Package ‘iml’

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**R topics documented:**

<table>
<thead>
<tr>
<th>Topic</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>iml-package</td>
<td>2</td>
</tr>
<tr>
<td>extract.glmnet.effects</td>
<td>3</td>
</tr>
<tr>
<td>FeatureEffect</td>
<td>3</td>
</tr>
<tr>
<td>FeatureEffects</td>
<td>8</td>
</tr>
<tr>
<td>FeatureImp</td>
<td>11</td>
</tr>
<tr>
<td>has.predict</td>
<td>15</td>
</tr>
<tr>
<td>Interaction</td>
<td>15</td>
</tr>
<tr>
<td>InterpretationMethod</td>
<td>17</td>
</tr>
<tr>
<td>LocalModel</td>
<td>19</td>
</tr>
<tr>
<td>order_levels</td>
<td>22</td>
</tr>
<tr>
<td>Partial</td>
<td>23</td>
</tr>
<tr>
<td>plot.FeatureEffect</td>
<td>25</td>
</tr>
<tr>
<td>plot.FeatureEffects</td>
<td>26</td>
</tr>
<tr>
<td>plot.FeatureImp</td>
<td>27</td>
</tr>
<tr>
<td>plot.Interaction</td>
<td>28</td>
</tr>
<tr>
<td>plot.LocalModel</td>
<td>29</td>
</tr>
<tr>
<td>plot.Shapley</td>
<td>30</td>
</tr>
<tr>
<td>plot.TreeSurrogate</td>
<td>31</td>
</tr>
<tr>
<td>predict.LocalModel</td>
<td>32</td>
</tr>
<tr>
<td>predict.TreeSurrogate</td>
<td>33</td>
</tr>
<tr>
<td>Predictor</td>
<td>34</td>
</tr>
<tr>
<td>probs.to.labels</td>
<td>36</td>
</tr>
<tr>
<td>Shapley</td>
<td>37</td>
</tr>
<tr>
<td>TreeSurrogate</td>
<td>39</td>
</tr>
</tbody>
</table>

Index: 42

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**iml-package**

*Make machine learning models and predictions interpretable*

**Description**

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

**Author(s)**

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**See Also**

Book on Interpretable Machine Learning

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**extract.glmnet.effects**

*Extract glmnet effects*

**Description**

Extract glmnet effects

**Usage**

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.


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$center()`
- `FeatureEffect$predict()`
- `FeatureEffect$clone()`

**Method** `new()`: Create a FeatureEffect object

**Usage:**

```r
FeatureEffect$new(
  predictor,
  feature,
  method = "ale",
  center.at = NULL,
  grid.size = 20,
  grid.points = NULL
)
```

**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.
- `grid.points` (numeric() | list(numeric(), numeric()))
  An optional grid along the feature. If `grid.points` are set, the `grid.size` argument is ignored. Provide a list of two vectors with the same order as in the 'feature' argument, if PDP/ALE for two features is to be computed with a user-defined grid.

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

**Usage:**

```r
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:*
deep 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("rpart")rf <- rpart(medv ~ ., data = Boston)mod <- Predictor$new(rf, data = Boston)

# Compute the accumulated local effects for the first featureeff <- 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) +
  ggtitle("Partial dependence") +
  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$resultshead(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:
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)
```

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:**

```r
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,
FeatureEffects

- '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()

# 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()
FeatureImp

# 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](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:

```r
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 \texttt{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:

\begin{verbatim}
future::plan(multisession, workers = 2)
<iml function here>
\end{verbatim}

Consult the resources of the \texttt{future} package for more parallel backend options.

Super class

\texttt{iml::InterpretationMethod} -> \texttt{FeatureImp}

Public fields

- \texttt{loss} (character(1) | function)
  - The loss function. Either the name of a loss (e.g. "ce" for classification or "mse") or a function.
- \texttt{original.error} (numeric(1))
  - The loss of the model before perturbing features.
- \texttt{n.repetitions} integer
  - Number of repetitions.
- \texttt{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.
- \texttt{features} (list)
  - Features for which importance scores are to be calculated. The names are the feature/group names, while the contents specify which feature(s) are to be permuted.

Methods

\textbf{Public methods:}

- \texttt{FeatureImp$new()}
- \texttt{FeatureImp$clone()}

\textbf{Method} \texttt{new()}: Create a FeatureImp object

\textit{Usage:}

\begin{verbatim}
FeatureImp$new(
  predictor,
  loss,
  compare = "ratio",
  n.repetitions = 5,
  features = NULL
)
\end{verbatim}

\textit{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 repetitions the more stable and accurate the results become.

**features (character or list)**

For which features do you want importance scores calculated. The default value of NULL implies all features. Use a named list of character vectors to define groups of features for which joint importance will be calculated. See examples.

**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:**

- `deep` Whether to make a deep clone.

**References**


**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)

# 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)

# We can calculate feature importance for a subset of features
imp <- FeatureImp$new(mod, loss = "mae", features = c("crim", "zn", "indus"))
plot(imp)

# We can calculate joint importance of groups of features
groups = list(
  grp1 = c("crim", "zn", "indus", "chas"),
  grp2 = c("nox", "rm", "age", "dis"),
  grp3 = c("rad", "tax", "ptratio", "black", "lstat")
)
imp <- FeatureImp$new(mod, loss = "mae", features = groups)
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$new(tree,  
data = X, y = y == "virginica",  
type = "prob", class = "virginica"  
)  
imp <- FeatureImp$new(mod, loss = "ce")  
plot(imp)

has.predict(object)

Arguments

object

The object to check.

Description

returns TRUE if object has predict function

Interaction

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 de-  
pendence 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).  
To learn more about interaction effects, read the Interpretable Machine Learning book: https://christophm.github.io/interpretable-ml-book/interaction.html
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
default::plan(multisession, workers = 2)
```

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

Super class

`iml::InterpretationMethod` <- 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:
```r
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:
```r
Interaction(clone(deep = FALSE)
```

Arguments:
- `deep`: Whether to make a deep clone.
References

Examples

## 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)

---

**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.

Please note that scaling continuous features in the machine learning method might be advisable when using LIME as an interpretation technique. LIME uses a distance measure to compute proximity weights for the weighted glm. Hence, the original scale of the features may influence the distance measure and therewith LIME results.

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: \( \sqrt{\exp(-\text{distance}^2)/(\text{kernel.width}^2)} \).

- **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",
   gower.power = 1,
   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.

gower.power numeric(1))
   The calculated gower proximity will be raised to the power of this value. Can be used to
   specify the size of the neighborhood for the LocalModel (similar to kernel.width for the
   euclidean distance).

kernel.width numeric(1))
   The width of the kernel for the proximity computation. Only used if dist.fun is not "gower".

k numeric(1)
   The number of features.
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
plot(lemon)

# 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).

• 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, when 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)

<table>
<thead>
<tr>
<th>Partial</th>
<th>Effect of one or two feature(s) on the model predictions (deprecated)</th>
</tr>
</thead>
</table>

Description

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

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

Details

Deprecated, please use FeatureEffect.

Super classes

iml::InterpretationMethod -> iml::FeatureEffect -> Partial
Methods

Public methods:

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

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

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

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:
```r
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**

```r
## 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()

**Details**

In contrast to other plot methods, 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
```
### plot.FeatureImp

**Description**

plot.FeatureImp() plots the feature importance results of a FeatureImp object.

**Usage**

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

**Arguments**

- `x` A `FeatureImp` object
- `sort` logical. Should the features be sorted in descending order? Defaults to TRUE.
- `...` Further arguments for the objects plot function

**Details**

The plot shows the importance per feature.

When `n.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)
```

---

**plot.Interaction**

**Plot Interaction**

**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**

```r
# 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**  
```r
## 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)
```
plot.Shapley

Description

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

Usage

## S3 method for class '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

## 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)
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

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.

Details

A Predictor object is a container for the prediction model and the data. This ensures that the machine learning model can be analyzed in a robust way.

Note: 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

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. You should use the column name of the predicted class,
    e.g. class="setosa".
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.
Shapley

Prediction explanations with game theory

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:*
deep 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
```
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

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)
Index

character, 26, 34, 35

data.frame, 6, 16, 18, 20, 21, 33–35, 37, 38, 40

extract.glmnet.effects, 3

factor, 35
FeatureEffect, 3, 4, 8, 23–26
FeatureEffects, 8, 8, 26
FeatureImp, 11, 27, 35
function, 12, 13, 34, 35

has.predict, 15

iml (iml-package), 2
iml-package, 2
iml::FeatureEffect, 23
iml::InterpretationMethod, 4, 9, 12, 16, 19, 23, 37, 39
integer, 12, 35
Interaction, 15, 28, 35
InterpretationMethod, 17

list, 9
LocalModel, 19, 29, 32, 38
logical, 24, 25, 30

numeric, 4, 9, 35, 37

order_levels, 22
ordered, 35

Partial, 23, 35
party::ctree(), 40
partykit::ctree, 39
partykit::ctree(), 41
plot.FeatureEffect, 6, 25, 26
plot.FeatureEffects, 10, 26
plot.FeatureImp, 27
plot.Interaction, 28

plot.LocalModel, 21, 29
plot.Shapley, 30
plot.TreeSurrogate, 31, 41
predict.LocalModel, 21, 32
predict.TreeSurrogate, 33, 40, 41
Predictor, 5, 9, 13, 16, 18, 20, 24, 34, 37, 40
probs.to.labels, 36
Shapley, 21, 30, 37, 38
stats::dist, 20
stats::dist(), 19
TreeSurrogate, 31, 33, 39