Package ‘pdp’

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Type Package

Title Partial Dependence Plots

Version 0.8.1

Description A general framework for constructing partial dependence (i.e., marginal effect) plots from various types machine learning models in R.

License GPL (>= 2)

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http://bgreenwell.github.io/pdp/

BugReports https://github.com/bgreenwell/pdp/issues

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autoplot.partial Plotting Partial Dependence Functions

Description

Plots partial dependence functions (i.e., marginal effects) using \texttt{ggplot2} graphics.

Usage

```r
## S3 method for class 'partial'
autoplot(
  object,
  center = FALSE,
  plot.pdp = TRUE,
  pdp.color = "red",
  pdp.size = 1,
  pdp.linetype = 1,
  rug = FALSE,
  smooth = FALSE,
  smooth.method = "auto",
  smooth.formula = y ~ x,
  smooth.span = 0.75,
  smooth.method.args = list(),
  contour = FALSE,
  contour.color = "white",
  train = NULL,
  xlab = NULL,
  ylab = NULL,
  main = NULL,
  legend.title = "yhat",
  ...
)

## S3 method for class 'ice'
autoplot(
```
autoplot.partial

object,
center = FALSE,
plot.pdp = TRUE,
pdp.color = "red",
pdp.size = 1,
pdp.linetype = 1,
rug = FALSE,
train = NULL,
xlab = NULL,
ylab = NULL,
main = NULL,
...
)

## S3 method for class 'cice'
autoplot(
  object,
  plot.pdp = TRUE,
pdp.color = "red",
pdp.size = 1,
pdp.linetype = 1,
rug = FALSE,
train = NULL,
xlab = NULL,
ylab = NULL,
main = NULL,
...
)

Arguments

object An object that inherits from the "partial" class.
center Logical indicating whether or not to produce centered ICE curves (c-ICE curves). Only useful when object represents a set of ICE curves; see partial for details. Default is FALSE.
plot.pdp Logical indicating whether or not to plot the partial dependence function on top of the ICE curves. Default is TRUE.
pdp.color Character string specifying the color to use for the partial dependence function when plot.pdp = TRUE. Default is "red".
pdp.size Positive number specifying the line width to use for the partial dependence function when plot.pdp = TRUE. Default is 1.
pdp.linetype Positive number specifying the line type to use for the partial dependence function when plot.pdp = TRUE. Default is 1.
rug Logical indicating whether or not to include rug marks on the predictor axes. Default is FALSE.
smooth Logical indicating whether or not to overlay a LOESS smooth. Default is FALSE.
autoplot.partial

- **smooth.method**: Character string specifying the smoothing method (function) to use (e.g., "auto", "lm", "glm", "gam", "loess", or "rlm"). Default is "auto". See `geom_smooth` for details.
- **smooth.formula**: Formula to use in smoothing function (e.g., `y ~ x`, `y ~ poly(x, 2)`, or `y ~ log(x)`).
- **smooth.span**: Controls the amount of smoothing for the default loess smoother. Smaller numbers produce wigglier lines, larger numbers produce smoother lines. Default is 0.75.
- **smooth.method.args**: List containing additional arguments to be passed on to the modeling function defined by `smooth.method`.
- **contour**: Logical indicating whether or not to add contour lines to the level plot.
- **contour.color**: Character string specifying the color to use for the contour lines when `contour = TRUE`. Default is "white".
- **train**: Data frame containing the original training data. Only required if `rug = TRUE` or `chull = TRUE`.
- **xlab**: Character string specifying the text for the x-axis label.
- **ylab**: Character string specifying the text for the y-axis label.
- **main**: Character string specifying the text for the main title of the plot.
- **legend.title**: Character string specifying the text for the legend title. Default is "yhat".
- **...**: Additional (optional) arguments to be passed onto `geom_line`, `geom_point`, or `scale_fill_viridis_c`.

**Value**

A "ggplot" object.

**Examples**

```r
## Not run:
#
# Regression example (requires randomForest package to run)
#
# Load required packages
library(ggplot2) # for autoplot() generic
library(gridExtra) # for `grid.arrange`
library(magrittr) # for forward pipe operator `%>%`
library(randomForest)

# Fit a random forest to the Boston housing data
data (boston) # load the boston housing data
set.seed(101) # for reproducibility
boston.rf <- randomForest(cmedv ~ ., data = boston)

# Partial dependence of cmedv on lstat
boston.rf %>%
  partial(pred.var = "lstat") %>%
```

```r
# Partial dependence of cmedv on lstat and rm
boston.rf %>%
partial(pred.var = c("lstat", "rm"), chull = TRUE, progress = TRUE) %>%
autoplot(contour = TRUE, legend.title = "cmedv",
option = "B", direction = -1) + theme_bw()

# ICE curves and c-ICE curves
age.ice <- partial(boston.rf, pred.var = "lstat", ice = TRUE)
grid.arrange(
  autoplot(age.ice, alpha = 0.1), # ICE curves
  autoplot(age.ice, center = TRUE, alpha = 0.1), # c-ICE curves
  ncol = 2
)

## End(Not run)
```

---

**boston**

*Boston Housing Data*

**Description**

Data on median housing values from 506 census tracts in the suburbs of Boston from the 1970 census. This data frame is a corrected version of the original data by Harrison and Rubinfeld (1978) with additional spatial information. The data were taken directly from BostonHousing2 and unneeded columns (i.e., name of town, census tract, and the uncorrected median home value) were removed.

**Usage**

```r
data(boston)
```

**Format**

A data frame with 506 rows and 16 variables.

- **lon** Longitude of census tract.
- **lat** Latitude of census tract.
- **cmedv** Corrected median value of owner-occupied homes in USD 1000’s
- **crim** Per capita crime rate by town.
- **zn** Proportion of residential land zoned for lots over 25,000 sq.ft.
- **indus** Proportion of non-retail business acres per town.
- **chas** Charles River dummy variable (= 1 if tract bounds river; 0 otherwise).
- **nox** Nitric oxides concentration (parts per 10 million).
- **rm** Average number of rooms per dwelling.
• age Proportion of owner-occupied units built prior to 1940.
• dis Weighted distances to five Boston employment centers.
• rad Index of accessibility to radial highways.
• tax Full-value property-tax rate per USD 10,000.
• ptratio Pupil-teacher ratio by town.
• b $1000(B - 0.63)^2$ where B is the proportion of blacks by town.
• lstat Percentage of lower status of the population.

References


Examples

head(boston)

---

exemplar

## S3 method for class 'data.frame'
exemplar(object)

## S3 method for class 'matrix'

Description

Construct a single "exemplar" record from a data frame. For now, all numeric columns (including "Date" objects) are replaced with their corresponding median value and non-numeric columns are replaced with their most frequent value.

Usage

exemplar(object)
exemplar(object)

## S3 method for class 'dgCMatrix'
exemplar(object)

Arguments

object A data frame, matrix, or dgCMatrix (the latter two are supported by xgboost).

Value

A data frame with the same number of columns as object and a single row.

Examples

set.seed(1554) # for reproducibility
train <- data.frame(
  x = rnorm(100),
  y = sample(letters[1L:3L], size = 100, replace = TRUE,
              prob = c(0.1, 0.1, 0.8))
)
exemplar(train)
inv.link = NULL,
which.class = 1L,
prob = FALSE,
recursive = TRUE,
plot = FALSE,
plot.engine = c("lattice", "ggplot2"),
smooth = FALSE,
rug = FALSE,
chull = FALSE,
levelplot = TRUE,
contour = FALSE,
contour.color = "white",
alpha = 1,
train,
cats = NULL,
check.class = TRUE,
progress = FALSE,
parallel = FALSE,
paropts = NULL,
... }

## S3 method for class 'model_fit'
partial(object, ...)

Arguments

  object   A fitted model object of appropriate class (e.g., "gbm", "lm", "randomForest", "train", etc.).
  ...      Additional optional arguments to be passed onto predict.
  pred.var Character string giving the names of the predictor variables of interest. For reasons of computation/interpretation, this should include no more than three variables.
  pred.grid Data frame containing the joint values of interest for the variables listed in pred.var.
  pred.fun Optiona prediction function that requires two arguments: object and newdata. If specified, then the function must return a single prediction or a vector of predictions (i.e., not a matrix or data frame). Default is NULL.
  grid.resolution Integer giving the number of equally spaced points to use for the continuous variables listed in pred.var when pred.grid is not supplied. If left NULL, it will default to the minimum between 51 and the number of unique data points for each of the continuous independent variables listed in pred.var.
  ice      Logical indicating whether or not to compute individual conditional expectation (ICE) curves. Default is FALSE. See Goldstein et al. (2014) for details.
  center   Logical indicating whether or not to produce centered ICE curves (c-ICE curves). Only used when ice = TRUE. Default is FALSE. See Goldstein et al. (2014) for details.
approx Logical indicating whether or not to compute a faster, but approximate, marginal
effect plot (similar in spirit to the plotmo package). If TRUE, then partial() will compute predictions across the predictors specified in pred.var while holding
the other predictors constant (a "poor man's partial dependence" function as
Stephen Milborrow, the author of plotmo, puts it). Default is FALSE. Note this
works with ice = TRUE as well. WARNING: This option is currently experimental.
Use at your own risk. It is possible (and arguably safer) to do this manually
by passing a specific "exemplar" observation to the train argument and specifying
pred.grid manually.

quantiles Logical indicating whether or not to use the sample quantiles of the continuous
predictors listed in pred.var. If quantiles = TRUE and grid.resolution =
NULL the sample quantiles will be used to generate the grid of joint values for
which the partial dependence is computed.

probs Numeric vector of probabilities with values in [0,1]. (Values up to 2e-14 out-
side that range are accepted and moved to the nearby endpoint.) Default is
1:9/10 which corresponds to the deciles of the predictor variables. These spec-
ify which quantiles to use for the continuous predictors listed in pred.var when
quantiles = TRUE.

trim.outliers Logical indicating whether or not to trim off outliers from the continuous pre-
dictors listed in pred.var (using the simple boxplot method) before generating
the grid of joint values for which the partial dependence is computed. Default is
FALSE.

type Character string specifying the type of supervised learning. Current options are
"auto", "regression" or "classification". If type = "auto" then partial
will try to extract the necessary information from object.

inv.link Function specifying the transformation to be applied to the predictions before
the partial dependence function is computed (experimental). Default is NULL
(i.e., no transformation). This option is intended to be used for models that
allow for non-Gaussian response variables (e.g., counts). For these models, pre-
dictions are not typically returned on the original response scale by default. For
example, Poisson GBMs typically return predictions on the log scale. In this
case setting inv.link = exp will return the partial dependence function on the
response (i.e., raw count) scale.

which.class Integer specifying which column of the matrix of predicted probabilities to use
as the "focus" class. Default is to use the first class. Only used for classification
problems (i.e., when type = "classification").

prob Logical indicating whether or not partial dependence for classification problems
should be returned on the probability scale, rather than the centered logit. If
FALSE, the partial dependence function is on a scale similar to the logit. Default
is FALSE.

recursive Logical indicating whether or not to use the weighted tree traversal method de-
scribed in Friedman (2001). This only applies to objects that inherit from class
"gbm". Default is TRUE which is much faster than the exact brute force approach
used for all other models. (Based on the C++ code behind plot.gbm.)

plot Logical indicating whether to return a data frame containing the partial depen-
dence values (FALSE) or plot the partial dependence function directly (TRUE).
Default is FALSE. See plotPartial for plotting details.
plot.engine  Character string specifying which plotting engine to use whenever plot = TRUE. Options include "lattice" (default) or "ggplot2".
smooth Logical indicating whether or not to overlay a LOESS smooth. Default is FALSE.
rug Logical indicating whether or not to include a rug display on the predictor axes. The tick marks indicate the min/max and deciles of the predictor distributions. This helps reduce the risk of interpreting the partial dependence plot outside the region of the data (i.e., extrapolating). Only used when plot = TRUE. Default is FALSE.
chull Logical indicating whether or not to restrict the values of the first two variables in pred.var to lie within the convex hull of their training values; this affects pred.grid. This helps reduce the risk of interpreting the partial dependence plot outside the region of the data (i.e., extrapolating). Default is FALSE.
levelplot Logical indicating whether or not to use a false color level plot (TRUE) or a 3-D surface (FALSE). Default is TRUE.
contour Logical indicating whether or not to add contour lines to the level plot. Only used when levelplot = TRUE. Default is FALSE.
contour.color Character string specifying the color to use for the contour lines when contour = TRUE. Default is "white".
alpha Numeric value in [0, 1] specifying the opacity alpha (most useful when plotting ICE/c-ICE curves). Default is 1 (i.e., no transparency). In fact, this option only affects ICE/c-ICE curves and level plots.
train An optional data frame, matrix, or sparse matrix containing the original training data. This may be required depending on the class of object. For objects that do not store a copy of the original training data, this argument is required. For reasons discussed below, it is good practice to always specify this argument.
cats Character string indicating which columns of train should be treated as categorical variables. Only used when train inherits from class "matrix" or "dgCMatrix".
check.class Logical indicating whether or not to make sure each column in pred.grid has the correct class, levels, etc. Default is TRUE.
progress Logical indicating whether or not to display a text-based progress bar. Default is FALSE.
parallel Logical indicating whether or not to run partial in parallel using a backend provided by the foreach package. Default is FALSE.
paropts List containing additional options to be passed onto foreach when parallel = TRUE.

Value

By default, partial returns an object of class c("data.frame", "partial"). If ice = TRUE and center = FALSE then an object of class c("data.frame", "ice") is returned. If ice = TRUE and center = TRUE then an object of class c("data.frame", "cice") is returned. These three classes determine the behavior of the plotPartial function which is automatically called whenever plot = TRUE. Specifically, when plot = TRUE, a "trellis" object is returned (see lattice for details); the "trellis" object will also include an additional attribute, "partial.data", containing the data displayed in the plot.
Note

In some cases it is difficult for `partial` to extract the original training data from `object`. In these cases an error message is displayed requesting the user to supply the training data via the `train` argument in the call to `partial`. In most cases where `partial` can extract the required training data from `object`, it is taken from the same environment in which `partial` is called. Therefore, it is important to not change the training data used to construct `object` before calling `partial`. This problem is completely avoided when the training data are passed to the `train` argument in the call to `partial`.

It is recommended to call `partial` with `plot = FALSE` and store the results. This allows for more flexible plotting, and the user will not have to waste time calling `partial` again if the default plot is not sufficient.

It is possible to retrieve the last printed "trellis" object, such as those produced by `plotPartial`, using `trellis.last.object()`.

If `ice = TRUE` or the prediction function given to `pred.fun` returns a prediction for each observation in `newdata`, then the result will be a curve for each observation. These are called individual conditional expectation (ICE) curves; see Goldstein et al. (2015) and `ice` for details.

References


Examples

```r
## Not run:
#
# Regression example (requires randomForest package to run)
#

# Fit a random forest to the boston housing data
library(randomForest)
data(boston) # load the boston housing data
set.seed(101) # for reproducibility
boston.rf <- randomForest(cmedv ~ ., data = boston)

# Using randomForest's partialPlot function
partialPlot(boston.rf, pred.data = boston, x.var = "lstat")

# Using pdp's partial function
head(partial(boston.rf, pred.var = "lstat")) # returns a data frame
partial(boston.rf, pred.var = "lstat", plot = TRUE, rug = TRUE)

# The partial function allows for multiple predictors
partial(boston.rf, pred.var = c("lstat", "rm"), grid.resolution = 40,
       plot = TRUE, chull = TRUE, progress = TRUE)
```
# The plotPartial function offers more flexible plotting
pd <- partial(boston.rf, pred.var = c("lstat", "rm"), grid.resolution = 40)
plotPartial(pd, levelplot = FALSE, zlab = "cmedv", drape = TRUE,
            colorkey = FALSE, screen = list(z = -20, x = -60))

# The autoplot function can be used to produce graphics based on ggplot2
library(ggplot2)
autoplot(pd, contour = TRUE, legend.title = "Partial\ndependence")

# Individual conditional expectation (ICE) curves

# Use partial to obtain ICE/c-ICE curves
rm.ice <- partial(boston.rf, pred.var = "rm", ice = TRUE)
plotPartial(rm.ice, rug = TRUE, train = boston, alpha = 0.2)
autoplot(rm.ice, center = TRUE, alpha = 0.2, rug = TRUE, train = boston)

# Classification example (requires randomForest package to run)

# Fit a random forest to the Pima Indians diabetes data
data (pima) # load the boston housing data
set.seed(102) # for reproducibility
pima.rf <- randomForest(diabetes ~ ., data = pima, na.action = na.omit)

# Partial dependence of positive test result on glucose (default logit scale)
partial(pima.rf, pred.var = "glucose", plot = TRUE, chull = TRUE,
       progress = TRUE)

# Partial dependence of positive test result on glucose (probability scale)
partial(pima.rf, pred.var = "glucose", prob = TRUE, plot = TRUE,
       chull = TRUE, progress = TRUE)

## End(Not run)

---

**pdp**

*pdp*: A general framework for constructing partial dependence (i.e., marginal effect) plots from various types of machine learning models in R.

**Description**

Partial dependence plots (PDPs) help visualize the relationship between a subset of the features (typically 1-3) and the response while accounting for the average effect of the other predictors in the model. They are particularly effective with black box models like random forests and support vector machines.
Details

The development version can be found on GitHub: https://github.com/bgreenwell/pdp. As of right now, pdp exports four functions:

- **partial** - construct partial dependence functions (i.e., objects of class "partial") from various fitted model objects;
- **plotPartial** - plot partial dependence functions (i.e., objects of class "partial") using *lattice* graphics;
- **autoplot** - plot partial dependence functions (i.e., objects of class "partial") using *ggplot2* graphics;
- **topPredictors** - extract most "important" predictors from various types of fitted models.

---

**pima**

*Pima Indians Diabetes Data*

Description

Diabetes test results collected by the US National Institute of Diabetes and Digestive and Kidney Diseases from a population of women who were at least 21 years old, of Pima Indian heritage, and living near Phoenix, Arizona. The data were taken directly from *PimaIndiansDiabetes2*.

Usage

data(pima)

Format

A data frame with 768 observations on 9 variables.

- **pregnant** Number of times pregnant.
- **glucose** Plasma glucose concentration (glucose tolerance test).
- **pressure** Diastolic blood pressure (mm Hg).
- **triceps** Triceps skin fold thickness (mm).
- **insulin** 2-Hour serum insulin (mu U/ml).
- **mass** Body mass index (weight in kg/(height in m)^2).
- **pedigree** Diabetes pedigree function.
- **age** Age (years).
- **diabetes** Factor indicating the diabetes test result (neg/pos).
plotPartial

References


Examples

head(pima)

plotPartial

Plotting Partial Dependence Functions

Description

Plots partial dependence functions (i.e., marginal effects) using lattice graphics.

Usage

plotPartial(object, ...)

## S3 method for class 'ice'
plotPartial(
  object,
  center = FALSE,
  plot.pdp = TRUE,
  pdp.col = "red2",
  pdp.lwd = 2,
  pdp.lty = 1,
  rug = FALSE,
  train = NULL,
  ...
)

## S3 method for class 'cice'
plotPartial(
  object,
  plot.pdp = TRUE,
  pdp.col = "red2",

plotPartial

pdp.lwd = 2,
pdp.lty = 1,
rug = FALSE,
train = NULL,
...
)

## S3 method for class 'partial'
plotPartial(
  object,
  center = FALSE,
  plot.pdp = TRUE,
pdp.col = "red2",
pdp.lwd = 2,
pdp.lty = 1,
smooth = FALSE,
rug = FALSE,
chull = FALSE,
levelplot = TRUE,
contour = FALSE,
contour.color = "white",
col.regions = NULL,
number = 4,
overlap = 0.1,
train = NULL,
...
)

Arguments

object An object that inherits from the "partial" class.
...
... Additional optional arguments to be passed onto dotplot, levelplot, xyplot,
or wireframe.

center Logical indicating whether or not to produce centered ICE curves (c-ICE curves).
Only useful when object represents a set of ICE curves; see partial for details. Default is FALSE.

plot.pdp Logical indicating whether or not to plot the partial dependence function on top
of the ICE curves. Default is TRUE.

pdp.col Character string specifying the color to use for the partial dependence function when plot.pdp = TRUE. Default is "red".

pdp.lwd Integer specifying the line width to use for the partial dependence function when plot.pdp = TRUE. Default is 1. See par for more details.

pdp.lty Integer or character string specifying the line type to use for the partial dependence function when plot.pdp = TRUE. Default is 1. See par for more details.

rug Logical indicating whether or not to include rug marks on the predictor axes. Default is FALSE.
plotPartial

Data frame containing the original training data. Only required if rug = TRUE or chull = TRUE.

Logical indicating whether or not to overlay a LOESS smooth. Default is FALSE.

Logical indicating whether or not to restrict the first two variables in pred. var to lie within the convex hull of their training values; this affects pred.grid. Default is FALSE.

Logical indicating whether or not to use a false color level plot (TRUE) or a 3-D surface (FALSE). Default is TRUE.

Logical indicating whether or not to add contour lines to the level plot. Only used when levelplot = TRUE. Default is FALSE.

Character string specifying the color to use for the contour lines when contour = TRUE. Default is "white".

Vector of colors to be passed on to levelplot's col.region argument. Defaults to grDevices::hcl.colors(100) (which is the same viridis color palette used in the past).

Integer specifying the number of conditional intervals to use for the continuous panel variables. See co.intervals and equal.count for further details.

The fraction of overlap of the conditioning variables. See co.intervals and equal.count for further details.

Examples

## Not run:
#
# Regression example (requires randomForest package to run)
#

# Load required packages
library(gridExtra) # for `grid.arrange`
library(magrittr) # for forward pipe operator `%>%`
library(randomForest)

# Fit a random forest to the Boston housing data
data (boston) # load the boston housing data
set.seed(101) # for reproducibility
boston.rf <- randomForest(cmedv ~ ., data = boston)

# Partial dependence of cmedv on lstat
boston.rf %>%
  partial(pred.var = "lstat") %>%
  plotPartial(rug = TRUE, train = boston)

# Partial dependence of cmedv on lstat and rm
boston.rf %>%
  partial(pred.var = c("lstat", "rm"), chull = TRUE, progress = TRUE) %>%
  plotPartial(contour = TRUE, legend.title = "rm")

# ICE curves and c-ICE curves
age.ice <- partial(boston.rf, pred.var = "lstat", ice = TRUE)
p1 <- plotPartial(age.ice, alpha = 0.1)
p2 <- plotPartial(age.ice, center = TRUE, alpha = 0.1)
grid.arrange(p1, p2, ncol = 2)
## End(Not run)

topPredictors

Extract Most "Important" Predictors (Experimental)

Description

Extract the most "important" predictors for regression and classification models.

Usage

topPredictors(object, n = 1L, ...)

## Default S3 method:
topPredictors(object, n = 1L, ...)

## S3 method for class 'train'
topPredictors(object, n = 1L, ...)

Arguments

object A fitted model object of appropriate class (e.g., "gbm", "lm", "randomForest", etc.).
n Integer specifying the number of predictors to return. Default is 1 meaning return the single most important predictor.
... Additional optional arguments to be passed onto varImp.

Details

This function uses the generic function varImp to calculate variable importance scores for each predictor. After that, they are sorted at the names of the n highest scoring predictors are returned.

Examples

## Not run:
#
# Regression example (requires randomForest package to run)
#

Load required packages
library(ggplot2)
library(randomForest)

# Fit a random forest to the mtcars dataset
```r
data(mtcars, package = "datasets")
set.seed(101)
mtcars.rf <- randomForest(mpg ~ ., data = mtcars, mtry = 5, importance = TRUE)

# Top four predictors
top4 <- topPredictors(mtcars.rf, n = 4)

# Construct partial dependence functions for top four predictors
pd <- NULL
for (i in top4) {
  tmp <- partial(mtcars.rf, pred.var = i)
  names(tmp) <- c("x", "y")
  pd <- rbind(pd, cbind(tmp, predictor = i))
}

# Display partial dependence functions
ggplot(pd, aes(x, y)) + geom_line() + facet_wrap(~ predictor, scales = "free") + theme_bw() + ylab("mpg")

## End(Not run)
```
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