Package 'fmeffects'

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Title Model-Agnostic Interpretations with Forward Marginal Effects

Version 0.1.2

Description Create local, regional, and global explanations for any machine learning model with forward marginal effects. You provide a model and data, and 'fmeffects' computes feature effects. The package is based on the theory in: C. A. Scholbeck, G. Casalicchio, C. Molnar, B. Bischl, and C. Heumann (2022) <arXiv:2201.08837>.

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Description

Computes forward marginal effects (FME) for arbitrary supervised machine learning models. You provide a model and data, and 'fmeffects' gives you feature effects.

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See Also

Useful links:

- https://holgstr.github.io/fmeffects/
- https://github.com/holgstr/fmeffects
- Report bugs at https://github.com/holgstr/fmeffects/issues

ame

Computes AMEs for every feature (or a subset of features) of a model.

Description

This is a wrapper function for AverageMarginalEffects\$new(...)\$compute(). It computes Average Marginal Effects (AME) based on Forward Marginal Effects (FME) for a model. The AME is a simple mean FME and computed w.r.t. a feature variable and a model.

Usage

```
ame(model, data, target, features = NULL, ep.method = "none")
```

or "envelope". Defaults to "none".

Arguments

model	The (trained) model, with the ability to predict on new data. This must be an Learner (mlr3) or train (caret) object.
data	The data used for computing AMEs, must be data.frame or data.table.
target	A string specifying the model's target variable.
features	A named character vector of the names of the feature variables for which AMEs should be computed, together with the desired step sizes.
ep.method	String specifying the method used for extrapolation detection. One of "none"

Value

An AverageMarginalEffects object, with a field results containing a list of summary statistics, including

- Feature: The name of the feature.
- step. size: The step. size w.r.t. the specified feature.
- AME: The Average Marginal Effect for a step of length step.size w.r.t. the specified feature.
- SD: The standard deviation of FMEs for the specified feature and step.size.
- 0.25: The 0.25-quantile of FMEs for the specified feature and step.size.
- 0.75: The 0.75-quantile of FMEs for the specified feature and step.size.
- n: The number of observations included for the computation of the AME. This can vary for the following reasons: For categorical features, FMEs are only computed for observations where the original category is not the step.size category. For numerical features, FMEs are only computed for observations that are not extrapolation points (if ep.method is set to "envelope").

References

Scholbeck, C. A., Casalicchio, G., Molnar, C., Bischl, B., & Heumann, C. (2022). Marginal Effects for Non-Linear Prediction Functions.

Examples

```
# Train a model:
library(mlr3verse)
library(ranger)
data(bikes, package = "fmeffects")
set.seed(123)
row.id = sample(1:nrow(bikes), 100)
task = as_task_regr(x = bikes, id = "bikes", target = "count")
forest = lrn("regr.ranger")$train(task)
# Compute AMEs for all features:
overview = ame(model = forest, data = bikes[row.id, ], target = "count")
summary(overview)
# Compute AMEs for a subset of features with non-default step.sizes:
overview = ame(model = forest,
               data = bikes[row.id, ],
               target = "count",
               features = c(humidity = 0.1, weather = c("clear", "rain")))
summary(overview)
# Extract results:
overview$results
```

AverageMarginalEffects

R6 Class computing Average Marginal Effects (AME) based on Forward Marginal Effects (FME) for a model

Description

The AME is a simple mean FME and computed w.r.t. a feature variable and a model.

Public fields

```
predictor Predictor object
features vector of features for which AMEs should be computed
ep.method string specifying extrapolation detection method
results data.table with AMEs computed
computed logical specifying if compute() has been run
```

Methods

Public methods:

```
    AverageMarginalEffects$new()
    AverageMarginalEffects$compute()
    AverageMarginalEffects$clone()
    Method new(): Create a new AME object.
        Usage:
        AverageMarginalEffects$new(
        model,
        data,
        target,
```

Arguments:

features = NULL,
ep.method = "none"

model The (trained) model, with the ability to predict on new data. This must be an Learner (mlr3) or train (caret) object.

data The data used for computing AMEs, must be data.frame or data.table.

target A string specifying the model's target variable.

features A named character vector of the names of the feature variables for which AMEs should be computed, together with the desired step sizes.

ep.method String specifying the method used for extrapolation detection. One of "none" or "envelope". Defaults to "none".

```
Returns: A new AME object.
Examples:
# Train a model:
library(mlr3verse)
library(ranger)
set.seed(123)
data(bikes, package = "fmeffects")
row.id = sample(1:nrow(bikes), 100)
task = as_task_regr(x = bikes, id = "bikes", target = "count")
forest = lrn("regr.ranger")$train(task)
# Compute AMEs for all features:
overview = AverageMarginalEffects$new(
 model = forest,
  data = bikes[row.id, ],
  target = "count")$compute()
summary(overview)
# Compute AMEs for a subset of features with non-default step.sizes:
overview = AverageMarginalEffects$new(model = forest,
```

```
data = bikes[row.id, ],
                                           target = "count",
                                           features = c(humidity = 0.1,
                                          weather = c("clear", "rain")))$compute()
 summary(overview)
Method compute(): Computes results, i.e., AMEs including the SD of FMEs, for an AME object.
 Usage:
 AverageMarginalEffects$compute()
 Returns: An AME object with results.
 Examples:
 # Compute results:
 overview$compute()
Method clone(): The objects of this class are cloneable with this method.
 Usage:
 AverageMarginalEffects$clone(deep = FALSE)
 Arguments:
 deep Whether to make a deep clone.
```

Examples

```
## Method `AverageMarginalEffects$new`
# Train a model:
library(mlr3verse)
library(ranger)
set.seed(123)
data(bikes, package = "fmeffects")
row.id = sample(1:nrow(bikes), 100)
task = as_task_regr(x = bikes, id = "bikes", target = "count")
forest = lrn("regr.ranger")$train(task)
# Compute AMEs for all features:
overview = AverageMarginalEffects$new(
 model = forest,
 data = bikes[row.id, ],
 target = "count")$compute()
summary(overview)
# Compute AMEs for a subset of features with non-default step.sizes:
overview = AverageMarginalEffects$new(model = forest,
                                      data = bikes[row.id, ],
                                      target = "count",
                                      features = c(humidity = 0.1,
```

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```
weather = c("clear", "rain")))$compute()

## ------
## Method `AverageMarginalEffects$compute`
## ------
## Compute results:
overview$compute()
```

bikes

Regression data of the usage of rental bikes in Washington D.C., USA

Description

This data set contains information on hourly bike sharing usage in Washington, D.C. for the years 2011-2012. The target variable is count, the total number of bikes lent out to users at a specific time.

Usage

```
data(bikes)
```

Format

An object of class data. table (inherits from data. frame) with 727 rows and 11 columns.

Details

This data frame contains the following columns:

```
season Season of the year
year Year; 0=2011, 1=2012
month Month of the year
holiday If a day is a public holiday (y/n)
weekday Day of the week
workingday If a day is aworking day (y/n)
weather Weather situation
temp Temperature in degrees celsius
humidity Humidity (relative)
windspeed Windspeed in miles per hour
count Total number of bikes lent out to users
```

Source

This is a subset of the original data, which can be found on the OpenML database (ID = 42712).

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References

Fanaee-T, Hadi, and Gama, Joao, "Event labeling combining ensemble detectors and background knowledge", Progress in Artificial Intelligence (2013): pp. 1-15, Springer Berlin Heidelberg, doi:10.1007/s13748-013-0040-3.

Vanschoren, Joaquin, et al. "OpenML: networked science in machine learning." ACM SIGKDD Explorations Newsletter 15.2 (2014): 49-60.

came

Computes a partitioning for a ForwardMarginalEffect

Description

This is a wrapper function that creates the correct subclass of Partitioning. It computes feature subspaces for semi-global interpretations of FMEs via recursive partitioning (RP).

Usage

```
came(
  effects,
  number.partitions = NULL,
  max.sd = Inf,
  rp.method = "ctree",
  tree.control = NULL
)
```

Arguments

effects A ForwardMarginalEffect object with FMEs computed.

number.partitions

The exact number of partitions required. Either number.partitions or max.sd

can be specified.

max.sd The maximum standard deviation required in each partition. Among multiple

partitionings with this criterion identified, the one with lowest number of parti-

tions is selected. Either number.partitions or max.sd can be specified.

rp.method One of "ctree" or "rpart". The RP algorithm used for growing the decision

tree. Defaults to "ctree".

tree.control Control parameters for the RP algorithm. One of "ctree.control(...)" or

"rpart.control(...)". #' @return Partitioning Object with identified fea-

ture subspaces.

References

Scholbeck, C. A., Casalicchio, G., Molnar, C., Bischl, B., & Heumann, C. (2022). Marginal Effects for Non-Linear Prediction Functions.

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Examples

```
# Train a model and compute FMEs:
library(mlr3verse)
library(ranger)
data(bikes, package = "fmeffects")
task = as_task_regr(x = bikes, id = "bikes", target = "count")
forest = lrn("regr.ranger")$train(task)
effects = fme(model = forest, data = bikes, target = "count", feature = "temp",
              step.size = 1, ep.method = "envelope")
# Find a partitioning with exactly 3 subspaces:
subspaces = came(effects, number.partitions = 3)
# Find a partitioning with a maximum standard deviation of 20, use `rpart`:
library(rpart)
subspaces = came(effects, max.sd = 20, rp.method = "rpart")
# Analyze results:
summary(subspaces)
plot(subspaces)
# Extract results:
subspaces$results
subspaces$tree
```

fme

Computes FMEs.

Description

This is a wrapper function for FME\$new(...)\$compute(). It computes forward marginal effects (FMEs) for a specified change in feature values.

Usage

```
fme(
  model,
  data,
  target,
  feature,
  step.size,
  ep.method = "none",
  compute.nlm = FALSE,
  nlm.intervals = 1
)
```

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Arguments

model	The (trained) model, with the ability to predict on new data. This must be an Learner (mlr3) or train (caret) object.
data	The data used for computing FMEs, must be data.frame or data.table.
target	A string specifying the model's target variable.
feature	A character vector of the names of the feature variables affected by the step. For numerical steps, this must have length 1 or 2. For categorical steps, this must have length 1.
step.size	A numeric vector of the step lengths in the features affected by the step. For numerical steps, this must have length 1 or 2. For categorical steps, this is the name of the reference category.
ep.method	String specifying the method used for extrapolation detection. One of "none" or "envelope". Defaults to "none".
compute.nlm	Compute NLMs for FMEs for numerical steps. Defaults to FALSE.
nlm.intervals	Number of intervals for computing NLMs. Results in longer computing time but more accurate approximation of NLMs. Defaults to 1.

Value

FME Object with FMEs computed.

References

Scholbeck, C. A., Casalicchio, G., Molnar, C., Bischl, B., & Heumann, C. (2022). Marginal Effects for Non-Linear Prediction Functions.

Examples

ForwardMarginalEffect R6 Class representing a forward marginal effect (FME)

Description

The FME is a forward difference in prediction due to a specified change in feature values.

Public fields

```
feature vector of features
predictor Predictor object
step.size vector of step sizes for features specified by "feature"
data.step the data.table with the data matrix after the step
ep.method string specifying extrapolation detection method
compute.nlm logical specifying if NLM should be computed
nlm.intervals number of intervals for computing NLMs
step.type "numerical" or "categorical"
extrapolation.ids vector of observation ids classified as extrapolation points
results data.table with FMEs and NLMs computed
ame Average Marginal Effect (AME) of observations in results
anlm Average Non-linearity Measure (ANLM) of observations in results
computed logical specifying if compute() has been run
```

Methods

Public methods:

- ForwardMarginalEffect\$new()
- ForwardMarginalEffect\$compute()
- ForwardMarginalEffect\$plot()
- ForwardMarginalEffect\$clone()

Method new(): Create a new ForwardMarginalEffect object.

```
Usage:
ForwardMarginalEffect$new(
  predictor,
  feature,
  step.size,
  ep.method = "none",
  compute.nlm = FALSE,
  nlm.intervals = 1
)
Arguments:
```

```
predictor Predictor object.
 feature Feature vector.
 step.size Vector of step sizes.
 ep.method String specifying extrapolation detection method.
 compute.nlm Compute NLM with FMEs? Defaults to FALSE.
 nlm.intervals How many intervals for NLM computation. Defaults to 1.
 Returns: A new ForwardMarginalEffect object.
 Examples:
 # Train a model:
 library(mlr3verse)
 library(ranger)
 data(bikes, package = "fmeffects")
 forest = lrn("regr.ranger")$train(as_task_regr(x = bikes, id = "bikes", target = "count"))
 # Create an `ForwardMarginalEffect` object:
 effects = ForwardMarginalEffect$new(makePredictor(forest, bikes, "count"),
                     feature = c("temp", "humidity"),
                     step.size = c(1, 0.01),
                     ep.method = "envelope")
Method compute(): Computes results, i.e., FME (and NLMs) for non-extrapolation points, for
a ForwardMarginalEffect object.
 Usage:
 ForwardMarginalEffect$compute()
 Returns: A ForwardMarginalEffect object with results.
 Examples:
 # Compute results:
 effects$compute()
Method plot(): Plots results, i.e., FME (and NLMs) for non-extrapolation points, for an FME
object.
 Usage:
 ForwardMarginalEffect$plot(with.nlm = FALSE, jitter = c(0, 0))
 Arguments:
 with.nlm Plots NLMs if computed, defaults to FALSE.
 jitter Jitters data. A two-dimensional numeric vector, corresponds to "width" and "height".
     See ?ggplot2::geom_jitter for details. Not available if step.type is categorical. De-
     faults to no jittering, i.e., c(0, 0).
 Examples:
 # Compute results:
 effects$plot()
```

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

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```
Usage:
ForwardMarginalEffect$clone(deep = FALSE)
Arguments:
deep Whether to make a deep clone.
```

Examples

```
## -----
## Method `ForwardMarginalEffect$new`
## -----
# Train a model:
library(mlr3verse)
library(ranger)
data(bikes, package = "fmeffects")
forest = lrn("regr.ranger")$train(as_task_regr(x = bikes, id = "bikes", target = "count"))
# Create an `ForwardMarginalEffect` object:
effects = ForwardMarginalEffect$new(makePredictor(forest, bikes, "count"),
            feature = c("temp", "humidity"),
            step.size = c(1, 0.01),
            ep.method = "envelope")
## -----
## Method `ForwardMarginalEffect$compute`
## -----
# Compute results:
effects$compute()
## -----
## Method `ForwardMarginalEffect$plot`
## -----
# Compute results:
effects$plot()
```

makePredictor

User-friendly function to create a Predictor.

Description

A wrapper function that creates the correct subclass of Predictor by automatically from model. Can be passed to the constructor of FME.

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Usage

```
makePredictor(model, data, target)
```

Arguments

model the (trained) model, with the ability to predict on new data.

data the data used for computing FMEs, must be data.frame or data.table.

target a string specifying the target variable.

Examples

```
# Train a model:
library(mlr3verse)
data(bikes, package = "fmeffects")
task = as_task_regr(x = bikes, id = "bikes", target = "count")
forest = lrn("regr.ranger")$train(task)

# Create the predictor:
predictor = makePredictor(forest, bikes, "count")

# This instantiated an object of the correct subclass of `Predictor`: class(predictor)
```

Partitioning

R6 Class representing a partitioning

Description

This is the abstract superclass for partitioning objects like PartitioningCtree and PartitioningRpart. A Partitioning contains information about feature subspaces with conditional average marginal effects (cAME) computed for ForwardMarginalEffect objects.

Public fields

```
object a ForwardMarginalEffect object with results computed method the method for finding feature subspaces value the value of method results descriptive statistics of the resulting feature subspaces tree the tree representing the partitioning, a party object tree.control control parameters for the RP algorithm computed logical specifying if compute() has been run
```

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Methods

```
Public methods:
```

```
• Partitioning$new()
```

- Partitioning\$compute()
- Partitioning\$plot()
- Partitioning\$clone()

```
Method new(): Create a Partitioning object
```

```
Usage:
```

```
Partitioning$new(...)
```

Arguments:

... Partitioning cannot be initialized, only its subclasses

Method compute(): Computes the partitioning, i.e., feature subspaces with more homogeneous FMEs, for a ForwardMarginalEffect object.

```
Usage:
```

Partitioning\$compute()

Returns: An Partitioning object with results.

Examples:

- # Compute results for an arbitrary partitioning:
- # subspaces\$compute()

Method plot(): Plots results, i.e., a decision tree and summary statistics of the feature subspaces, for an Partitioning object after \$compute() has been run.

Usage:

Partitioning\$plot()

Examples:

- # Plot an arbitrary partitioning:
- # subspaces\$plot()

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

Usage:

Partitioning\$clone(deep = FALSE)

Arguments:

deep Whether to make a deep clone.

Examples

```
## -----
## Method `Partitioning$compute`
## -----
## Compute results for an arbitrary partitioning:
```

PartitioningCtree

```
# subspaces$compute()
## ------
## Method `Partitioning$plot`
## ------
# Plot an arbitrary partitioning:
# subspaces$plot()
```

PartitioningCtree

PartitioningCtree

Description

This task specializes Partitioning for the ctree algorithm for recursive partitioning.

It is recommended to use came() for construction of Partitioning objects.

Super class

```
fmeffects::Partitioning -> PartitioningCtree
```

Methods

Public methods:

- PartitioningCtree\$new()
- PartitioningCtree\$clone()

Method new(): Create a new PartitioningCtree object.

```
Usage:
```

PartitioningCtree\$new(object, method, value, tree.control = NULL)

Arguments:

object an FME object with results computed.

method the method for finding feature subspaces.

value the value of method.

tree.control control parameters for the RP algorithm.

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

Usage:

PartitioningCtree\$clone(deep = FALSE)

Arguments:

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PartitioningRpart

PartitioningRpart

Description

This task specializes Partitioning for the rpart algorithm for recursive partitioning.

It is recommended to use came() for construction of Partitioning objects.

Super class

```
fmeffects::Partitioning -> PartitioningRpart
```

Methods

Public methods:

- PartitioningRpart\$new()
- PartitioningRpart\$clone()

Method new(): Create a new PartitioningRpart object.

```
Usage:
```

```
PartitioningRpart$new(object, method, value, tree.control = NULL)
```

Arguments:

object An FME object with results computed.

method The method for finding feature subspaces.

value The value of method.

tree.control Control parameters for the RP algorithm.

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

Usage:

```
PartitioningRpart$clone(deep = FALSE)
```

Arguments:

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```
\verb|plot.ForwardMarginalEffect|\\
```

 $Plots\ an\ Forward Marginal Effect\ object.$

Description

Plots an ForwardMarginalEffect object.

Usage

```
## S3 method for class 'ForwardMarginalEffect' plot(x, ...)
```

Arguments

- x object of class ForwardMarginalEffect.
- ... additional arguments affecting the summary produced.

plot.Partitioning

Plots an FME Partitioning.

Description

Plots an FME Partitioning.

Usage

```
## S3 method for class 'Partitioning' plot(x, ...)
```

Arguments

- x object of class Partitioning.
- ... additional arguments affecting the summary produced.

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Predictor

R6 Class representing a predictor

Description

This is the abstract superclass for predictor objects like PredictorMLR3 and PredictorCaret. A Predictor contains information about an ML model's prediction function and training data.

Public fields

model The (trained) model, with the ability to predict on new data.

X A data.table with feature and target variables.

feature.names A character vector with the names of the features in X.

feature.types A character vector with the types (numerical or categorical) of the features in X.

Methods

Public methods:

- Predictor\$new()
- Predictor\$clone()

```
Method new(): Create a Predictor object
```

```
Usage:
Predictor$new(...)
Arguments:
```

... Predictor cannot be initialized, only its subclasses

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.
```

20 PredictorCaret

PredictorCaret

PredictorCaret

Description

This task specializes Predictor for caret regression models. The model is assumed to be a c("train", "train.formula").

It is recommended to use makePredictor() for construction of Predictor objects.

Super class

```
fmeffects::Predictor -> PredictorCaret
```

Methods

Public methods:

- PredictorCaret\$new()
- PredictorCaret\$predict()
- PredictorCaret\$clone()

Method new(): Create a new PredictorCaret object.

```
Usage:
```

PredictorCaret\$new(model, data, target)

Arguments:

model train, train.formula object.

data The data used for computing FMEs, must be data.frame or data.table.

target A string specifying the target variable.

Method predict(): Predicts on an observation "newdata".

Usage:

PredictorCaret\$predict(newdata)

Arguments:

newdata The feature vector for which the target should be predicted.

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

Usage:

PredictorCaret\$clone(deep = FALSE)

Arguments:

PredictorMLR3 21

PredictorMLR3

PredictorMLR3

Description

This task specializes Predictor for mlr3 models. The model is assumed to be a LearnerRegr or LearnerClassif.

It is recommended to use makePredictor() for construction of Predictor objects.

Super class

```
fmeffects::Predictor -> PredictorMLR3
```

Methods

Public methods:

- PredictorMLR3\$new()
- PredictorMLR3\$predict()
- PredictorMLR3\$clone()

Method new(): Create a new PredictorMLR3 object.

Usage:

PredictorMLR3\$new(model, data, target)

Arguments:

model LearnerRegr or LearnerClassif object.

data The data used for computing FMEs, must be data.frame or data.table.

target A string specifying the target variable.

Method predict(): Predicts on an observation "newdata".

Usage:

PredictorMLR3\$predict(newdata)

Arguments:

newdata The feature vector for which the target should be predicted.

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

Usage:

PredictorMLR3\$clone(deep = FALSE)

Arguments:

22 PredictorParsnip

PredictorParsnip

PredictorParsnip

Description

This task specializes Predictor for parsnip models. The model is assumed to be a model_fit object.

It is recommended to use makePredictor() for construction of Predictor objects.

Super class

```
fmeffects::Predictor -> PredictorParsnip
```

Methods

Public methods:

- PredictorParsnip\$new()
- PredictorParsnip\$predict()
- PredictorParsnip\$clone()

Method new(): Create a new PredictorParsnip object.

Usage:

PredictorParsnip\$new(model, data, target)

Arguments:

model model_fit object.

data The data used for computing FMEs, must be data.frame or data.table.

target A string specifying the target variable.

Method predict(): Predicts on an observation "newdata".

Usage:

PredictorParsnip\$predict(newdata)

Arguments:

newdata The feature vector for which the target should be predicted.

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

Usage:

PredictorParsnip\$clone(deep = FALSE)

Arguments:

```
\verb|print.ForwardMarginalEffect|\\
```

Prints an ForwardMarginalEffect object.

Description

Prints an ForwardMarginalEffect object.

Usage

```
## S3 method for class 'ForwardMarginalEffect' print(x, ...)
```

Arguments

- x object of class ForwardMarginalEffect.
- ... additional arguments affecting the summary produced.

print.Partitioning

Prints an FME Partitioning.

Description

Prints an FME Partitioning.

Usage

```
## S3 method for class 'Partitioning' print(x, ...)
```

Arguments

- x object of class Partitioning.
- ... additional arguments affecting the summary produced.

```
\verb|summary.AverageMarginalEffects| \\
```

Prints summary of an AverageMarginalEffects object.

Description

Prints summary of an AverageMarginalEffects object.

Usage

```
## S3 method for class 'AverageMarginalEffects'
summary(object, ...)
```

Arguments

object of class AverageMarginalEffects.
... additional arguments affecting the summary produced.

```
summary. Forward Marginal Effect\\
```

Prints summary of an ForwardMarginalEffect object.

Description

Prints summary of an ForwardMarginalEffect object.

Usage

```
## S3 method for class 'ForwardMarginalEffect'
summary(object, ...)
```

Arguments

```
object of class ForwardMarginalEffect.
```

... additional arguments affecting the summary produced.

summary.Partitioning 25

summary.Partitioning Prints summary of an FME Partitioning.

Description

Prints summary of an FME Partitioning.

Usage

```
## S3 method for class 'Partitioning'
summary(object, ...)
```

Arguments

object of class Partitioning.

... additional arguments affecting the summary produced.

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