Package ‘fmeffects’

July 19, 2023

Title Model-Agnostic Interpretations with Forward Marginal Effects

Version 0.1.0

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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Encoding UTF-8

RoxygenNote 7.2.3

Suggests caret, knitr, mlr3verse, ranger, rmarkdown, rpart

Imports checkmate, data.table, partykit, ggparty, ggplot2, cowplot, R6, testthat

Collate 'ExtrapolationDetector.R' 'FME.R' 'FMEPlot.R'
    'NonLinearityMeasure.R' 'Partitioning.R' 'PartitioningCtree.R'
    'PartitioningPlot.R' 'PartitioningRpart.R' 'Predictor.R'
    'PredictorCaret.R' 'PredictorMLR3.R' 'Pruner.R' 'S3.R' 'ame.R'
    'bikes.R' 'misc.R' 'zzz.R'

URL https://github.com/holgstr/fme

BugReports https://github.com/holgstr/fme/issues

VignetteBuilder knitr

NeedsCompilation no

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Depends R (>= 3.5.0)

Repository CRAN

Date/Publication 2023-07-19 11:00:02 UTC
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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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ame

See Also

Useful links:
  - https://github.com/holgstr/fme
  - Report bugs at https://github.com/holgstr/fme/issues

```r
ame

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")

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" or "envelope". Defaults to "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.
  - SD/AME: The coefficient of variation 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").
```
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,
  features = NULL,
  ep.method = "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" 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,
AverageMarginalEffects

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,
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 a working 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).
References


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 partitions 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(...)".

References

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

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


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"))

# Compute FMEs:
effects = fme(model = forest, data = bikes, target = "count", feature = "temp",
              step.size = 1, ep.method = "envelope")

# Analyze results:
summary(effects)
plot(effects)

# Extract results:
effects$results
**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. Defaults 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.
Usage:
ForwardMarginalEffect$clone(deep = FALSE)

Arguments:
deep  Whether to make a deep clone.

Examples

```r
## 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.
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
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

```r
## ------------------------------------------------
## Method `Partitioning$compute`
## ------------------------------------------------

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

## Method `Partitioning$plot`

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

---

### 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:*

- `deep` Whether to make a deep clone.
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:
- deep: Whether to make a deep clone.
plot.ForwardMarginalEffect

Plots an ForwardMarginalEffect 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.
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.
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` -&gt; `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:
- `deep` Whether to make a deep clone.
Description

This task specializes Predictor for mlr3 regression 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:
deep Whether to make a deep clone.
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.
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 object of class AverageMarginalEffects.
...
additional arguments affecting the summary produced.

summary.ForwardMarginalEffect

Prints summary of an ForwardMarginalEffect object.

Description

Prints summary of an ForwardMarginalEffect object.

Usage

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

Arguments

object object of class ForwardMarginalEffect.
...
additional arguments affecting the summary produced.
summary.Partitioning

Prints summary of an FME Partitioning.

Description

Prints summary of an FME Partitioning.

Usage

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

Arguments

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