pdp: An R Package for Constructing Partial Dependence Plots

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Abstract Complex nonparametric models—like neural networks, random forests, and support vector machines—are more common than ever in predictive analytics, especially when dealing with large observational databases that don't adhere to the strict assumptions imposed by traditional statistical techniques (e.g., multiple linear regression which assumes linearity, homoscedasticity, and normality). Unfortunately, it can be challenging to understand the results of such models and explain them to management. Partial dependence plots offer a simple solution. Partial dependence plots are low-dimensional graphical renderings of the prediction function $\widehat{f}(x)$ so that the relationship between the outcome and predictors of interest can be more easily understood. These plots are especially useful in explaining the output from black box models. In this paper, we introduce **pdp**, a general R package for constructing partial dependence plots.

Introduction

Harrison and Rubinfeld (1978) were among the first to analyze the well-known Boston housing data. One of their goals was to find a housing value equation using data on median housing values from 506 census tracts in the suburbs of Boston from the 1970 census. The prediction equation from one of there regression analyses is reproduced in Equation (1). Harrison and Rubinfeld (1978) took great care and time to find this model which obtained an R^2 of roughly 0.81. Part of the payoff for there efforts was a reasonable fitting model with an interpretable equation. For example, the equation tells us that an increase in median home value is associated with an increase in the average number of rooms per dwelling.

$$
\begin{aligned}
\log\widehat{(MV)} = {} & 9.76 + 0.0063RM^2 + 8.98 \times 10^{-5}AGE - 0.19\log{(DIS)} + 0.096\log{(RAD)} \\
& - 4.20 \times 10^{-4}TAX - 0.031PTRATIO + 0.36{(B - 0.63)}^2 - 0.37\log{(LSTAT)} \\
& - 0.012CRIM + 8.03^{-5}ZN + 2.41 \times 10^{-4}INDUS + 0.088CHAS - 0.0064NOX^2
\end{aligned}
\tag{1}
$$

Many modern nonparametric models, however, can fit the data automatically in seconds—typically with higher accuracy. The downfall, however, is some loss of interpretation; for example, there is usually no prediction formula like in Equation (1). Fortunately, these methods can still provide insight into the data, but it is not in the form of simple equations. For example, many modern methods, like boosting and random forests, can assign importance scores to all of the predictors.

Determining predictor importance is a crucial task in any supervised learning problem. However, ranking variables is only part of the story and once a subset of "important" features is identified it is often necessary to assess the relationship between them (or subset thereof) and the response. This can be done in many ways, but in machine learning it is often accomplished by constructing *partial dependence plots* (PDPs); see Friedman (2000) for details. 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.

Let $x = \left\{x_1, x_2, \dots, x_p\right\}$ represent the predictors in a model whose prediction function is $\widehat{f}(x)$. If we partition x into an interest set, z_s, and its compliment, $z_c = x \setminus z_s$, then the "partial dependence" of the response on z_s is defined as

$$
f_s(z_s) = E_{z_c}\left[\widehat{f}(z_s, z_c)\right] = \int \widehat{f}(z_s, z_c) \, p_c(z_c) \, dz_c,
\tag{2}
$$

where $p_c(z_c)$ is the marginal probability density of z_c: $p_c(z_c) = \int p(x) \, dz_s$. Equation (2) can be estimated from a set of training data by

$$
\bar{f}_s(z_s) = \frac{1}{n} \sum_{i=1}^{n} \widehat{f}(z_s, z_{i,c}),
\tag{3}
$$

where $z_{i,c}$ $(i = 1, 2, \dots, n)$ are the values of z_c that occur in the training sample; that is, we average out the effects of all the other predictors in the model.

Constructing a PDP (3) in practice is rather straightforward. To simplify, let $z_s = x_1$ be the predictor

variable of interest with unique values $\{x_{11}, x_{12}, \ldots, x_{1k}\}$. The partial dependence of the response on x_1 can be constructed as follows:

1. For $i \in \{1, 2, \ldots, k\}$:

   (a) Copy the training data and replace the original values of x_1 with the constant x_{1i}.

   (b) Compute the vector of predicted values from the modified copy of the training data.

   (c) Compute the average prediction to obtain $\bar{f}_1(x_{1i})$.

2. Plot the pairs $\{x_{1i}, \bar{f}_1(x_{1i})\}$ for $i = 1, 2, \ldots, k$.

This can be quite computationally intensive since the algorithm involves k passes over the training records. Fortunately, this can be parallelized quite easily (more on this in a later section). This algorithm can also be easily extended to larger subsets of two or more features as well.

Limited implementations of Friedman's PDPs are available in packages **randomForest** (Liaw and Wiener, 2002) and **gbm**, among others; these are all limited in the sense that they only apply to the models fit using the respective package. For example, the `partialPlot` function in **randomForest** only applies to objects of class `"randomForest"` and the `plot` function in **gbm** only applies to `"gbm"` objects. While the **randomForest** implementation will only allow for a single predictor, the **gbm** implementation can deal with any subset of the predictor space. Partial dependence functions are not restricted to tree-based models; they can be applied to any supervised learning algorithm (e.g., multiple linear regression and neural networks). However, to our knowledge, there is no general package for constructing PDPs in R. For example, PDPs for a *conditional random forest* as implemented by the `cforest` function in the **party** and **partykit** packages; see Torsten Hothorn and Zeileis (2015) and Hothorn and Zeileis (2016), respectively. The **pdp** (Greenwell, 2016) package tries to close this gap by offering a general framework for constructing PDPs that can be applied to several classes of fitted models.

The **plotmo** package (Milborrow, 2015) is one alternative to **pdp**. According to its author, **plotmo** constructs "a poor man's partial dependence plot." In particular, it plots a model's response when varying one or two predictors while holding the other predictors in the model constant (continuous features are fixed at their median value, while factors are held at their first level). These plots allow for up to two variables at a time. They are also less accurate than PDPs, but are faster to construct. For additive models (i.e., models with no interactions), these plots are identical in shape to PDPs.

PDPs can be misleading in the presence of substantial interactions (Goldstein et al., 2015). To overcome this issue Goldstein, Kapelner, Bleich, and Pitkin developed the concept of *individual conditional expectation* (ICE) plots—available in the **ICEbox** package. **ICEbox** only allows for one variable at a time (i.e., no multivariate displays), though color can be used effectively to display information about an additional predictor. The ability to construct derivative plots is also available in **ICEbox**.

Many other techniques exist for visualizing relationships between the predictors and the response based on a fitted model. For example, the **car** package (Fox and Weisberg, 2011) contains many functions for constructing partial-residual and marginal-model plots. The **effects** package (Fox, 2003) is also of interest. It provides tabular and graphical displays for the terms in parametric models. However, these methods were designed for simpler parametric models (e.g., linear and generalized linear models), whereas **plotmo**, **ICEbox**, and **pdp** are more useful for black box models (although, they can be used for simple parametric models as well).

Constructing PDPs in R

The **pdp** package is useful for constructing PDPs for many classes of fitted models in R. PDPs are especially useful for visualizing the relationships discovered by complex machine learning algorithms such as a random forest. The latest stable release is available from CRAN. The development version is located on GitHub: https://github.com/bgreenwell/pdp. Bug reports and suggestions are appreciated and should be submitted to https://github.com/bgreenwell/pdp/issues. Currently, only two functions are exported by **pdp**:

- `partial`

- `plotPartial`

The `partial` function evaluates the partial dependence (3) from a fitted model over a grid of predictor values; the fitted model and predictors are specified using the `object` and `pred.var` arguments, respectively—these are the only required arguments. If `plot = FALSE` (the default), `partial` returns an object of class `"partial"` which inherits from the class `"data.frame"`; put another way, by default, `partial` returns a data frame with an additional class that is recognized by the `plotPartial` function.

The columns of the data frame are labeled in the same order as the features supplied to pred.var, and the last column is always labeled y and contains the values of the partial dependence function $\bar{f}_s(z_s)$. If plot = TRUE, then partial makes an internal call to plotPartial and returns the PDP in the form of a **lattice** plot (Sarkar, 2008).

The plotPartial function can be used for displaying more advanced PDPs; it operates on objects of class "partial" and has many useful plotting options. For example, plotPartial makes it straight forward to add a LOESS smooth, or produce a 3-D surface instead of a false color level plot (the default). Of course, since the default output produced by partial is still a data frame, the user can easily use any plotting package he/she desires to visualize the results—**ggplot2** (Wickham, 2009), for instance.

Note: as mentioned above, **pdp** relies on **lattice** for its graphics. **lattice** itself is built on top of **grid** (R Core Team, 2016). **grid** graphics behave a little differently than traditional R graphics, and two points are worth making (see ?lattice for more details):

1. **lattice** functions return a "trellis" object, but do not display it; the print method produces the actual display. However, due to R's automatic printing rule, the result is automatically printed when using these functions in the command line. If plotPartial is called inside of source or inside a loop (e.g., for or while), an explicit print statement is required to display the resulting graph.

2. Setting graphical parameters via par typically has no effect on **lattice** plots. Instead, **lattice** provides its own trellis.par.set function for modifying graphical parameters.

A consequence of the second point is that the par function cannot be used to control the layout of multiple **lattice** (and hence **pdp**) plots. Simple solutions are available in packages **latticeExtra** (Sarkar and Andrews, 2016) and **gridExtra** (Auguie, 2016). For convenience, **pdp** imports the grid.arrange function from **gridExtra** which makes it easy to display multiple **pdp** plots on a single page.

Currently supported models are described in Table 1. In a lot of these cases, partial should be able to automatically determine appropriate values for the options type (i.e., "regression" or "classification") and train (the original training data). In other situations, the user may need to specify one or both of these additional arguments. These two arguments allow partial to be flexible enough to handle many of the model types not listed in Table 1; for example, neural networks from the **nnet** package (Venables and Ripley, 2002) and projection pursuit regression (Friedman and Stuetzle, 1981) using the ppr function in the **stats** package.

Type of model	R package	Object class
Decision tree	**C50** (Kuhn et al., 2015)	"C5.0"
	party	"BinaryTree"
	partykit	"constparty"/"party"
	rpart (Therneau et al., 2015)	"rpart"
Bagged decision trees	**adabag** (Alfaro et al., 2013)	"bagging"
	ipred (Peters and Hothorn, 2015)	"classbagg", "regbagg"
Boosted decision trees	**adabag** (Alfaro et al., 2013)	"boosting"
	gbm	"gbm"
	xgboost	"xgb.Booster"
Cubist	**Cubist** (Kuhn et al., 2014)	"cubist"
Random forest	**randomForest**	"randomForest"
Conditional random forest	**party**	"RandomForest"
	partykit	"cforest"
Linear model	**stats**	"lm"
Generalized linear model	**stats**	"glm", "lm"
Nonlinear least squares	**stats**	"nls"
Multivariate adaptive regression splines (MARS)	**earth** (Milborrow, 2016)	"earth"
Support vector machine	**e1071** (Meyer et al., 2015)	"svm"
	kernlab (Karatzoglou et al., 2004)	"ksvm"

Table 1: Models specifically supported by the **pdp** package. **Note:** for some of these cases, the user may still need to supply additional arguments in the call to partial.

When additional arguments are necessary, the user will be prompted with an informative error

message. For instance, the user may occasionally see the following:

```
Error: The training data could not be extracted from object. Please supply
the raw training data using the `train` argument in the call to `partial`.
```

This will occur, for example, when using partial with the "xgb.Booster" class (see Section 2.2.6). In fact, using `partial` with any object that does not store the original training data will result in the above error message.

The partial function also supports object of class "train" produced using the train function from the well-known **caret** package (Kuhn, 2016). This means that `partial` can be used with any classification or regression model that has been fit using **caret**'s train function; see http://topepo.github.io/caret/available-models.html for a current list of models supported by **caret**. An example is given in Section 2.2.6.

For illustration, we will use the (corrected) Boston housing data which are available from the **mlbench** package (Dimitriadou, 2010). These data contain the median value of owner-occupied homes in 506 U.S. census tracts in the Boston area, along with 13 independent variables such as the per capita crime rate by town. We begin by loading the data and omitting unimportant columns.

```
data(BostonHousing2, package = "mlbench")  # mlbench must be installed!
boston <- BostonHousing2[, -c(1, 2, 5)]
```

Next, we fit a random forest to the entire data set with default tuning parameters and 500 trees:

```
library(randomForest)
set.seed(101)  # for reproducibility
boston.rf <- randomForest(cmedv ~ ., data = boston, importance = TRUE)
varImpPlot(boston.rf)  # Figure 1
```

The model fit is reasonable, with an *out-of-bag* (pseudo) R^2 of 0.89. The variable importance scores are displayed in Figure 1. Both plots indicate that the percentage of lower status of the population (lstat) and the average number of rooms per dwelling (rm) are highly associated with the median value of owner-occupied homes (cmedv). The question then arises, "What is the nature of these associations?" To help answer this, we can look at the partial dependence of cmedv on lstat and rm, both individually and together.
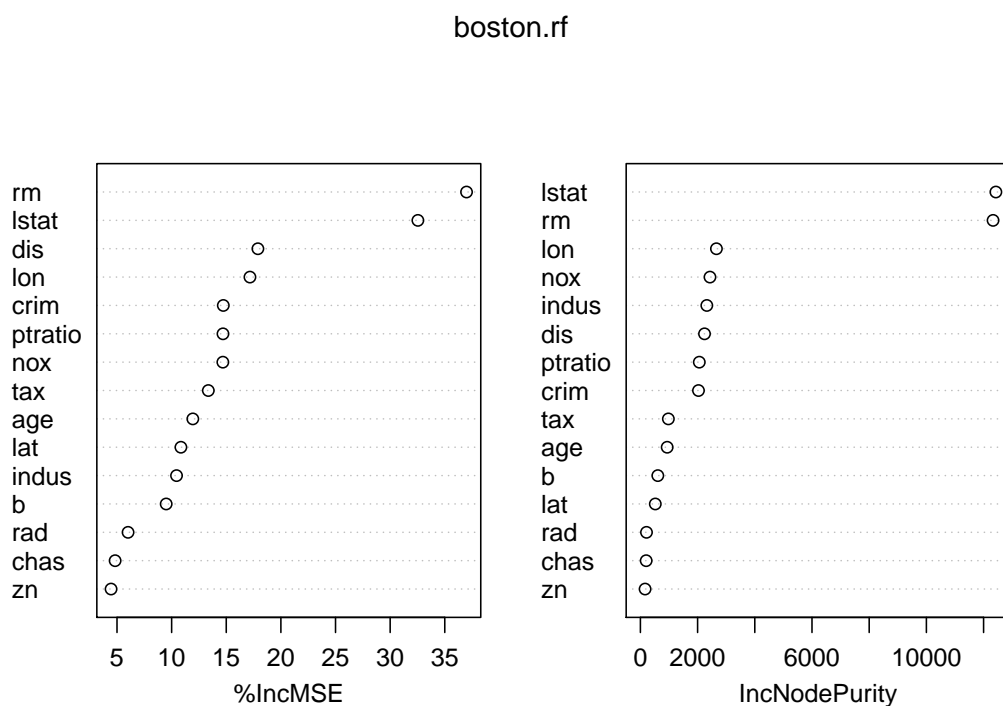
Figure 1: Dotchart of variable importance scores for the Boston housing data based on a random forest with 500 trees.

Single predictor PDPs

As previously mentioned, the randomForest package has its own partialPlot function for visualizing the partial dependence of the response on a single predictor—the keywords here are "single predictor". For example, the following snippet of code plots the partial dependence of cmedv on lstat:

```
partialPlot(boston.rf, pred.data = boston, x.var = "lstat")
```

The same plot can be achieved using the partial function and setting plot = TRUE (see the left side of Figure 2):

```
library(pdp)
partial(boston.rf, pred.var = "lstat", plot = TRUE)  # Figure 2 (left)
```

The only difference is that **pdp** uses the **lattice** graphics package to produce all of its displays.

For a more customizable plot, we can set plot = FALSE in the call to partial and then use the plotPartial function on the resulting data frame. This is illustrated in the example below which increases the line width, adds a LOESS smooth, and customizes the *y*-axis label. The result is displayed in the right side of Figure 2. **Note:** to encourage writing more readable code, the *pipe* operator %>% provided by the **magrittr** package (Bache and Wickham, 2014) is exported whenever **pdp** is loaded.

```
# Figure 2 (right)
boston.rf %>%  # the %>% operator is read as "and then"
  partial(pred.var = "lstat") %>%
  plotPartial(smooth = TRUE, lwd = 2, ylab = expression(f(lstat)))
```
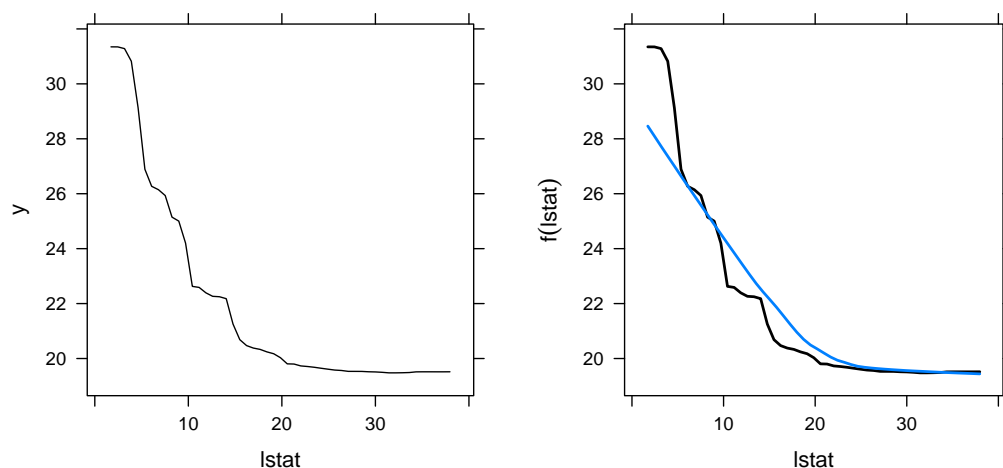

Figure 2: Partial dependence of cmedv on lstat based on a random forest. *Left*: Default plot. *Right*: Customized plot obtained using the plotPartial function.

Multi-predictor PDPs

The benefit of using partial is threefold: (1) it is a generic function that can be used for various types of fitted models (not just random forests), (2) it will allow for any number of predictors to be used (e.g., multivariate displays), and (3) it can utilize any of the parallel backends supported by the **foreach** package (Analytics and Weston, 2015c); we discuss parallel execution in a later section. For example, the following code chunk uses the random forest model to assess the joint effect of lstat and rm on cmedv. The grid.arrange function is then used to display three PDPs, which make use of various plotPartial options[1], on the same graph. The result is displayed in Figure 3.

```
rwb <- colorRampPalette(c("red", "white", "blue"))
pd <- partial(boston.rf, pred.var = c("lstat", "rm"))
grid.arrange(
  # Figure 3 (left)
  plotPartial(pd),
```

---

[1]See Section 2.2.4 for an example of how to add a label to the colorkey in these types of graphs.

```
  # Figure 3 (middle)
  plotPartial(pd, contour = TRUE, col.regions = rwb),
  # Figure 3 (right)
  plotPartial(pd, levelplot = FALSE, zlab = "cmedv", drape = TRUE,
              colorkey = TRUE, screen = list(z = -20, x = -60)),
  ncol = 3
)
```

Note: the default color map for level plots is the color blind-friendly matplotlib (Hunter, 2007) 'viridis' color map provided by the **viridis** package (Garnier, 2016).
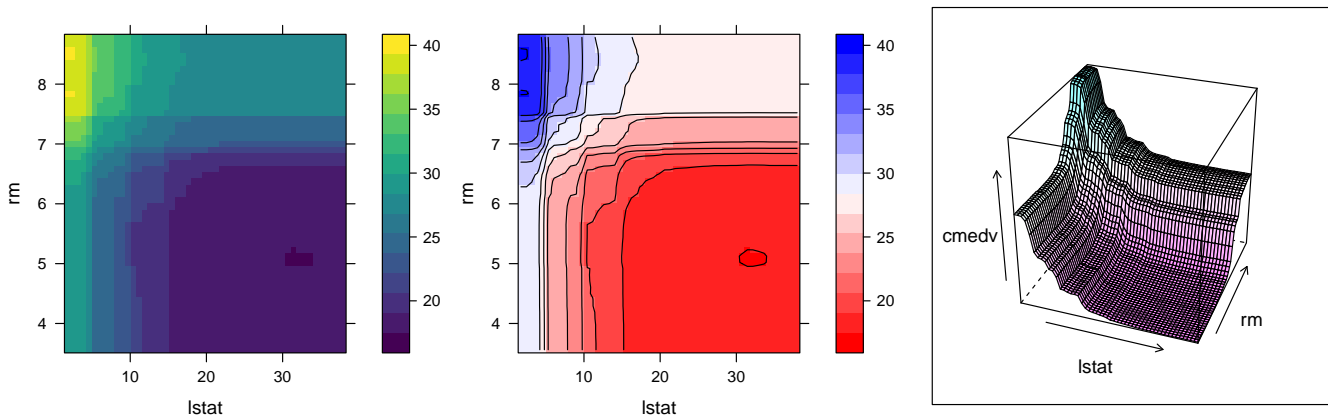
Figure 3: Partial dependence of `cmedv` on `lstat` and `rm` based on a random forest. *Left*: Default plot. *Middle*: With contour lines and a different color palette. *Right*: Using a 3-D surface.

Avoiding extrapolation

It is not wise to draw conclusions from PDPs in regions outside the area of the training data. Here we describe two ways to mitigate the risk of extrapolation in PDPs: rug displays and convex hulls. Rug displays are one-dimensional plots added to the axes. Both `partial` and `plotPartial` have a `rug` option that, when set to `TRUE`, will display the deciles of the distribution (as well as the minimum and maximum values) for the predictors on the horizontal and vertical axes. The following snippet of code produces the left display in Figure 4.

```
# Figure 4 (left)
partial(boston.rf, pred.var = "lstat", plot = TRUE, rug = TRUE)
```

In two or more dimensions, plotting the convex hull is more informative; it outlines the region of the predictor space that the model was trained on. When `chull = TRUE`, the convex hull of the first two dimensions of z_s (i.e., the first two variables supplied to `pred.var`) is computed; for example, if you set `chull = TRUE` in the call to `partial` only the region within the convex hull of the first two variables is plotted. Over interpreting the PDP outside of this region is considered extrapolation and is ill-advised. The right display in Figure 4 was produced using:

```
# Figure 4 (right)
partial(boston.rf, pred.var = c("lstat", "rm"), plot = TRUE, chull = TRUE)
```

Addressing computational concerns

Constructing PDPs can be quite computationally expensive. Several strategies are available to ease the computational burden in larger problems. For example, there is no need to compute partial dependence of `cmedv` using each unique value of `rm` in the training data (which would require $k = 446$ passes over the data!). We could get very reasonable results using a reduced number of points. Current options are to use a grid of equally spaced values in the range of the variable of interest; the number of points can be controlled using the `grid.resolution` option in the call to `partial`. Alternatively, a user-specified grid of values (e.g., containing specific quantiles of interest) can be supplied through the `pred.grid` argument. To demonstrate, the following snippet of code computes the partial dependence of `cmedv` on `rm` using each option, then uses `grid.arrange` to display all three PDPs on the same page; the results are displayed in Figure 5.
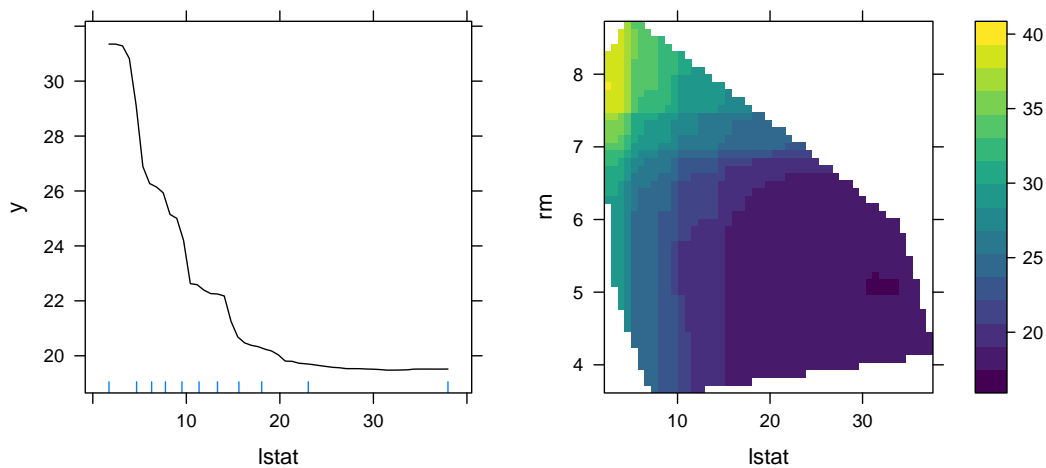
Figure 4: Examples of PDPs with the addition of a rug display (left) and a convex hull (right).

```
grid.arrange(
  # Figure 5 (left)
  partial(boston.rf, "rm", plot = TRUE),
  # Figure 5 (middle)
  partial(boston.rf, "rm", grid.resolution = 30, plot = TRUE),
  # Figure 5 (right)
  partial(boston.rf, "rm", pred.grid = data.frame(rm = 3:9), plot = TRUE),
  ncol = 3
)
```
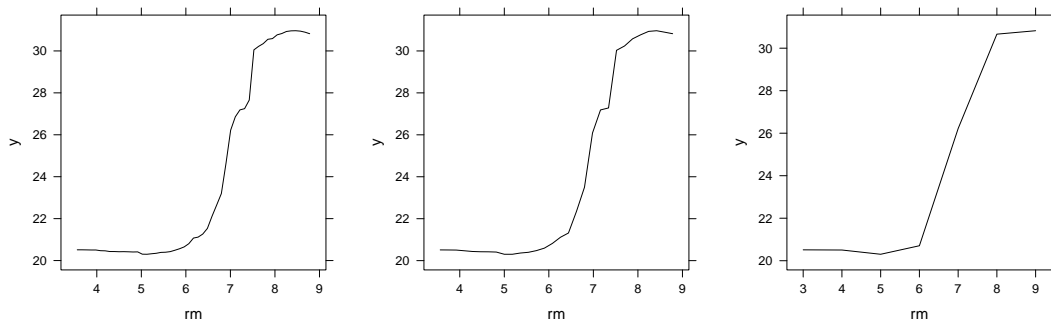

Figure 5: Partial dependence of cmedv on rm. *Left*: Default plot. *Middle*: Using a reduced grid size. *Right*: Using a user-specified grid.

The partial function relies on the **plyr** package (Wickham, 2011), rather than R's built-in for loops. This makes it easy to request progress bars (e.g., progress = "text") or run partial in parallel. In fact, partial can use any of the parallel backends supported by the **foreach** package. To use this functionality, we must first load and register a supported parallel backend [e.g., **doMC** (Analytics and Weston, 2015a) or **doParallel** (Analytics and Weston, 2015b)].

To illustrate, we will use the Los Angeles ozone pollution data described in Breiman and Friedman (1985). The data contain daily measurements of ozone concentration (ozone) along with eight meteorological quantities for 330 days in the Los Angeles basin in 1976. The data are available from http://statweb.stanford.edu/~tibs/ElemStatLearn/datasets/LAozone.data. Details, including variable information, are available from http://statweb.stanford.edu/~tibs/ElemStatLearn/datasets/LAozone.info. The following code chunk loads the data into R:

```
ozone <- read.csv(paste0("http://statweb.stanford.edu/~tibs/ElemStatLearn/",
                         "datasets/LAozone.data"), header = TRUE)
```

Next, we use the multivariate adaptive regression splines (MARS) algorithm introduced in Friedman (1991) to model ozone concentration as a nonlinear function of the eight meteorological variables

plus day of the year; we allow for up to three-way interactions.

```
ozone.mars <- earth(ozone ~ ., data = ozone, degree = 3)
summary(ozone.mars)
```

The MARS model produced a generalized R^2 of 0.79, similar to what was reported in Breiman and Friedman (1985). A single three-way interaction was found involving the predictors

- wind: wind speed (mph) at Los Angeles International Airport (LAX)
- temp: temperature (^oF) at Sandburg Air Force Base
- dpg: the pressure gradient (mm Hg) from LAX to Dagget, CA

To understand this interaction, we can use a PDP. However, since the partial dependence between three continuous variables can be computationally expensive, we will run partial in parallel.

Setting up a parallel backend is rather straightforward. To demonstrate, the following snippet of code sets up the partial function to run in parallel on both Windows and Unix-like systems using the **doParallel** package.

```
library(doParallel)  # load the parallel backend
cl <- makeCluster(4)  # use 4 workers
registerDoParallel(cl)  # register the parallel backend
```

Now, to run partial in parallel, all we have to do is invoke the parallel = TRUE and paropts options and the rest is taken care of by the internal call to **plyr** and the parallel backend we loaded[2]. This is illustrated in the code chunk below which obtains the partial dependence of ozone on wind, temp, and dpg in parallel. The last three lines of code simply add a label to the colorkey. The result is displayed in Figure 6. **Note:** it is considered good practice to shut down the workers by calling stopCluster when finished.

```
partial(ozone.mars, pred.var = c("wind", "temp", "dpg"), plot = TRUE,
        chull = TRUE, parallel = TRUE, paropts = list(.packages = "earth"))  # Figure 6
stopCluster(cl)  # good practice

# Add a label to the colorkey
lattice::trellis.focus("legend", side = "right", clipp.off = TRUE, highlight = FALSE)
grid::grid.text("ozone", x = 0.2, y = 1.05, hjust = 0.5, vjust = 1)
lattice::trellis.unfocus()
```
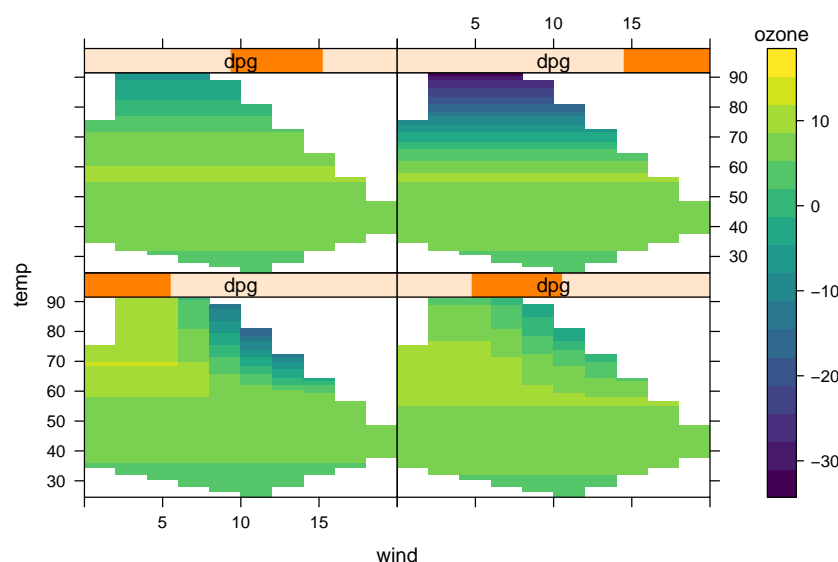

Figure 6: Partial dependence of ozone on wind, temp, and dpg. Since dpg is contiuous, it is first converted to a shingle; in this case, four groups with 10% overlap.

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[2]Notice we have to pass the names of external packages that the tasks depend on via the paropts argument; in this case, "earth". See ?plyr::adply for details.

It is important to note that when using more than two predictor variables, `plotPartial` produces a trellis display. The first two variables given to `pred.var` are used for the horizontal and vertical axes, and additional variables define the panels. If the panel variables are continuous, then shingles[3] are produced first using the equal count algorithm (see, for example, `?lattice::equal.count`). Hence, it will be more effective to use categorical variables to define the panels in higher dimensional displays when possible.

Classification problems

For classification problems, partial dependence functions are on a scale similar to the logit; see, for example, Hastie et al. (2009, pp. 369—370). Suppose the response is categorical with K levels, then for each class we compute

$$f_k(x) = \log\left[p_k(x)\right] - \frac{1}{K}\sum_{k=1}^{K}\log\left[p_k(x)\right], \quad k = 1, 2, \dots, K, \tag{4}$$

where $p_k(x)$ is the predicted probability for the k-th class. Plotting $f_k(x)$ helps us understand how the log-odds for the k-th class depends on different subsets of the predictor variables.

To illustrate, we consider Edgar Anderson's iris data from the **datasets** package. The `iris` data frame contains the sepal length, sepal width, petal length, and petal width (in centimeters) for 50 flowers from each of three species of iris: setosa, versicolor, and virginica. We fit a support vector machine with a Gaussian radial basis function kernel to the data using the `svm` function in the **e1071** package (the tuning parameters were determined using 5-fold cross-validation).

```
library(e1071)
iris.svm <- svm(Species ~ ., data = iris, kernel = "radial", gamma = 0.75,
                cost = 0.25, probability = TRUE)
```

Note: the `partial` function has to be able to extract the predicted probabilities for each class, so it is necessary to set `probability = TRUE` in the call to `svm`.

Next, we plot the partial dependence of `Species` on both `Petal.Width` and `Petal.Length` for each of the three classes. The result is displayed in Figure 7.

```
pd <- NULL
for (i in 1:3) {
  tmp <- partial(iris.svm, pred.var = c("Petal.Width", "Petal.Length"),
                 which.class = i, grid.resolution = 101, progress = "text")
  pd <- rbind(pd, cbind(tmp, Species = levels(iris$Species)[i]))
}

# Figure 7
library(ggplot2)
ggplot(pd, aes(x = Petal.Width, y = Petal.Length, z = y, fill = y)) +
  geom_tile() +
  geom_contour(color = "white", alpha = 0.5) +
  scale_fill_distiller(name = "Logit", palette = "Spectral") +
  theme_bw() +
  facet_grid(~ Species)
```

Using partial with the XGBoost library

To round out our discussion, we provide one last example using a recently popular (and successful!) machine learning tool. XGBoost, short for eXtreme Gradient Boosting, is a popular library providing optimized distributed gradient boosting that is specifically designed to be highly efficient, flexible and portable. The associated R package **xgboost** has been used to win a number of Kaggle competitions. It has been shown to be many times faster than the well-known **gbm** package. However, unlike **gbm**, **xgboost** does not have built-in functions for constructing PDPs. Fortunately, the **pdp** package can be used to fill this gap.

For illustration, we return to the Boston housing data. The code chunk below uses **caret** to train an XGBoost model to the `boston` data frame from Section 2.2 over a grid of tuning values (see

---

[3]A shingle is a special Trellis data structure that consists of a numeric vector along with intervals that define the "levels" of the shingle. The intervals may be allowed to overlap.
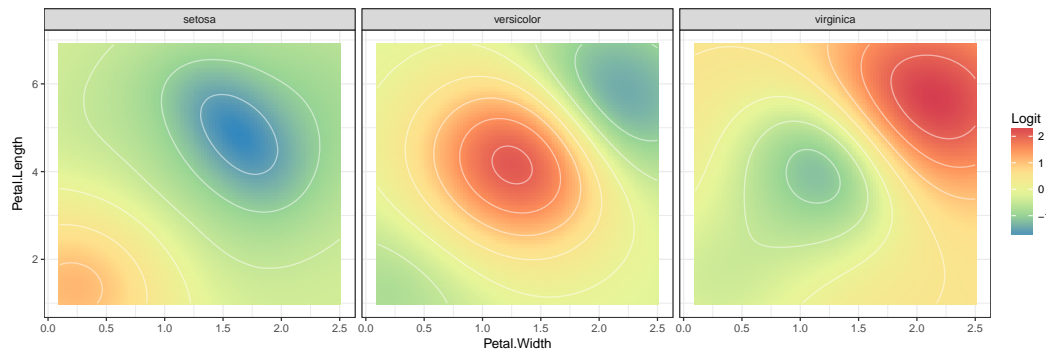
Figure 7: Partial dependence of species on petal width and petal length for the iris data.

?xgboost::xgboost for an explanation of the various tuning parameters). The optimal combination of tuning parameter values is selected via 5-fold cross-validation.

```
library(caret)

# Setup for 5-fold cross-validation
ctrl <- trainControl(method = "cv", number = 5, verboseIter = TRUE)

# Grid of tuning values for XGBoost.
xgb.grid <- expand.grid(nrounds = c(100, 500, 1000, 2000, 5000),
                        max_depth = 1:6,
                        eta = c(0.001, 0.01, 0.1, 0.5, 1),
                        gamma = 0,
                        colsample_bytree = 1,
                        min_child_weight = 1)

# Train an XGBoost model
set.seed(202)
boston.xgb <- train(x = data.matrix(subset(boston, select = -cmedv)),
                    y = boston$cmedv,
                    method = "xgbTree",
                    metric = "RMSE",
                    trControl = ctrl,
                    tuneGrid = xgb.grid)
```

The model with the smallest root-mean-squared error (RMSE) had nrounds = 2000, max_depth = 3, eta = 0.01, and achieved a cross-validated RMSE and R^2 of 2.819 and 0.905, respectively. The following snippet of code computes the partial dependence of cmedv on both rm and lstat, individually and together, and then uses grid.arrange to display all three PDPs on the same page. The results are displayed in Figure 8.

```
grid.arrange(
  # Figure 8 (left)
  partial(boston.xgb, pred.var = "rm", plot = TRUE, rug = TRUE),
  # Figure 8 (middle)
  partial(boston.xgb, pred.var = "lstat", plot = TRUE, rug = TRUE),
  # Figure 8 (right)
  partial(boston.xgb, pred.var = c("lstat", "rm"), plot = TRUE, chull = TRUE),
  ncol = 3
)
```

Since train always stores a copy of the training data as part of the "train" object in a component called trainingData (e.g., boston.xgb.tune$trainingData) there is no need to supply the training data in the call to partial. However, this is not the case when using the **xgboost** package directly. For example, the following code fits the same model using the xgboost function.

```
set.seed(203)  # for reproducibility
boston.xgb <- xgboost(data = data.matrix(subset(boston, select = -cmedv)),
                      label = boston$cmedv, objective = "reg:linear",
                      nrounds = 2000, max_depth = 3, eta = 0.01)
```
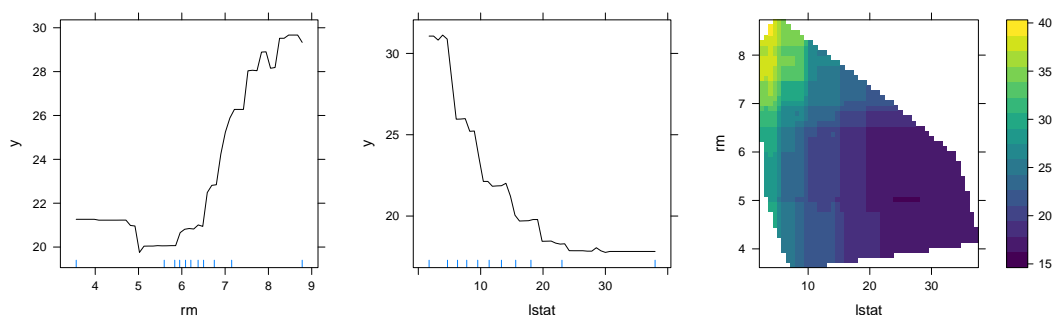
Figure 8: PDPs for the top two most important variables in the Boston housing data using XGBoost. Compare this to the random forest results displayed in Figures 4-5.

To use `partial` with the `"xgb.Booster"` class, we need to supply the original training data (minus the response) in the call to `partial`. The following snippet of code computes the partial dependence of cmedv on rm (plot not shown). (Make sure you are using version 0.6-0 or later of **xgboost**: https://github.com/dmlc/xgboost/tree/master/R-package.) **Note:** while xgboost requires the training data to be an object of class `"matrix"`, `"dgCMatrix"`, or `"xgb.DMatrix"`, `partial` requires a `"data.frame"`.

```
partial(boston.xgb, pred.var = "rm", plot = TRUE, rug = TRUE,
        train = subset(boston, select = -cmedv))
```

Summary

PDPs can be used to graphically examine the dependence of the response on low cardinality subsets of the features, accounting for the average effect of the other predictors. In this paper, we showed how to construct PDPs for various types of black box models in R using the **pdp** package. We also briefly discussed related approaches available in other R packages. Suggestions to avoid extrapolation and high execution times were discussed and demonstrated via examples.

In terms of future development, **pdp** can be expanded in a number of ways. For example, it would be useful to have the ability to construct PDPs for black box survival models—like conditional random forests with censored response. It would also be worthwhile to implement the partial dependence-based *H*-statistic (Friedman and Popescu, 2008) for assessing the strength of interaction between predictors.

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TBD.

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