot and ice curves within the same plot.
center.at  (numeric(1))
  Value at which the plot should be centered. Ignored in the case of two features.
grid.size  (numeric(1) | numeric(2))
  The size of the grid for evaluating the predictions.
feature  (character(1) | character(2) | numeric(1) | numeric(2))
  The feature name or index for which to compute the effects.

Method clone(): The objects of this class are cloneable with this method.

Usage:
FeatureEffects$clone(deep = FALSE)

Arguments:
deep  Whether to make a deep clone.

References


See Also

plot.FeatureEffects

Examples

# We train a random forest on the Boston dataset:
library("rpart")
data("Boston", package = "MASS")
rf <- rpart(medv ~ ., data = Boston)
mod <- Predictor$new(rf, data = Boston)

# Compute the accumulated local effects for all features
eff <- FeatureEffects$new(mod)
eff$plot()
## Not run:
# Again, but this time with a partial dependence plot
eff <- FeatureEffects$new(mod, method = "pdp")
eff$plot()

# Only a subset of features
eff <- FeatureEffects$new(mod, features = c("nox", "crim"))
eff$plot()

# You can access each FeatureEffect individually
eff.nox <- eff$effects[["nox"]]
eff.nox$plot()

# FeatureEffects also works with multiclass classification
rf <- rpart(Species ~ ., data = iris)
mod <- Predictor$new(rf, data = iris, type = "prob")
FeatureEffects$new(mod)$plot(ncol = 2)
## End(Not run)

FeatureImp | Feature importance
--- | ---

Description

FeatureImp computes feature importance for prediction models. The importance is measured as the factor by which the model’s prediction error increases when the feature is shuffled.
Details

To compute the feature importance for a single feature, the model prediction loss (error) is measured before and after shuffling the values of the feature. By shuffling the feature values, the association between the outcome and the feature is destroyed. The larger the increase in prediction error, the more important the feature was. The shuffling is repeated to get more accurate results, since the permutation feature importance tends to be quite unstable. Read the Interpretable Machine Learning book to learn about feature importance in detail: https://christophm.github.io/interpretable-ml-book/feature-importance.html

The loss function can be either specified via a string, or by handing a function to FeatureImp(). If you want to use your own loss function it should have this signature:

function(actual, predicted)

Using the string is a shortcut to using loss functions from the Metrics package. Only use functions that return a single performance value, not a vector. Allowed losses are: "ce", "f1", "logLoss", "mae", "mse", "rmse", "mape", "mdae", "msle", "percent_bias", "rae", "rmse", "rmsle", "rse", "rrse" and "smape".

See library(help = "Metrics") to get a list of functions.

Parallelization

Parallelization is supported via package future. To initialize future-based parallelization, select an appropriate backend and specify the amount of workers. For example, to use a PSOCK based cluster backend do:

future::plan(multisession, workers = 2)
<iml function here>

Consult the resources of the future package for more parallel backend options.

Super class

iml::InterpretationMethod -> FeatureImp

Public fields

loss (character(1) | function)
    The loss function. Either the name of a loss (e.g. "ce" for classification or "mse") or a function.
original.error (numeric(1))
    The loss of the model before perturbing features.
n.repetitions integer
    Number of repetitions.
compare (character(1))
    Either "ratio" or "difference", depending on whether the importance was calculated as difference between original model error and model error after permutation or as ratio.
Methods

Public methods:

- FeatureImp$new()
- FeatureImp$clone()

Method new(): Create a FeatureImp object

Usage:
FeatureImp$new(predictor, loss, compare = "ratio", n.repetitions = 5)

Arguments:

predictor  Predictor
  The object (created with Predictor$new()) holding the machine learning model and the
data.

loss (character(1) | function)
  The loss function. Either the name of a loss (e.g. "ce" for classification or "mse") or a
  function. See Details for allowed losses.

compare (character(1))
  Either "ratio" or "difference". Should importance be measured as the difference or as
  the ratio of original model error and model error after permutation?
  - Ratio: error.permutation/error.orig
  - Difference: error.permutation - error.orig

n.repetitions (numeric(1))
  How often should the shuffling of the feature be repeated? The higher the number of re-
etitions the more stable and accurate the results become.

Returns: (data.frame)
data.frame with the results of the feature importance computation. One row per feature with the
following columns:
  - importance.05 (5% quantile of importance values from the repetitions)
  - importance (median importance)
  - importance.95 (95% quantile) and the permutation.error (median error over all repetitions).
The distribution of the importance is also visualized as a bar in the plots, the median importance
over the repetitions as a point.

Method clone(): The objects of this class are cloneable with this method.

Usage:
FeatureImp$clone(deep = FALSE)

Arguments:
dee Whether to make a deep clone.

References

sures for any Machine Learning Model Class, from the "Rashomon" Perspective. Retrieved from
http://arxiv.org/abs/1801.01489
library("rpart")
# We train a tree on the Boston dataset:
data("Boston", package = "MASS")
tree <- rpart(medv ~ ., data = Boston)
y <- Boston$medv
X <- Boston[-which(names(Boston) == "medv")]
mod <- Predictor$new(tree, data = X, y = y)

# Compute feature importances as the performance drop in mean absolute error
imp <- FeatureImp$new(mod, loss = "mae")

# Plot the results directly
plot(imp)

# Since the result is a ggplot object, you can extend it:
library("ggplot2")
plot(imp) + theme_bw()
# If you want to do your own thing, just extract the data:
imp.dat <- imp$results
head(imp.dat)
ggplot(imp.dat, aes(x = feature, y = importance)) +
  geom_point() +
  theme_bw()

# We can also look at the difference in model error instead of the ratio
imp <- FeatureImp$new(mod, loss = "mae", compare = "difference")

# Plot the results directly
plot(imp)

# FeatureImp also works with multiclass classification.
# In this case, the importance measurement regards all classes
tree <- rpart(Species ~ ., data = iris)
X <- iris[-which(names(iris) == "Species")]
y <- iris$Species
mod <- Predictor$new(tree, data = X, y = y, type = "prob")

# For some models we have to specify additional arguments for the predict function
imp <- FeatureImp$new(mod, loss = "ce")
plot(imp)

# For multiclass classification models, you can choose to only compute
# performance for one class.
# Make sure to adapt y
mod <- Predictor$new(tree,
data = X, y = y == "virginica",
type = "prob", class = "virginica")
)
Interaction

```r
imp <- FeatureImp$new(mod, loss = "ce")
plot(imp)
```

### Description

returns TRUE if object has predict function

### Usage

```r
has.predict(object)
```

### Arguments

- **object**
  - The object to check.

### Interaction

**Feature interactions**

### Description

Feature interactions

### Details

Interaction estimates the feature interactions in a prediction model.

Interactions between features are measured via the decomposition of the prediction function: If a feature \( j \) has no interaction with any other feature, the prediction function can be expressed as the sum of the partial function that depends only on \( j \) and the partial function that only depends on features other than \( j \). If the variance of the full function is completely explained by the sum of the partial functions, there is no interaction between feature \( j \) and the other features. Any variance that is not explained can be attributed to the interaction and is used as a measure of interaction strength.

The interaction strength between two features is the proportion of the variance of the 2-dimensional partial dependence function that is not explained by the sum of the two 1-dimensional partial dependence functions.

The interaction is measured by Friedman’s H-statistic (square root of the H-squared test statistic) and takes on values between 0 (no interaction) to 1 (100% of standard deviation of \( f(x) \) due to interaction).

Parallelization

Parallelization is supported via package `future`. To initialize future-based parallelization, select an appropriate backend and specify the amount of workers. For example, to use a PSOCK based cluster backend do:

```r
future::plan(multisession, workers = 2)
<iml function here>
```

Consult the resources of the `future` package for more parallel backend options.

Super class

`iml::InterpretationMethod` $\rightarrow$ Interaction

Public fields

`grid.size` (logical(1))

The number of values per feature that should be used to estimate the interaction strength.

Methods

Public methods:

- `Interaction$new()`
- `Interaction$clone()`

Method `new()`: Create an Interaction object

Usage:

`Interaction$new(predictor, feature = NULL, grid.size = 30)`

Arguments:

predictor  Predictor

The object (created with `Predictor$new()`) holding the machine learning model and the data.

feature (character(1) | character(2) | numeric(1) | numeric(2))

The feature name or index for which to compute the effects.

grid.size (numeric(1) | numeric(2))

The size of the grid for evaluating the predictions.

Returns:  `data.frame` with the interaction strength (column `.interaction`) per feature calculated as Friedman’s H-statistic and - in the case of a multi-dimensional outcome - per class.

Method `clone()`: The objects of this class are cloneable with this method.

Usage:

`Interaction$clone(deep = FALSE)`

Arguments:

depth  Whether to make a deep clone.
References


Examples

```r
## Not run:
library("rpart")
set.seed(42)
# Fit a CART on the Boston housing data set
data("Boston", package = "MASS")
rf <- rpart(medv ~ ., data = Boston)
# Create a model object
mod <- Predictor$new(rf, data = Boston[-which(names(Boston) == "medv")])

# Measure the interaction strength
ia <- Interaction$new(mod)

# Plot the resulting leaf nodes
plot(ia)

# Extract the results
dat <- ia$results
head(dat)

# Interaction also works with multiclass classification
rf <- rpart(Species ~ ., data = iris)
mod <- Predictor$new(rf, data = iris, type = "prob")

# For some models we have to specify additional arguments for the predict function
ia <- Interaction$new(mod)

ia$plot()

# For multiclass classification models, you can choose to only show one class:
mod <- Predictor$new(rf, data = iris, type = "prob", class = "virginica")
plot(Interaction$new(mod))

## End(Not run)
```

InterpretationMethod  Interpretation Method

Description

Superclass container for Interpretation Method objects
**Public fields**

results data.frame
   The aggregated results of the experiment

predictor Predictor object.

**Methods**

**Public methods:**

- InterpretationMethod$new()
- InterpretationMethod$plot()
- InterpretationMethod$print()
- InterpretationMethod$clone()

**Method new():** Create an InterpretationMethod object

*Usage:*
InterpretationMethod$new(predictor)

*Arguments:*
predictor Predictor
   The object (created with Predictor$new()) holding the machine learning model and the data.

**Method plot():** Plot function. Calls private$generatePlot() of the respective subclass.

*Usage:*
InterpretationMethod$plot(...)

*Arguments:*
... Passed to private$generatePlot().

**Method print():** Printer for InterpretationMethod objects

*Usage:*
InterpretationMethod$print()

**Method clone():** The objects of this class are cloneable with this method.

*Usage:*
InterpretationMethod$clone(deep = FALSE)

*Arguments:*
deep Whether to make a deep clone.
LocalModel fits locally weighted linear regression models (logistic regression for classification) to explain single predictions of a prediction model.

Details

A weighted glm is fitted with the machine learning model prediction as target. Data points are weighted by their proximity to the instance to be explained, using the gower proximity measure. L1-regularization is used to make the results sparse.

The resulting model can be seen as a surrogate for the machine learning model, which is only valid for that one point. Categorical features are binarized, depending on the category of the instance to be explained: 1 if the category is the same, 0 otherwise.

To learn more about local models, read the Interpretable Machine Learning book: https://christophm.github.io/interpretable-ml-book/lime.html

The approach is similar to LIME, but has the following differences:

- **Distance measure**: Uses as default the gower proximity (= 1 - gower distance) instead of a kernel based on the Euclidean distance. Has the advantage to have a meaningful neighborhood and no kernel width to tune. When the distance is not "gower", then the stats::dist() function with the chosen method will be used, and turned into a similarity measure: \( \sqrt{\exp\left(-\frac{distance^2}{\text{kernel.width}^2}\right)} \).

- **Sampling**: Uses the original data instead of sampling from normal distributions. Has the advantage to follow the original data distribution.

- **Visualization**: Plots effects instead of betas. Both are the same for binary features, but are different for numerical features. For numerical features, plotting the betas makes no sense, because a negative beta might still increase the prediction when the feature value is also negative.

To learn more about local surrogate models, read the Interpretable Machine Learning book: https://christophm.github.io/interpretable-ml-book/lime.html

Super class

`iml::InterpretationMethod` -> LocalModel

Public fields

- `x.interest` data.frame
  Single row with the instance to be explained.

- `k` numeric(1)
  The number of features as set by the user.

- `model` glmnet
  The fitted local model.
best.fit.index numeric(1)
The index of the best glmnet fit.

Methods

Public methods:

• LocalModel$new()
• LocalModel$predict()
• LocalModel$explain()
• LocalModel$clone()

Method new(): Create a Local Model object.

Usage:
LocalModel$new(
  predictor,
  x.interest,
  dist.fun = "gower",
  kernel.width = NULL,
  k = 3
)

Arguments:
predictor Predictor
  The object (created with Predictor$new()) holding the machine learning model and the data.
x.interest data.frame
  Single row with the instance to be explained.
dist.fun character(1)
  The name of the distance function for computing proximities (weights in the linear model).
  Defaults to "gower". Otherwise will be forwarded to stats::dist.
k numeric(1)
  The width of the kernel for the proximity computation. Only used if dist.fun is not "gower".

Returns: data.frame
  Results with the feature names (feature) and contributions to the prediction.

Method predict(): Method to predict new data with the local model See also predict.LocalModel.

Usage:
LocalModel$predict(newdata = NULL, ...)

Arguments:
newdata data.frame
  Data to predict on.
... Not used

Method explain(): Set a new data point to explain.
Usage:
LocalModel$explain(x.interest)

Arguments:
x.interest data.frame
   Single row with the instance to be explained.

Method clone(): The objects of this class are cloneable with this method.

Usage:
LocalModel$clone(deep = FALSE)

Arguments:
deep Whether to make a deep clone.

References


See Also

plot.LocalModel and predict.LocalModel

Shapley can also be used to explain single predictions

The package lime with the original implementation

Examples

library("randomForest")
# First we fit a machine learning model on the Boston housing data
data("Boston", package = "MASS")
X <- Boston[-which(names(Boston) == "medv")]
rf <- randomForest(medv ~ ., data = Boston, ntree = 50)
mod <- Predictor$new(rf, data = X)

# Explain the first instance of the dataset with the LocalModel method:
x.interest <- X[1,]
lemon <- LocalModel$new(mod, x.interest = x.interest, k = 2)
lemon

# Look at the results in a table
lemon$results
# Or as a plot
plot(lemon)

# Reuse the object with a new instance to explain
lemon$x.interest
lemon$explain(X[2,])
lemon$x.interest
# LocalModel also works with multiclass classification
rf <- randomForest(Species ~ ., data = iris, ntree = 50)
X <- iris[-which(names(iris) == "Species")]
mod <- Predictor$new(rf, data = X, type = "prob", class = "setosa")
# Then we explain the first instance of the dataset with the LocalModel method:
lemon <- LocalModel$new(mod, x.interest = X[1, ], k = 2)
lemon$results
plot(lemon)

---

## order_levels

**Order levels of a categorical features**

### Description

Orders the levels by their similarity in other features. Computes per feature the distance, sums up all distances and does multi-dimensional scaling

### Usage

`order_levels(dat, feature.name)`

### Arguments

- **dat**: data.frame with the training data
- **feature.name**: the name of the categorical feature

### Details

**Goal**: Compute the distances between two categories. **Input**: Instances from category 1 and 2

1. For all features, do (excluding the categorical feature for which we are computing the order):

   - If the feature is numerical: Take instances from category 1, calculate the empirical cumulative probability distribution function (ecdf) of the feature. The ecdf is a function that tells us for a given feature value, how many values are smaller. Do the same for category 2. The distance is the absolute maximum point-wise distance of the two ecdf. Practically, this value is high when the distribution from one category is strongly shifted far away from the other. This measure is also known as the Kolmogorov-Smirnov distance ([https://en.wikipedia.org/wiki/Kolmogorov%E2%80%93Smirnov_test](https://en.wikipedia.org/wiki/Kolmogorov%E2%80%93Smirnov_test)).

   - If the feature is categorical: Take instances from category 1 and calculate a table with the relative frequency of each category of the other feature. Do the same for instances from category 2. The distance is the sum of the absolute difference of both relative frequency tables.

1. Sum up the distances over all features
This algorithm we run for all pairs of categories. Then we have a \( k \times k \) matrix, where \( k \) is the number of categories, where each entry is the distance between two categories. Still not enough to have a single order, because, a (dis)similarity tells you the pair-wise distances, but does not give you a one-dimensional ordering of the classes. To kind of force this thing into a single dimension, we have to use a dimension reduction trick called multi-dimensional scaling. This can be solved using multi-dimensional scaling, which takes in a distance matrix and returns a distance matrix with reduced dimension. In our case, we only want 1 dimension left, so that we have a single ordering of the categories and can compute the accumulated local effects. After reducing it to a single ordering, we are done and can use this ordering to compute ALE. This is not the Holy Grail how to order the factors, but one possibility.

**Value**

the order of the levels (not levels itself)

---

**Partial**

*Effect of one or two feature(s) on the model predictions (deprecated)*

---

**Description**

Effect of one or two feature(s) on the model predictions (deprecated)

---

**Details**

Deprecated, please use `FeatureEffect`.

---

**Super classes**

`iml::InterpretationMethod` \(\rightarrow\) `iml::FeatureEffect` \(\rightarrow\) Partial

---

**Methods**

**Public methods:**

- `Partial$new()`
- `Partial$clone()`

**Method** `new()`: Effect of one or two feature(s) on the model predictions

*Usage:*

```r
Partial$new(
    predictor,
    feature,
    aggregation = "pdp",
    ice = TRUE,
    center.at = NULL,
    grid.size = 20
)
```
Arguments:
predictor Predictor
    The object (created with Predictor$new()) holding the machine learning model and the
data.
feature (character(1) | character(2) | numeric(1) | numeric(2))
    The feature name or index for which to compute the effects.
aggregation (character(1))
    The aggregation approach to use. Possible values are "pdp", "ale" or "none".
ice logical
    Whether to compute ice plots.
center.at (numeric(1))
    Value at which the plot should be centered. Ignored in the case of two features.
grid.size (numeric(1) | numeric(2))
    The size of the grid for evaluating the predictions.

Method clone(): The objects of this class are cloneable with this method.

Usage:
Partial$clone(deep = FALSE)

Arguments:
deep Whether to make a deep clone.

See Also
FeatureEffect

plot.FeatureEffect

Description
plot.FeatureEffect() plots the results of a FeatureEffect object.

Usage
## S3 method for class 'FeatureEffect'
plot(x, rug = TRUE, show.data = FALSE, ylim = NULL)

Arguments
x A FeatureEffect object.
rug logical
    Should a rug be plotted to indicate the feature distribution? The rug will be
    jittered a bit, so the location may not be exact, but it avoids overplotting.
show.data (logical(1))
    Should the data points be shown? Only affects 2D plots, and ignored for 1D
    plots, because rug has the same information.
ylim (numeric(2))

Vector with two coordinates for the y-axis. Only works when one feature is used in FeatureEffect, ignored when two are used.

Value

ggplot2 plot object

See Also

FeatureEffect

Examples

# We train a random forest on the Boston dataset:
if (require(“randomForest”)) {
  data(“Boston”, package = “MASS”)
  rf <- randomForest(medv ~ ., data = Boston, ntree = 50)
  mod <- Predictor$new(rf, data = Boston)

  # Compute the ALE for the first feature
  eff <- FeatureEffect$new(mod, feature = “crim”)

  # Plot the results directly
  plot(eff)
}

plot.FeatureEffects  Plot FeatureEffect

Description

plot.FeatureEffect() plots the results of a FeatureEffect object.

Usage

## S3 method for class ’FeatureEffects’
plot(x, features = NULL, nrows = NULL, ncols = NULL, fixed_y = TRUE, ...)

Arguments

x A FeatureEffect object.

features character For which features should the effects be plotted? Default is all features.
You can also sort the order of the plots with this argument.

nrows The number of rows in the table of graphics

ncols The number of columns in the table of graphics

fixed_y Should the y-axis range be the same for all effects? Defaults to TRUE.

... Further arguments for FeatureEffect$plot()
In contrast to other plot methods in iml, for FeatureEffects the returned plot is not a ggplot2 object, but a grid object, a collection of multiple ggplot2 plots.

Value
grid object

See Also
FeatureEffects plot.FeatureEffect

Examples
# We train a random forest on the Boston dataset:
library("randomForest")
data("Boston", package = "MASS")
rf <- randomForest(medv ~ ., data = Boston, ntree = 50)
mod <- Predictor$new(rf, data = Boston)

# Compute the partial dependence for the first feature
eff <- FeatureEffects$new(mod)

# Plot the results directly
eff$plot()

# For a subset of features
eff$plot(features = c("lstat", "crim"))

# With a different layout
eff$plot(nrows = 2)
plot.Interaction

Details

The plot shows the importance per feature.

When \( n\text{.repetitions} \) in FeatureImp$new was larger than 1, then we get multiple importance estimates per feature. The importance are aggregated and the plot shows the median importance per feature (as dots) and also the 90%-quantile, which helps to understand how much variance the computation has per feature.

Value

ggplot2 plot object

See Also

FeatureImp

Examples

```r
library("rpart")
# We train a tree on the Boston dataset:
data("Boston", package = "MASS")
tree <- rpart(medv ~ ., data = Boston)
y <- Boston$medv
X <- Boston[-which(names(Boston) == "medv")]
mod <- Predictor$new(tree, data = X, y = y)

# Compute feature importances as the performance drop in mean absolute error
imp <- FeatureImp$new(mod, loss = "mae")

# Plot the results directly
plot(imp)
```

Description

plot.Interaction() plots the results of an Interaction object.

Usage

```r
## S3 method for class 'Interaction'
plot(x, sort = TRUE)
```

Arguments

- \( x \) An Interaction R6 object
- \( sort \) logical. Should the features be sorted in descending order? Defaults to TRUE.
Value

   ggplot2 plot object

See Also

   Interaction

Examples

  # We train a tree on the Boston dataset:
  ## Not run:
  library("rpart")
  data("Boston", package = "MASS")
  rf <- rpart(medv ~ ., data = Boston)
  mod <- Predictor$new(rf, data = Boston)

  # Compute the interactions
  ia <- Interaction$new(mod)

  # Plot the results directly
  plot(ia)

  ## End(Not run)

plot.LocalModel

Plot Local Model

Description

   plot.LocalModel() plots the feature effects of a LocalModel object.

Usage

   ## S3 method for class 'LocalModel'
   plot(object)

Arguments

   object   A LocalModel R6 object

Value

   ggplot2 plot object

See Also

   LocalModel
Examples

```r
library("randomForest")
# First we fit a machine learning model on the Boston housing data
data("Boston", package = "MASS")
X <- Boston[-which(names(Boston) == "medv")]
rf <- randomForest(medv ~ ., data = Boston, ntree = 50)
mod <- Predictor$new(rf, data = X)

# Explain the first instance of the dataset with the LocalModel method:
x.interest <- X[1, ]
lemon <- LocalModel$new(mod, x.interest = x.interest, k = 2)
plot(lemon)
```

Description

`plot.Shapley()` plots the Shapley values - the contributions of feature values to the prediction.

Usage

```r
## S3 method for class 'Var/Shapley'
plot(object, sort = TRUE)
```

Arguments

- `object`: A Shapley R6 object
- `sort`: logical
  Should the feature values be sorted by Shapley value? Ignored for multi.class output.

Value

ggplot2 plot object

See Also

Shapley

Examples

```r
## Not run:
library("rpart")
# First we fit a machine learning model on the Boston housing data
data("Boston", package = "MASS")
rf <- rpart(medv ~ ., data = Boston)
X <- Boston[-which(names(Boston) == "medv")]
```
mod <- Predictor$new(rf, data = X)

# Then we explain the first instance of the dataset with the Shapley method:
x.interest <- X[1,]
shapley <- Shapley$new(mod, x.interest = x.interest)
plot(shapley)

## End(Not run)

---

plot.TreeSurrogate

**Plot Tree Surrogate**

**Description**

Plot the response for newdata of a TreeSurrogate object. Each plot facet is one leaf node and visualizes the distribution of the $\hat{y}$ from the machine learning model.

**Usage**

```
## S3 method for class 'TreeSurrogate'
plot(object)
```

**Arguments**

- **object**
  
  A TreeSurrogate object.

**Value**

ggplot2 plot object

**See Also**

TreeSurrogate

**Examples**

```r
library("randomForest")
# Fit a Random Forest on the Boston housing data set
data("Boston", package = "MASS")
rf <- randomForest(medv ~ ., data = Boston, ntree = 50)
# Create a model object
mod <- Predictor$new(rf, data = Boston[-which(names(Boston) == "medv")])

# Fit a decision tree as a surrogate for the whole random forest
dt <- TreeSurrogate$new(mod)

# Plot the resulting leaf nodes
plot(dt)
```
predict.LocalModel

Description

Predict the response for newdata with the LocalModel model.

Usage

```r
## S3 method for class 'LocalModel'
predict(object, newdata = NULL, ...)
```

Arguments

- `object` A LocalModel R6 object
- `newdata` A data.frame for which to predict
- `...` Further arguments for the objects predict function

Value

A data.frame with the predicted outcome.

See Also

LocalModel

Examples

```r
library("randomForest")
# First we fit a machine learning model on the Boston housing data
data("Boston", package = "MASS")
X <- Boston[-which(names(Boston) == "medv")]
rf <- randomForest(medv ~ ., data = Boston, ntree = 50)
mod <- Predictor$new(rf, data = X)

# Explain the first instance of the dataset with the LocalModel method:
x.interest <- X[1, ]
lemon <- LocalModel$new(mod, x.interest = x.interest, k = 2)
predict(lemon, newdata = x.interest)
```
predict.TreeSurrogate

**Description**

Predict the response for newdata of a `TreeSurrogate` object.

This function makes the `TreeSurrogate` object call its internal `$predict()` method.

**Usage**

```r
## S3 method for class 'TreeSurrogate'
predict(object, newdata, type = "prob", ...)  
```

**Arguments**

- `object`: The surrogate tree. A `TreeSurrogate` object.
- `newdata`: A `data.frame` for which to predict.
- `type`: Either "prob" or "class". Ignored if the surrogate tree does regression.
- `...`: Further arguments for `predict_party`.

**Value**

A `data.frame` with the predicted outcome. In case of regression it is the predicted \( \hat{y} \). In case of classification it is either the class probabilities (for type "prob") or the class label (type "class").

**See Also**

- `TreeSurrogate`

**Examples**

```r
library("randomForest")
# Fit a Random Forest on the Boston housing data set
data("Boston", package = "MASS")
rf <- randomForest(medv ~ ., data = Boston, ntree = 50)
# Create a model object
mod <- Predictor$new(rf, data = Boston[-which(names(Boston) == "medv")])

# Fit a decision tree as a surrogate for the whole random forest
dt <- TreeSurrogate$new(mod)

# Plot the resulting leaf nodes
predict(dt, newdata = Boston)
```
A Predictor object holds any machine learning model (mlr, caret, randomForest, ...) and the data to be used for analyzing the model. The interpretation methods in the iml package need the machine learning model to be wrapped in a Predictor object.

In case of classification, the model should return one column per class with the class probability.

Public fields

- **data** (data.frame) Data object with the data for the model interpretation.
- **model** (any) The machine learning model.
- **batch.size** (numeric(1)) The number of rows to be input the model for prediction at once.
- **class** (character(1)) The class column to be returned.
- **prediction.colnames** (character) The column names of the predictions.
- **prediction.function** (function) The function to predict newdata.
- **task** (character(1)) The inferred prediction task: "classification" or "regression".

Methods

Public methods:

- Predictor$new()
- Predictor$predict()
- Predictor$print()
- Predictor$clone()

Method `new()`: Create a Predictor object

Usage:
Predictor$new(
  model = NULL,
  data = NULL,
  predict.function = NULL,
  y = NULL,
  class = NULL,
  type = NULL,
  batch.size = 1000
)

Arguments:

model any
  The machine learning model. Recommended are models from mlr and caret. Other machine learning with a S3 predict functions work as well, but less robust (e.g. randomForest).

data data.frame
  The data to be used for analyzing the prediction model. Allowed column classes are: numeric, factor, integer, ordered and character For some models the data can be extracted automatically. Predictor$new() throws an error when it can’t extract the data automatically.

predict.function function
  The function to predict newdata. Only needed if model is not a model from mlr or caret package. The first argument of predict.fun has to be the model, the second the newdata: function(model, newdata)

y character(1) | numeric | factor
  The target vector or (preferably) the name of the target column in the data argument. Predictor tries to infer the target automatically from the model.

class character(1))
  The class column to be returned in case of multiclass output. You can either use numbers, e.g. class=2 would take the 2nd column from the predictions, or the column name of the predicted class, e.g. class="dog".

type character(1))
  This argument is passed to the prediction function of the model. For regression models you usually don’t have to provide the type argument. The classic use case is to say type="prob" for classification models. Consult the documentation of the machine learning package you use to find which type options you have. If both predict.fun and type are used, then type is passed as an argument to predict.fun.

batch.size numeric(1)
  The maximum number of rows to be input the model for prediction at once. Currently only respected for FeatureImp, Partial and Interaction.

Method predict(): Predict new data with the machine learning model.

Usage:
Predictor$predict(newdata)

Arguments:
newdata data.frame
  Data to predict on.

Method print(): Print the Predictor object.
Usage:
Predictor$print()

Method clone(): The objects of this class are cloneable with this method.

Usage:
Predictor$clone(deep = FALSE)

Arguments:
  deep  Whether to make a deep clone.

Examples

library("mlr")
task <- makeClassifTask(data = iris, target = "Species")
learner <- makeLearner("classif.rpart", minsplit = 7, predict.type = "prob")
mod.mlr <- train(learner, task)
mod <- Predictor$new(mod.mlr, data = iris)
mod$predict(iris[1:5, ])

mod <- Predictor$new(mod.mlr, data = iris, class = "setosa")
mod$predict(iris[1:5, ])

library("randomForest")
rf <- randomForest(Species ~ ., data = iris, ntree = 20)

mod <- Predictor$new(rf, data = iris, type = "prob")
mod$predict(iris[50:55, ])

# Feature importance needs the target vector, which needs to be supplied:
mod <- Predictor$new(rf, data = iris, y = "Species", type = "prob")

probs.to.labels  

Turn class probabilities into class labels

Description

Turn class probabilities into class labels

Usage

probs.to.labels(prediction)

Arguments

  prediction  Prediction object.
Description

Shapley computes feature contributions for single predictions with the Shapley value, an approach from cooperative game theory. The features values of an instance cooperate to achieve the prediction. The Shapley value fairly distributes the difference of the instance's prediction and the datasets average prediction among the features.

Details

For more details on the algorithm see https://christophm.github.io/interpretable-ml-book/shapley.html

Super class

`iml::InterpretationMethod` -> Shapley

Public fields

- `x.interest` data.frame
  - Single row with the instance to be explained.
- `y.hat.interest` numeric
  - Predicted value for instance of interest.
- `y.hat.average` numeric(1)
  - Average predicted value for data X.
- `sample.size` numeric(1)
  - The number of times coalitions/marginals are sampled from data X. The higher the more accurate the explanations become.

Methods

Public methods:

- Shapley$new()
- Shapley$explain()
- Shapley$clone()

Method `new()`: Create a Shapley object

Usage:

Shapley$new(predictor, x.interest = NULL, sample.size = 100)

Arguments:

predictor Predictor

The object (created with Predictor$new()) holding the machine learning model and the data.
x.interest `data.frame`
  Single row with the instance to be explained.
sample.size numeric(1)
  The number of Monte Carlo samples for estimating the Shapley value.

*Returns:* `data.frame`
`data.frame` with the Shapley values (phi) per feature.

**Method** `explain()`: Set a new data point which to explain.

*Usage:*
Shapley$explain(x.interest)

*Arguments:*
x.interest `data.frame`
  Single row with the instance to be explained.

**Method** `clone()`: The objects of this class are cloneable with this method.

*Usage:*
Shapley$clone(deep = FALSE)

*Arguments:*
depth Whether to make a deep clone.

**References**

**See Also**
Shapley
A different way to explain predictions: `LocalModel`

**Examples**

```r
library("rpart")
# First we fit a machine learning model on the Boston housing data
data("Boston", package = "MASS")
rf <- rpart(medv ~ ., data = Boston)
X <- Boston[-which(names(Boston) == "medv")]
mod <- Predictor$new(rf, data = X)

# Then we explain the first instance of the dataset with the Shapley method:
x.interest <- X[1, ]
shapley <- Shapley$new(mod, x.interest = x.interest)
shapley

# Look at the results in a table
shapley$results
# Or as a plot
```

TreeSurrogate

plot(shapley)

# Explain another instance
shapley$explain(X[2, ])
plot(shapley)

## Not run:
# Shapley() also works with multiclass classification
rf <- rpart(Species ~ ., data = iris)
X <- iris[-which(names(iris) == "Species")]
mod <- Predictor$new(rf, data = X, type = "prob")

# Then we explain the first instance of the dataset with the Shapley() method:
shapley <- Shapley$new(mod, x.interest = X[1, ])
shapley$results
plot(shapley)

# You can also focus on one class
mod <- Predictor$new(rf, data = X, type = "prob", class = "setosa")
shapley <- Shapley$new(mod, x.interest = X[1, ])
shapley$results
plot(shapley)

## End(Not run)

---

**TreeSurrogate**

**Decision tree surrogate model**

**Description**

TreeSurrogate fits a decision tree on the predictions of a prediction model.

**Details**

A conditional inference tree is fitted on the predicted $\hat{y}$ from the machine learning model and the data. The partykit package and function are used to fit the tree. By default a tree of maximum depth of 2 is fitted to improve interpretability.


**Super class**

`iml::InterpretationMethod` -> TreeSurrogate

**Public fields**

- `tree` party
  - The fitted tree. See also partykit::ctree.

- `maxdepth` numeric(1)
  - The maximum tree depth.
r.squared numeric(1|n.classes)
R squared measures how well the decision tree approximates the underlying model. It is calculated as 1 - (variance of prediction differences / variance of black box model predictions).
For the multi-class case, r.squared contains one measure per class.

Methods

Public methods:
• TreeSurrogate$new()
• TreeSurrogate$predict()
• TreeSurrogate$clone()

Method new(): Create a TreeSurrogate object

Usage:
TreeSurrogate$new(predictor, maxdepth = 2, tree.args = NULL)

Arguments:
predictor Predictor
The object (created with Predictor$new()) holding the machine learning model and the data.
maxdepth numeric(1)
The maximum depth of the tree. Default is 2.
tree.args (named list)
Further arguments for party::ctree().

Method predict(): Predict new data with the tree. See also predict.TreeSurrogate

Usage:
TreeSurrogate$predict(newdata, type = "prob", ...)

Arguments:
newdata data.frame
Data to predict on.
type Prediction type.
... Further arguments passed to predict().

Method clone(): The objects of this class are cloneable with this method.

Usage:
TreeSurrogate$clone(deep = FALSE)

Arguments:
deep Whether to make a deep clone.

References
In Advances in neural information processing systems (pp. 24-30).
See Also

predict.TreeSurrogate plot.TreeSurrogate

For the tree implementation partykit::ctree()

Examples

library("randomForest")
# Fit a Random Forest on the Boston housing data set
data("Boston", package = "MASS")
rf <- randomForest(medv ~ ., data = Boston, ntree = 50)
# Create a model object
mod <- Predictor$new(rf, data = Boston[-which(names(Boston) == "medv")])

# Fit a decision tree as a surrogate for the whole random forest
dt <- TreeSurrogate$new(mod)

# Plot the resulting leaf nodes
plot(dt)

# Use the tree to predict new data
predict(dt, Boston[1:10, ])

# Extract the results
dat <- dt$results
head(dat)

# It also works for classification
rf <- randomForest(Species ~ ., data = iris, ntree = 50)
X <- iris[-which(names(iris) == "Species")]
mod <- Predictor$new(rf, data = X, type = "prob")

# Fit a decision tree as a surrogate for the whole random forest
dt <- TreeSurrogate$new(mod, maxdepth = 2)

# Plot the resulting leaf nodes
plot(dt)

# If you want to visualize the tree directly:
plot(dt$tree)

# Use the tree to predict new data
set.seed(42)
iris.sample <- X[sample(1:nrow(X), 10), ]
predict(dt, iris.sample)
predict(dt, iris.sample, type = "class")

# Extract the dataset
dat <- dt$results
head(dat)
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