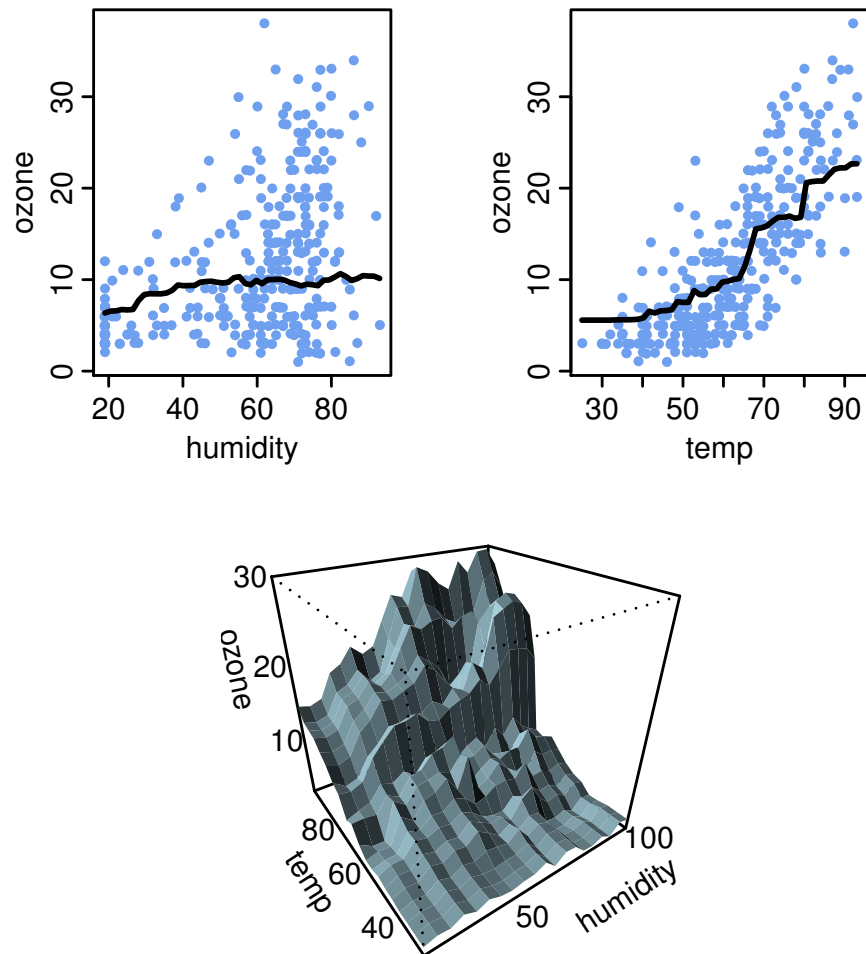


## Plotting regression surfaces with plotmo



Stephen Milborrow

May 31, 2018

# Contents

<b>1</b>	<b>Introduction</b>	<b>2</b>
<b>2</b>	<b>Examples</b>	<b>2</b>
<b>3</b>	<b>Limitations</b>	<b>4</b>
3.1	Inherent limitations . . . . .	4
3.2	Practical limitations . . . . .	5
<b>4</b>	<b>Alternatives to plotmo</b>	<b>6</b>
<b>5</b>	<b>Some details</b>	<b>7</b>
5.1	Page layout . . . . .	7
5.2	The <code>type</code> and <code>nresponse</code> arguments . . . . .	7
5.3	Background variables . . . . .	7
5.4	The <code>ylim</code> and <code>clip</code> arguments . . . . .	8
<b>6</b>	<b>Which variables get plotted?</b>	<b>9</b>
<b>7</b>	<b>Notes on miscellaneous packages</b>	<b>10</b>
7.1	The MASS package and <code>lda</code> and <code>qda</code> . . . . .	11
7.2	The <code>mlr</code> package . . . . .	12
<b>8</b>	<b>Classification models</b>	<b>13</b>
8.1	Multinomial models . . . . .	15
<b>9</b>	<b>Partial-dependence plots (the <code>pmethod</code> argument)</b>	<b>16</b>
9.1	An example . . . . .	16
9.2	Approximate partial-dependence plots . . . . .	17
9.3	Transforming the response for partial dependencies . . . . .	17
<b>10</b>	<b>Prediction intervals (the <code>level</code> argument)</b>	<b>19</b>
<b>11</b>	<b>FAQ</b>	<b>21</b>
<b>12</b>	<b>Common error messages</b>	<b>23</b>
<b>13</b>	<b>Accessing the model data</b>	<b>24</b>
13.1	Method functions . . . . .	24
13.2	Environment for the model data . . . . .	25

# 1 Introduction

The `plotmo` function in the `plotmo` R package [17] makes it easy to plot regression surfaces for a model. These plots can be useful for understanding the model.

The plots on the title page of this document are examples—those plots are for a random forest, but `plotmo` can be used on a wide variety of R models.

`Plotmo` automatically creates a separate plot for each variable in the model. Each such *degree1* plot is generated by plotting the predicted response as the variable changes. The top two plots on the title page are examples. The variables that don't appear in a plot are the *background* variables (or simply the “other” variables). In each plot the background variables are held fixed at their median values (the medians are calculated from the training data).

`Plotmo` can also show interactions between pairs of variables. A *degree2* plot is generated by plotting the predicted response as two variables are changed (once again with all other variables held at their median values). The bottom plot on the title page is an example.

`Plotmo` invokes `predict` internally to generate the predicted response. Which specific `predict` method gets invoked is determined by the model's class — thus for say a `randomForest` model, `predict.randomForest` is invoked.

`Plotmo` also supports partial dependence plots (Section 9), as an alternative to its default method of plotting which simply holds the background variables at their medians.

## 2 Examples

Here are some examples which illustrate `plotmo` on various models. Figure 1 shows the resulting plots.

```
# use a small set of variables for illustration
library(earth) # for ozone1 data
data(ozone1)
oz <- ozone1[, c("O3", "humidity", "temp", "ibt")]

lm.mod <- lm(O3 ~ humidity + temp*ibt, data=oz)          ## linear model
plotmo(lm.mod)

library(rpart)                                          ## rpart
rpart.mod <- rpart(O3 ~ ., data=oz)
plotmo(rpart.mod)

library(randomForest)                                  ## randomForest
rf.mod <- randomForest(O3 ~ ., data=oz)
plotmo(rf.mod)
# partialPlot(rf.mod, oz, temp)          # compare to partial dependence plot
```

```

library(gbm)                                     ## gbm
gbm.mod <- gbm(O3 ~ ., data=oz, dist="gaussian", inter=2, n.trees=1000)
plotmo(gbm.mod)
# plot(gbm.mod, i.var=2)                         # compare to partial-dependence plots
# plot(gbm.mod, i.var=c(2,3))

library(gam)                                     ## gam
gam.mod <- gam(O3 ~ s(humidity) + s(temp) + s(ibt), data=oz)
plotmo(gam.mod, all2=TRUE)                       # all2=TRUE to show interaction plots

library(nnet)                                     ## nnet
set.seed(4)
nnet.mod <- nnet(O3 ~ ., data=scale(oz), size=2, decay=0.01, trace=FALSE)
plotmo(nnet.mod, type="raw", all2=T)             # type="raw" gets passed to predict

```

This is by no means an exhaustive list of models supported by plotmo. The packages used in the above code are [9, 11, 20, 21, 23].

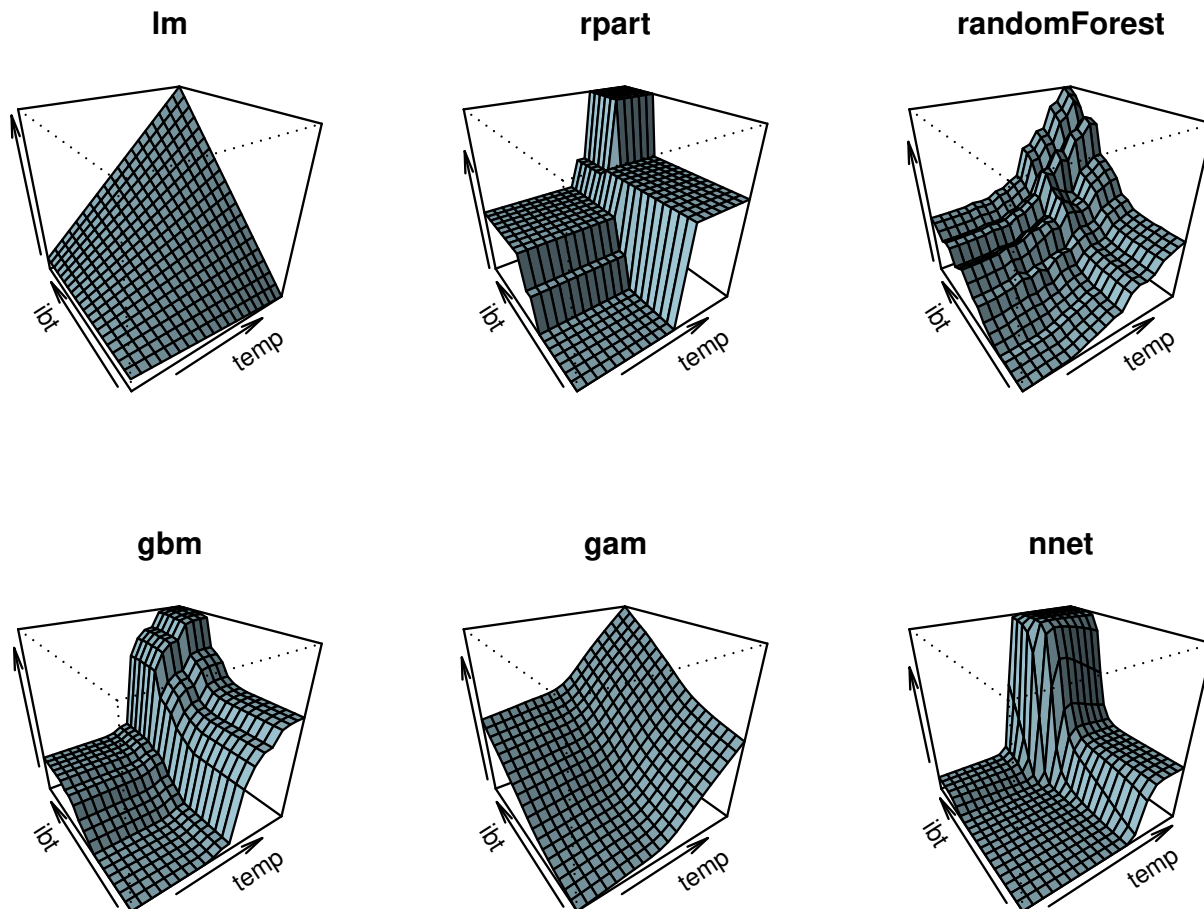


Figure 1: *Plotmo graphs on various models, generated by the code in the text.*

A single degree2 plot for each model is illustrated here, but by default plotmo displays a set of plots on the same page for each model. See Section 6 “Which variables get plotted?”.

## 3 Limitations

There are inherent limitations because the plots give only a partial view of the model. There are also practical limitations to do with the way some models are built in R. This section discusses these limitations in turn.

### 3.1 Inherent limitations

The plots can give only a partial view of the model. Each plot shows only a thin slice<sup>1</sup> of the data with the background variables pegged at fixed values.

For example, in Figure 2 the response curve as  $x_1$  varies depends greatly on the value of the other variable  $x_2$ . Compare the response curve when  $x_2$  is at 15 (say) to the curve when  $x_2$  is pegged at its median 72. Please be aware of this loss of information when interpreting the graphs. Over-interpretation is a temptation.

Similar issues arise for partial-dependence plots, although harder to illustrate.

For a one variable model the regression surface is fully described by a degree1 plot, and for a two variable model by a degree2 plot. For additive models (no variable interactions), the regression surface is fully described by the set of degree1 plots.

More generally, models with many variables must be viewed in a piecemeal fashion by looking at the action of one or two predictors at a time. The plots are most informative when the variables being plotted do not have strong interactions with the other variables. Chapter 10 in the [vignette for the rpart.plot package](#) has a short discussion on these topics.

---

<sup>1</sup>Each plot is a lower-dimensional “slice” through a higher-dimensional space, like a slice of bread is a 2D plane through a 3D loaf. The slice doesn’t tell you what’s going on at the other end of the loaf.

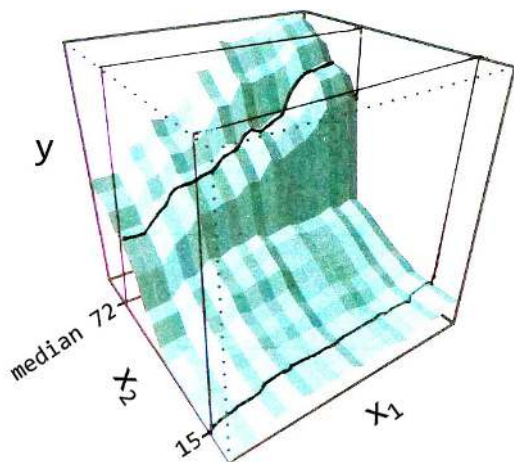


Figure 2: *The shape of the response curve as  $x_1$  varies is quite different for slices at different values of  $x_2$ .*

*This image illustrates 2D slices through a 3D space. With a typical multivariate model the plotmo slices are through a much higher-dimensional space.*

## 3.2 Practical limitations

There are practical limitations to do with the way some models are built in R.

Plotmo needs to access the data used when building the model, so it can formulate new data to pass to `predict`. For some models this isn't possible. Some models don't save the `call` or any references to the original data. For details see Section 13 “Accessing the model data”.

For the model to work with plotmo, it's best to keep the variable names and formula in the original call to the model-building function simple. Use temporary variables or `attach` rather than using `$` and similar in formulas. Error messages may be issued if there are NAs in the data (it depends on the model). For more details see Section 12 “Common error messages”.

## 4 Alternatives to plotmo

There are many ways of condensing a multi-dimensional model onto the two dimensions of a page. The technique used by plotmo is one of them. There is no silver bullet; large amounts of information are necessarily discarded when the complexities of a model must be plotted on a page.

Arguably the most important plot, although often overlooked, is the humble *residuals-vs-fitted* plot. The `plotres` function (also in the `plotmo` package) is an easy way to make various residual plots for “any” model. See the [plotres vignette](#). Sometimes it’s also worthwhile plotting the residuals against the variables or the model basis functions.

The `termplot` function in the standard `stats` package can be helpful, but it’s supported by only a few models (the `predict` method for the model must support `type="terms"`), and it doesn’t generate degree2 plots.

**Partial dependence plots** are a well-known technique for plotting regression surfaces. (See e.g. Hastie et al. [8] Section 10.13.2. To my knowledge, partial-dependence plots were first described in Friedman’s gradient boosting paper [5].) Plotmo sets the background variables to their median values, whereas in a partial-dependence plot at each plotted point the effect of the background variables is averaged. Computing this can take a long time. But for decision trees the effect of averaging can be determined without actual brute force summation, so partial-dependence plots for random forests and `gbm`’s can be generated quite quickly.

In general, partial-dependence plots and plotmo plots will differ, but for additive models (no interaction terms) the *shape* of the curves is identical although the scale may differ. Partial-dependence plots incorporate more overall information than plotmo plots, but it’s easier to understand in principle what the graph *doesn’t* show with plotmo than with partial-dependence plots (Section 3.1 “Inherent limitations”).

The `randomForest` and `gbm` packages have functions for generating partial-dependence plots for their respective models. The `pdp` [7] package, similar in spirit to plotmo, offers partial dependence plots for a variety of models

**Note added Nov 2016:** Plotmo now supports partial-dependence plots (Section 9).

Some other possibilities for plotting the response on a per-predictor basis are partial-residual plots, partial-regression variable plots, and marginal-model plots (e.g. `crPlots`, `avPlots`, and `marginalModelPlot` in the `car` package [2]). The `effects` package is also of interest [3]. These packages are orientated towards linear and parametric models, whereas plotmo is mainly for non-parametric models.

Quite a few methods have been invented specifically for random forests. Although each tree in the forest is easy to interpret (a white box), the interaction between the large number of trees in a random forest makes the model as a whole a black box. Techniques such as plotmo thus become useful. See also the discussion on the CrossValidated web page [Obtaining-knowledge-from-a-random-forest](#).

## 5 Some details

This section covers a few details that are useful to know when using plotmo.

### 5.1 Page layout

Plotmo puts all the plots on a single page. That can be overridden with the `do.par` argument.

Plotmo has special knowledge of some kinds of model. It uses that knowledge to plot only important plots, to limit crowding on the page. For example, for `earth` models it plots only the variables that are used in the final model, and for `randomForest` models it plots only the most important variables. We can also explicitly specify which variables get plotted by passing arguments to plotmo. For details see Section 6 “Which variables get plotted?”.

### 5.2 The type and nresponse arguments

Some models can make different kinds of predictions. For example, for classification models we can typically predict a response class or predict a probability. When calling `predict` internally, by default plotmo tries to automatically select a suitable response type for the model (often `type="response"`; use `trace=1` to see what plotmo uses). Explicitly tell plotmo what kind of prediction to plot using plotmo’s `type` argument. This gets passed internally to `predict`.

The `predict` function for some models returns a *matrix* rather than a vector of predicted values. For example, the `predict` function may return a two column matrix showing `absent` and `present` probabilities. By default, plotmo tries to automatically select which of these columns to display. Explicitly specify which column to use with plotmo’s `ncolumn` argument, which can be a column number or column name if columns are named.

Section 8 “Plotting classification models” gives some examples of using the `type` and `nresponse` arguments.

Plotmo tries to use sensible default arguments for `predict`, but they won’t always be correct (plotmo can’t know about the `predict` method for every kind of model). Change the defaults if necessary using plotmo arguments with a `predict.` prefix. Plotmo passes any argument prefixed with `predict.` directly to `predict`, after removing the prefix. The [plotres vignette](#) has an example.

### 5.3 Background variables

As mentioned in the introduction, plotmo holds the background variables at their medians. But if a background variable is a factor, then the first level is used instead of the median.



Change what values are used for the background variables with the `grid.func` and `grid.levels` arguments. For example

```
grid.func = mean
```

or

```
grid.levels = list(sex="male", age=21)
```

Use these arguments in a for loop to make a grid of plots conditioned on background variable values.

## 5.4 The `ylim` and `clip` arguments

Plotmo determines `ylim` (the vertical range) for the graphs automatically. If the automatic `ylim` isn't correct for the model, specify `ylim` when invoking plotmo.

Here are some details. Typically we want all plots on a page to have the same `ylim` (the same vertical axis limits), so we can see the effect of each variable relative to the other variables. The range of predicted values over all the plots is the obvious way for plotmo to automatically set `ylim`. However, a few wild predictions can make this range very wide, and reduce resolution over all graphs. Therefore when determining the range, plotmo ignores outlying predictions (unless `clip=FALSE`). Predictions that are more than 50% beyond the range of the observed response are considered outlying. In practice such outlying predictions seem quite rare.

## 6 Which variables get plotted?

The default set of variables plotted for some common models is listed below [11, 18, 20–22].

The default set of plots for the model may leave out some variables that we would like to see. In that case, use `all1=TRUE` and/or `all2=TRUE`.

To limit the set of displayed variables use the `degree1` and `degree2` arguments. Sometimes it's useful to use all those arguments: first expand the set with `all1` and `all2`, then trim that back with `degree1` and `degree2`.

- **earth**

- `degree1` variables in additive (non interaction) terms

- `degree2` variables appearing together in interaction terms

- **rpart**

- `degree1` variables used in the tree

- `degree2` variables which appear in parent-child pairs in the tree

- **randomForest**

- A  $4 \times 4$  grid of plots (or less if fewer variables) as follows:

- `degree1` The ten most important variables.

- How importance is measured depends on whether model was built with `importance=TRUE`, and whether the model is a regression or classification model. Use `trace=1` in the call to `plotmo` to see which measure of importance is used.

- `degree2` Pairs of the four most important variables (thus six `degree2` plots).

- **gbm**

- A  $4 \times 4$  grid of plots (or less if fewer variables) as follows:

- `degree1` The ten most important variables (measured by `relative.influence`).

- Variables with `relative.influence < 1%` are ignored.

- `degree2` Pairs of the four variables with the largest importance (thus six `degree2` plots)

- **lm, glm, gam, lda, etc.**

- These are processed using `plotmo`'s default methods (Section 13):

- `degree1` all variables

- `degree2` variables in the formula associated with each other by terms like `x1 * x2`, `x1:x2`, and `s(x1,x2)`

## 7 Notes on miscellaneous packages

This section gives some specifics on how `plotmo` and `plotres` handle some miscellaneous models [4, 6, 10, 12, 13, 19–22, 26].

By default, `predict.gbm` is called with `n.trees = object$n.trees`

By default, `predict.glmnet` is called with `type="response"` and `s = 0`. Change that by passing say `predict.s=.02` to `plotmo` or `plotres`.

By default, `predict.quantregForest` is called with `quantiles = .5`

By default, `predict.cosso` is called with `M = min(ncol(newdata), 2)`

By default, `predict.svm` (e1071 package) is called with `decision.values` and `probability` set to `FALSE`, but as usual we can change that by passing those arguments to `plotmo` with a `predict.` prefix, and `plotmo` will use those values if specified.

For `rpart` models, `plotres` uses the `rpart.plot` package [14] if it's available, else it uses the plotting routines built into the `rpart` package.

For models built with the `adabag` package, `plotmo`'s `type` argument should be `"votes"`, `"prob"` (default), or `"class"` to select the corresponding field in `predict.boosting`'s returned value. `Plotmo`'s `nresponse` argument will typically also be necessary to select a column in the matrix of predicted values.

The `predict` methods for `rq` and `rqs` models (`quantreg` package) return multiple columns, and `plotmo` chooses the column corresponding to `tau=0.5`. `Plotmo` will plot prediction intervals if the `quantreg` model is built with say `tau=c(.05, .5, .95)` and `plotmo` is called with the corresponding `level` argument, in this case `level=0.90`.

The `neuralnet` package doesn't provide a `predict` method, but `plotmo` provides one internally:

```
predict.nn(object, newdata=NULL, rep="mean", trace=FALSE)
```

where `rep` can be an integer, `"best"`, or `"mean"` (default). These last two are equivalent if the model was built with `nrep=1`. Examples:

```
plotres(nn.model, predict.rep="mean") # resids for mean prediction over all reps
plotres(nn.model)                    # same
plotres(nn.model, predict.rep="best") # resids for prediction from best rep
```

For `biglm` objects, only the residuals from the first call to `biglm` are plotted by `plotres` (the residuals for subsequent calls to `update` aren't plotted).

For `C5.0` models (from the `C50` package), variable selection works as in `gbm` models (page 9) but with relative importance measured using `C5imp`.

## 7.1 The MASS package and lda and qda

The predict methods for lda and qda models (MASS package) are extended internally within plotmo to take a `type` argument. This can be one of "class" (default), "posterior", or "response". This selects the "class", "posterior", or "x" field in the value returned by `predict.lda` and `predict.qda`. Use the `nresponse` argument to select a column within the selected field. Example (Figure 3):

```
library(MASS)
lcush <- data.frame(Type=as.numeric(Cushings$Type), log(Cushings[,1:2]))[1:21,]
qda.mod <- qda(Type ~ ., data=lcush)

plotmo(qda.mod,                                # figure shown below
       all2=TRUE,                               # show all interact plots
       type2="image",                           # use image instead of persp for interact plot
       ngrid2=200,                              # increase resolution in image plot
       image.col=c("lightpink", "palegreen1", "lightblue"),
       pt.col=as.numeric(Cushings$Type)+1, pt.pch=as.character(Cushings$Type))

for(nresponse in 1:3)                          # not shown
  plotmo(qda.mod, type="post", nresponse=nresponse,
        all2=TRUE, persp.border=NA)
        persp.theta=30)                        # same theta for all plots so can compare
```

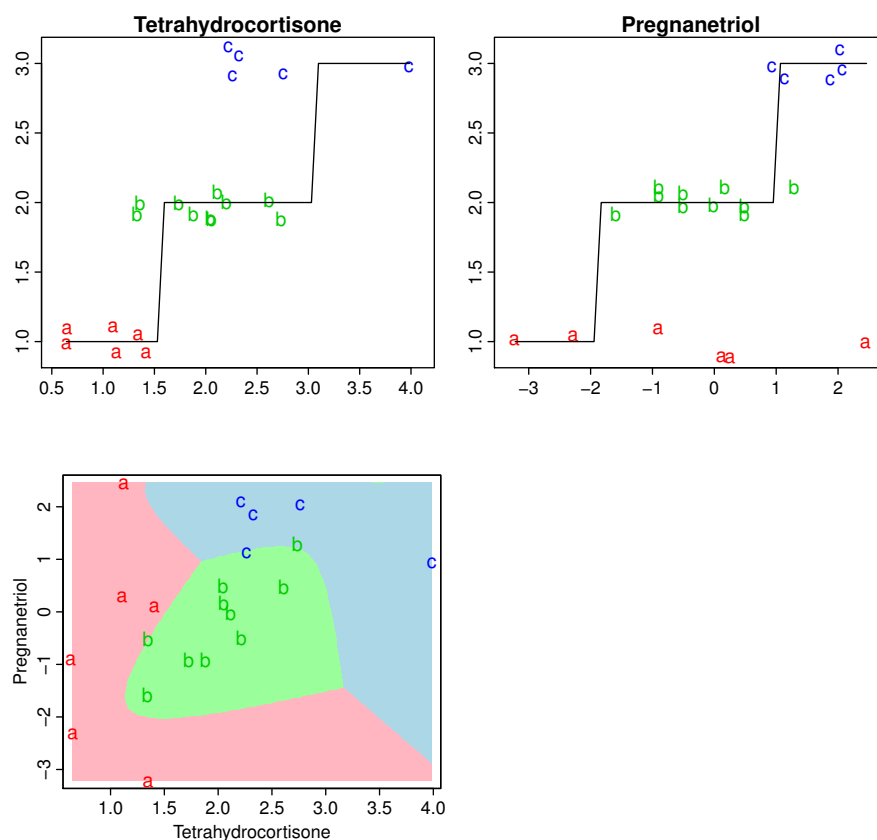


Figure 3: A qda model of the log Cushings data.

The background colors in the interaction plot show the predicted class.

The slightly messy look of the a,b,c labels in the top two plots is caused by plotmo's automatic jittering of factor labels (see the `jitter` argument).

## 7.2 The mlr package

Some examples with the `mlr` package are given below. For more examples, see the file `test.mlr.R` in the `slowtests` directory of the `plotmo` package.

Note that `plotmo` automatically plots all variables of interest, including interaction (degree2) plots. `Plotmo` can handle factor predictors—whereas with factor predictors the function `plotPartialDependence` in the `mlr` package (always?) fails with `Error: Discrete value supplied to continuous scale`.

Note that `plotmo` also works with the classic `caret` package, which has many of the same goals as `mlr`. The file `test.caret.R` has some examples.

```
#-- Regression model with mlr -----

library(mlr)
library(plotmo)
lrn <- makeLearner("regr.svm")
fit1 <- train(lrn, bh.task)

# generate partial dependence plots for all variables
plotmo(fit1$learner.model, pmethod="partdep")

# generate partial dependence plot for just "lstat"
plotmo(fit1$learner.model,
       degree1="lstat",           # what predictor(s) to plot
       degree2=0,                # no interaction plots
       pmethod="partdep",        # generate partial dependence plot
       pt.col=2, grid.col="gray") # optional bells and whistles

#-- Classification model with mlr -----
# For discussion on the arguments to plotmo for classification models,
# see Section 8 "Classification models".

lrn <- makeLearner("classif.rpart", predict.type="prob", minsplit=10)
fit2 <- train(lrn, iris.task)

# generate partial dependence plots for all variables
# (note that plotmo can plot the response for only one class at a time)
plotmo(fit2$learner.model,
       nresponse="virginica",    # what response to plot
       type="prob",              # type gets passed to predict.rpart
       pmethod="partdep")        # generate partial dependence plot

# generate partial dependence plot for just "Petal.Length"
plotmo(fit2$learner.model,
       degree1="Petal.Length",   # what predictor(s) to plot
       degree2=0,                # no interaction plots
       nresponse="virginica",    # what response to plot
       type="prob",              # type gets passed to predict.rpart
       pmethod="partdep")        # generate partial dependence plot
```

## 8 Classification models

This section discusses classification models, focusing on models with a two-class response (where the classes simply may be `TRUE` and `FALSE`). This section repeats information in other parts of this documents, but is geared towards users of classification models.

With classification models we often have to take care to set `plotmo`'s `type` and `nresponse` arguments appropriately (Section 5.2). The scale of the response plotted by `plotmo` is determined by the `type` argument and possibly other arguments for `predict`. (These get passed to `predict` via `plotmo`.) For example, for binomial `glm` models we can predict probabilities (`type="response"`, which can vary from 0 to 1) or log-odds (`type="link"`, which can vary from -infinity to +infinity, although in practice the response is restrained to a reasonable range).

For some models, the `predict` method returns multiple columns, and we need to select the appropriate column using `plotmo`'s `nresponse` argument. For example, when predicting probabilities for `randomForest` two-class models, `predict.randomForest` returns two columns. We must use `plotmo`'s `nresponse` argument to select the column for the class of interest. If we select the other column, the plotted curves will be upside down.

For some classification models, `plotmo` doesn't calculate `ylim` correctly. In that case, explicitly pass `ylim` to `plotmo`. We see that being done in the `svm` example below.

Here are some example models with a two-class response. We use a subset of the `iris` data for simplicity, and plot the probability of a `virginica` response. Figure 4 shows the plots. Optionally add `pmethod="partdep"` to the calls to `plotmo` below to generate partial-dependence instead of classical `plotmo` plots.

```
data(iris)
data <- data.frame(virginica = iris$Species == "virginica",
                  length    = iris$Sepal.Length,
                  width     = iris$Sepal.Width)

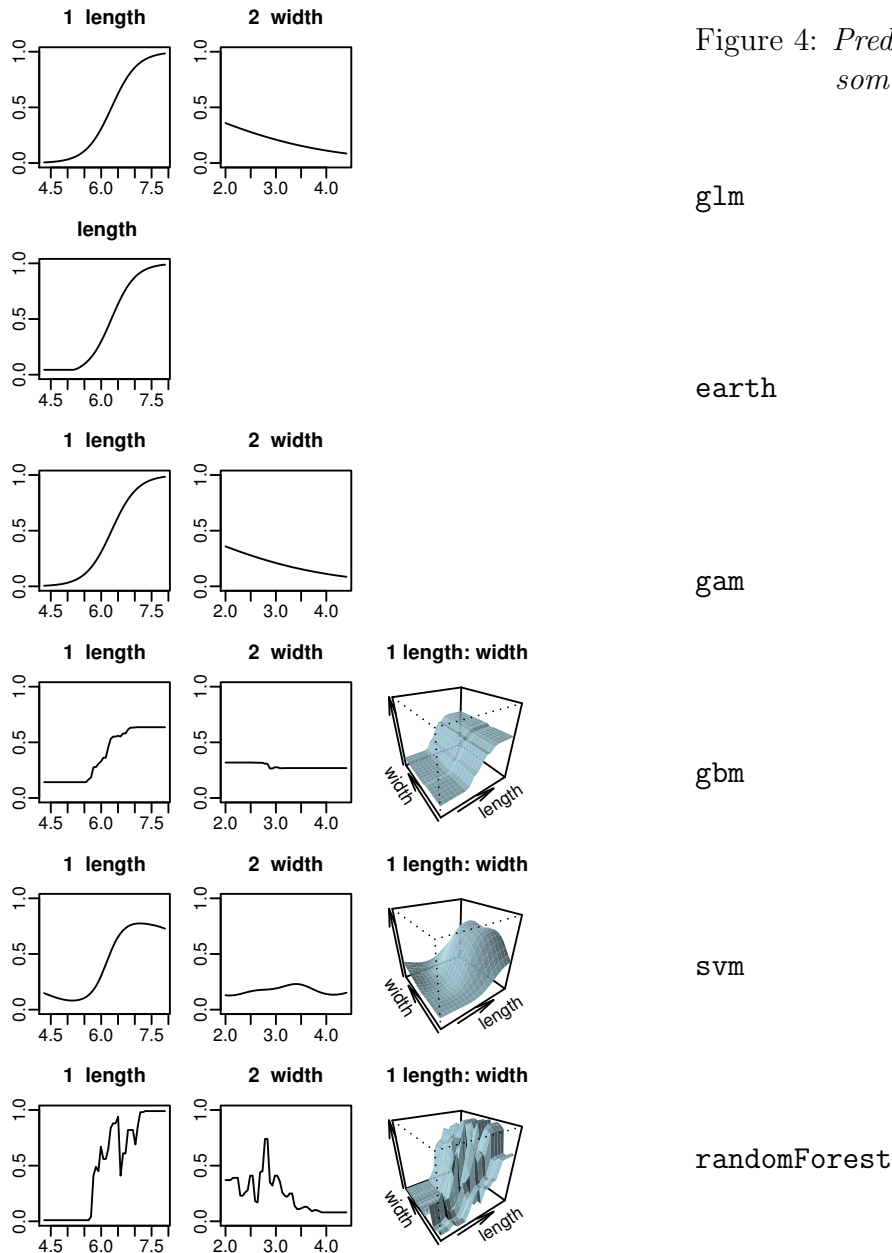
glm.mod <- glm(virginica~., data=data, family="binomial") ## glm
plotmo(glm.mod) # default type="response" returns probabilities

library(earth) ## earth
earth.mod <- earth(virginica~., data=data, degree=2, glm=list(family=binomial))
plotmo(earth.mod)

library(mgcv) ## mgcv gam
gam.mod <- gam(virginica~ s(length)+s(width), data=data, family=binomial())
plotmo(gam.mod)

library(gbm) ## gbm
gbm.mod <- gbm(virginica~., data=data, dist="bernoulli", inter=2, n.trees=1000)
plotmo(gbm.mod)
```

Figure 4: *Predicted probabilities for some two-class models.*



```
library(e1071) ## svm
data.fac <- data # svm requires a factor for classification (not a logical)
data.fac$virginica <- factor(ifelse(data$virginica,"yes","no"))
svm.mod <- svm(virginica~., data=data.fac, type="C-classification", probability=TRUE)
# plotmo knows how to handle predict.svm probability=TRUE
plotmo(svm.mod, predict.probability=TRUE, nresponse="yes", ylim=c(0,1))

library(randomForest) ## randomForest
data.fac <- data # randomForest requires a factor for classification (not a logical)
data.fac$virginica <- factor(ifelse(data$virginica,"yes","no"))
rf.mod <- randomForest(virginica~., data=data.fac, ntree=100)
plotmo(rf.mod, type="prob", nresponse="yes")
```

## 8.1 Multinomial models

For multinomial models we must plot the probabilities for each class one at a time. (Plotmo doesn't allow us to plot probability curves for more than one class on the same plot.) Typically we select the class of interest by using `nresponse` to select the appropriate column in the matrix returned by `predict`, but exactly how that works depends on the `predict` method for the model in question.



## 9 Partial-dependence plots (the pmethod argument)

By default `plotmo` fixes the background variables in each plot at their medians (or first level for factors). In contrast, in *partial-dependence* plots the effect of the background variables is averaged. We tell `plotmo` to generate partial-dependence plots by setting `plotmo`'s `pmethod` argument to `"partdep"`. Further discussion of partial-dependence plots can be found in Section 4 “Alternatives to `plotmo`”.

### 9.1 An example

This section demonstrates partial-dependence plots using artificial data with two variables `x1` and `x2` and a response `y`. The data is plotted on the left of Figure 5. There are large interactions between the variables.

The code to generate the data is:

```
f <- function(x1, x2) {  
  ifelse(x2 > .7, x1,                # big x2  
    ifelse(x2 > .4, 1 - x1,          # medium x2  
      .5 * sin(pi * x1))) # small x2  
}  
n <- 5000; x1 <- runif(n); x2 <- runif(n) # uniformly distributed  
data <- data.frame(x1=x1, x2=x2, y=f(x1, x2))
```

From this data we generate a random forest model (although any model could be used). We also generate a default `plotmo` plot and a partial-dependence plot:

```
library(randomForest)  
mod <- randomForest(y~., data=data)  
plotmo(mod) # middle figure, default plotmo plot  
plotmo(mod, pmethod="partdep") # right figure, partial-dependence plot
```

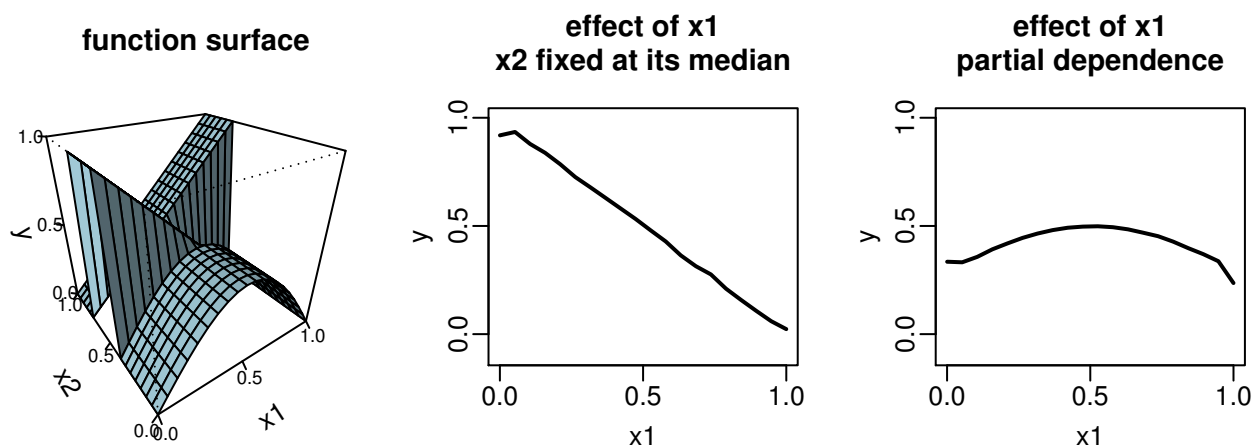


Figure 5:

- Left** A function surface showing strong interaction between `x1` and `x2`.
- Middle** A classical `plotmo` plot showing the predicted response varying as `x1` changes, with `x2` fixed at its median 0.5.
- Right** In a partial-dependence plot the effect of `x2` is averaged.

For simplicity we show results only for the `x1` variable (though the above code generates plots for the other variable too).

The middle figure is the default `plotmo` plot for `x1`. It shows the downward slope in the left figure when `x2` is at its median 0.5. In contrast, in the partial-dependence plot in the right figure the effects of downward and upward slopes cancel, leaving just the effect of the hump at low values of `x2`. (The small kinks at the extremes of the plotted curves are artifacts of the way the random forest handles the borders of the distribution.)

## 9.2 Approximate partial-dependence plots

Calculating partial dependencies can be slow. At each point in the plot we have to make `n` predictions (where `n` is the number of cases in the training data), and then average these predictions. For certain models there are techniques to calculate the plots quickly, but `plotmo` currently doesn't avail itself of these techniques. To increase speed, `plotmo` reduces the number of repeated internal calls to `predict` by accumulating data for each call. This may require quite a lot of temporary memory.

`Plotmo` can also plot *approximate* partial-dependence plots<sup>2</sup> (`pmethod="apartdep"`). These are like partial-dependence plots but the background variables are averaged over a subset of cases, rather than all cases in the training data. Approximate plots are much faster for large datasets. The plots are usually similar to standard partial-dependence plots, but guarantees can't be made.

How do we choose the subset of cases? We must select cases that are representative of the distribution of the data—for example if the data is concentrated in a banana shape in multi-dimensional space, we should select points along the banana. In general estimating which cases are representative is a very difficult problem, so `plotmo` makes a compromise estimate: the subset is created by selecting 50 rows at equally spaced intervals in the training matrix, after sorting the rows of the matrix on the response values. The idea here is that the density of the response values gives some indication of the density of the data locations. For responses with a small number of discrete values (classification models) this sorting approach doesn't really work.

Some details: Ties in the response value are randomly broken (so the subset isn't dependent on the original order of rows in the training matrix). The number 50 can be changed using the `ngrid1` argument. If `ngrid1` is greater than the number of cases then all cases are used, and `"apartdep"` is identical to `"partdep"`.

## 9.3 Transforming the response for partial dependencies

When doing the averaging for partial-dependencies, `plotmo` directly averages the predicted responses. The vertical axis of the plots is thus on the same scale as the values returned by `predict`.

---

<sup>2</sup>Bear in mind that we in fact are already making an approximation for *all* empirical partial-distribution plots, because we approximate the distribution of the background variables by using the training sample.

This point is raised because for classification models some partial-dependence functions transform the predicted probabilities before taking their average (for example `plotPartial` in the `randomForest` package). The transform is described by Equation 10.48 in Hastie et al. [8].

There seems to be no compelling reason to implement the transformation, especially for two-class (binomial) models—for most models we can use `predict type="link"` to get the same result, and in any case plotted probabilities are usually easier to work with than link functions.

Finally, it should be mentioned that different implementations of partial-dependence plots give slightly different curves. For example, we have to set `ngrid1=100` for `plotmo`'s partial-dependence curves to exactly match `gbm` package plots.

## 10 Prediction intervals (the level argument)

Use `plotmo`'s `level` argument to plot pointwise confidence or prediction intervals. The `predict` method of the model object must support this. Examples (Figure 6):

```
par(mfrow=c(2,3))
log.trees <- log(trees) # make the resids more homoscedastic
                        # (necessary for lm)

                                                                    ## lm
lm.model <- lm(Volume~Height, data=log.trees)
plot(lm.model, which=1) # residual vs fitted graph, check homoscedasticity
plotmo(lm.model, level=.90, pt.col=1,
       main="lm\n(conf and pred intervals)", do.par=F)

                                                                    ## earth
library(earth)
earth.model <- earth(Volume~Height, data=log.trees,
                    nfold=5, ncross=30, varmod.method="lm")
plotmo(earth.model, level=.90, pt.col=1, main="earth", do.par=F)

                                                                    ## quantreg
library(quantreg)
rq.model <- rq(Volume~Height, data=log.trees, tau=c(.05, .5, .95))
plotmo(rq.model, level=.90, pt.col=1, main="rq", do.par=F)

                                                                    ## quantregForest
# quantregForest is a layer on randomForest that allows prediction intervals
library(quantregForest)
x <- data.frame(Height=log.trees$Height)
qrf.model <- quantregForest(x, log.trees$Volume)
plotmo(qrf.model, level=.90, pt.col=1, main="qrf", do.par=F)

                                                                    ## gam
library(mgcv)
gam.model <- gam(Volume~s(Height), data=log.trees)
plotmo(gam.model, level=.90, pt.col=1,
       main="gam\n(conf not pred intervals)", do.par=F)
```

The packages used in the above code are [10,12,18,25].

### Confidence intervals versus prediction intervals

Be aware of the distinction between the two types of interval:

- (i) intervals for the prediction of the mean response (often called *confidence intervals*)
- (ii) intervals for the prediction of a future value (often called *prediction intervals*).

The model's `predict` method determines which of these intervals get returned and plotted by `plotmo`. Currently only `lm` supports both types of interval on new data (see

`predict.lm`'s `interval` argument), and both are plotted by `plotmo`.

A reference is Section 3.5 of Julian Faraway's online [linear regression book](#) [1]. See also the vignette [Variance models in earth](#) [16], which comes with the `earth` package.

## Assumptions for prediction intervals

Just because the intervals are displayed doesn't mean that they can be trusted. Be aware of the assumptions made to estimate the limits. At the very least, the model needs to fit the data adequately. Most models will impose further conditions. For example, linear model residuals must be homoscedastic.

Examination of the "Residual versus Fitted" plot is the standard way of detecting issues. So for example, with linear models use `plot.lm(mod, which=1)` and with `earth` models use `plot(mod, which=3)`. More generally, for any model use `plotres(mod, which=3)`, making use of the `plotres` function in the `plotmo` package.

Look at the distribution of residual points to detect non-homoscedasticity. Also look at the smooth line (the lowess line) in the residuals plot to detect non-linearity. If this is highly curved, we can't trust the intervals. One good place for more background on residual analysis is the *Regression Diagnostics: Residuals* section in Weisberg [24].

These are *pointwise* limits. They should only be interpreted in a pointwise fashion. So for non-parametric models they shouldn't be used to infer bumps or dips that are dependent on a range of the curve. For that we need *simultaneous* confidence bands, which none of the above models support.

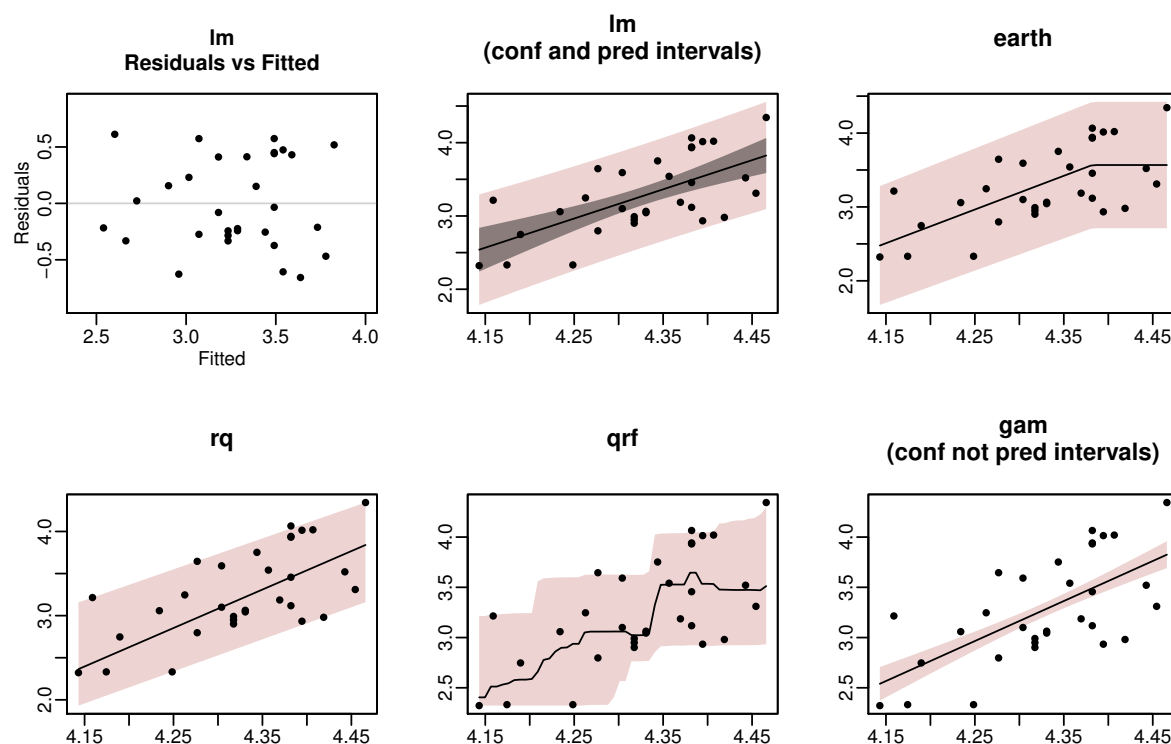


Figure 6: *Prediction intervals with plotmo. These plots were produced by the code on the previous page.*

## 11 FAQ

### I'm not seeing any interaction plots

Use `all2=TRUE` to force the display of interaction plots. By default, `degree2` plots are drawn only for some types of model (Section 6). When `all2=TRUE` is used, the `degree1` and `degree2` arguments can be useful to limit the number of plots.

### Plotmo always prints messages. How do I make it silent?

Use `trace = -1`. The grid message printed by default is a reminder that plotmo is displaying just a slice of the data.

### On what scale are the vertical axes of the plotmo plots?

Plotmo calls `predict` internally to generate the plots. So the vertical axis will be plotted in whatever units `predict` returns for your model. Plotmo sets the same vertical axis `ylim` for all plots on the page.

For more details, see Section 5.4 “The `ylim` and `clip` arguments” and Section 5.2 “The `type` and `nresponse` arguments”.

For further discussion, see the following CrossValidated web page:  
[Interpreting partial dependence plots \(marginal effects\) using plotmo.](#)

### How do I get more detail on the axes of `degree2` plots?

Get more information on the axes by invoking `persp` with `ticktype="detailed"`.

To do this, pass `persp.ticktype="detailed"` to `plotmo`. Example:

```
plotmo(model, persp.ticktype="detailed")
```

Any `plotmo` argument prefixed by `persp.` gets passed on internally to `persp`. In the `plotmo` help page, see the `type2` argument and the description of the `dots` argument near the bottom of the help page.

### How do I display the image plots in color (instead of black and white)?

Pass a vector of colors to `plotmo` using `image.col`. Example:

```
library(earth)
earth.mod <- earth(Volume ~ ., data = trees)
plotmo(earth.mod, all2=TRUE, type2="image",
       ngrid2=50,                               # increase resolution in image plot
       image.col=terrain.colors(30)) # 30 is arbitrary
```

Any `plotmo` argument prefixed by `image.` gets passed on internally to R's standard `image` function. In the `plotmo` help page, see the `type2` argument and the description of the `dots` argument near the bottom of the help page.

## The image display has blue “holes” in it. What gives?

The light blue holes are areas where the predicted response is out-of-range. Try using `clip=FALSE` (Section 5.4).

## I want to add lines or points to a plot created by `plotmo.` and am having trouble getting my axis scaling right.

Use `do.par=FALSE` or `do.par=2`. With the default `do.par=TRUE`, `plotmo` restores the `par` parameters and axis scales to their values before `plotmo` was called.

## After `plotmo` reports an error, `traceback()` says “No traceback available”

Try using `trace = -1` when invoking `plotmo`. This will often (but not always) allow `traceback` at the point of failure.

## How to cite `plotmo`

Stephen Milborrow. *plotmo: Plot a Model's Residuals, Response, and Partial Dependence Plots*. R Package (2018).

```
@Manual{plotmopackage,  
  title = {plotmo: Plot a Model's Residuals, Response, and Partial Dependence Plots},  
  author = {Stephen Milborrow},  
  year = {2018},  
  note = {R package},  
  url = {http://CRAN.R-project.org/package=plotmo }  
}
```

## 12 Common error messages

This section list some common error messages.

- `Error in match.arg(type): 'arg' should be one of ...`

The message is probably issued by the `predict` method for the model. Set `plotmo`'s `type` argument to a legal value for the model, as described on the help page for the `predict` method for the model.

- `Error: cannot get the original model predictors`
- `Error: model does not have a 'call' field or an 'x' field`

These and similar messages mean that `plotmo` cannot get the data it needs from the model (Section 13).

Try simplifying the way the model function is called. Try using the `x,y` interface instead of the `formula` interface, or vice versa.

Perhaps `keepxy` or similar is needed in the call to the model function, so the data is attached to the model object and available for `plotmo`.

A workaround is to manually add the `x` and `y` fields to the model object before calling `plotmo`, like this

```
model$x <- xdata
model$y <- ydata
```

where `xdata` and `ydata` are the `x` and `y` matrices used to build the model. This workaround often suffices for `plotmo` to do its job, assuming the model has a standard `predict` method that accepts `data.frames` (some `predict` methods accept only matrices).

Certain types of model built with NAs in the data will cause the above error messages.

- `Error: predict.lm(xgrid, type="response") returned the wrong length`
- `Warning: 'newdata' had 100 rows but variable(s) found have 30 rows`
- `Error: variable 'x' was fitted with type "nmatrix.2" but type "numeric" was supplied`
- `Error in model.frame: invalid type (list) for variable 'x[,3]'`

These and similar messages usually mean that `predict` is misinterpreting the new data generated by `plotmo`.

The underlying issue is that many `predict` methods, including `predict.lm`, seem to reject any reasonably constructed new data if the function used to create the model was called in an unconventional way.

The workaround is to simplify the way the model function is called. Use a formula and a data frame, or at least explicitly name the variables rather than passing a matrix on the right hand side of the formula. Use simple variable names (so `x1` rather than `dat$x1`, for example).

If the symptoms persist after changing the way the model is called, it's possible that the model doesn't save the data in a form accessible by `plotmo` (Section 13).



## 13 Accessing the model data

This section discusses some of `plotmo`'s internals. `Plotmo` needs to access the data used to build the model. It does that with the method functions listed below.

As an example, the job of the `plotmo.x` function is to return the `x` matrix used when the model was built. The default function `plotmo.x.default` essentially<sup>3</sup> does the following:

- (i) it uses `model$x`
- (i) if that doesn't exist, it uses the rhs of the model formula (so if the model was built with a formula, it must have a `terms` field)
- (i) if it can't access that, it uses `model$call$x`
- (i) if all that fails, it prints an error message.

The default method suffices for models that save the call and data with the model in a standard way (described in detail in the [Guidelines for S3 Regression Models](#) [15]). Specific method functions have been written to handle some other situations. For certain models this isn't possible—for example `xgboost` models save an incorrect `call` and use a custom matrix class from which the data can't be retrieved using R functions.

### 13.1 Method functions

The `plotmo` method functions are listed below. Use `trace=2` to see `plotmo` calling these functions.

- `plotmo.x` Return the model `x` matrix. The default method is described above.
- `plotmo.y` Return the model `y` matrix. Similar to `plotmo.x`.
- `plotmo.predict` Make predictions on new data. This is invoked for each subplot. The default method calls the usual `predict` method for the model. The prediction `newdata` for each subplot is the grid of values for the subplot. The `newdata` is a `data.frame` and not a matrix to allow both numerics and factors.  
  
Model-specific predict methods exist for some model classes, usually because a minor tweak is needed. For example `plotmo` has an internal one-line function `plotmo.predict.lars`—this converts `newdata` to a `matrix` before passing it to `predict.lars`, because `predict.lars` accepts only matrices.
- `plotmo.type` Select a `type` argument suitable for the current model's `predict` method.
- `plotmo.prolog` Called at the start of `plotmo` to do any model-specific initialization.

---

<sup>3</sup>There are actually a few more complications. For example, it also tries the `model` field saved with some `lm` models.

- `plotmo.singles` Figure out which variables should appear in degree1 plots.
- `plotmo.pairs` Figure out which variables should appear in degree2 plots.
- `plotmo.convert.na.nresponse` Convert the default `nresponse` argument to a column number for multiple response models.
- `plotmo.pint` Get the prediction intervals when `plotmo`'s `level` argument is used.

## 13.2 Environment for the model data

One `x` isn't necessarily the same as another `x`. `Plotmo` must access the data used to build the model in the correct environment:

- It uses the `.Environment` attribute of `model$terms`. (The `terms` field is standard for models built with a formula.)
- If that isn't available it uses `model$.Environment`. (Most models don't have such a field.)
- If that isn't available it uses `parent.frame()`. This last resort is correct if the model was built in the user's workspace and `plotmo` is called from the same workspace. But all bets are off if the model was created within a function and `plotmo` is called from a different function.

Note that the environment isn't actually necessary if the data is saved with the model, typically in the `x` and `y` fields of the model. Some models allow us to save `x` and `y` with a `keepxy` or similar argument (`plotmo` will use those fields if available).

# References

- [1] Julian Faraway. *Linear Models With R*. CRC, 2009. Cited on page 20.
- [2] John Fox, Sanford Weisberg, et al. *car: Companion to Applied Regression*, 2014. R package, <https://CRAN.R-project.org/package=car>. Cited on page 6.
- [3] John Fox, Sanford Weisberg, et al. *effects: Effect Displays for Linear, Generalized Linear, Multinomial-Logit, Proportional-Odds Logit Models and Mixed-Effects Models*, 2014. R package, <https://CRAN.R-project.org/package=effects>. Cited on page 6.
- [4] Jerome Friedman, Trevor Hastie, and Robert Tibshirani. *Regularization Paths for Generalized Linear Models via Coordinate Descent*. JASS, 2010. Cited on page 10.
- [5] Jerome H. Friedman. *Greedy Function Approximation: A Gradient Boosting Machine*. Annals of Statistics 19/1, 2001. <https://statistics.stanford.edu/research/multivariate-adaptive-regression-splines>. Cited on page 6.
- [6] Stefan Fritsch and Frauke Guenther; following earlier work by Marc Suling. *neuralnet: Training of neural networks*, 2012. R package, <https://CRAN.R-project.org/package=neuralnet>. Cited on page 10.
- [7] Brandon Greenwell. *pdp: Partial Dependence Plots*, 2016. R package, <https://CRAN.R-project.org/package=pdp>. Cited on page 6.
- [8] T. Hastie, R. Tibshirani, and J. Friedman. *The Elements of Statistical Learning: Data Mining, Inference, and Prediction (2nd Edition)*. Springer, 2009. Downloadable from <http://web.stanford.edu/~hastie/ElemStatLearn>. Cited on pages 6 and 18.
- [9] Trevor Hastie. *gam: Generalized Additive Models*, 2014. R package, <https://CRAN.R-project.org/package=gam>. Cited on page 3.
- [10] Roger Koenker. *quantreg: Quantile Regression*, 2014. R package, <https://CRAN.R-project.org/package=quantreg>. Cited on pages 10 and 19.
- [11] Andy Liaw, Mathew Weiner; Fortran original by Leo Breiman, and Adele Cutler. *randomForest: Breiman and Cutler's random forests for regression and classification*, 2014. R package, <https://CRAN.R-project.org/package=randomForest>. Cited on pages 3 and 9.
- [12] Nicolai Meinshausen. *quantregForest: Quantile Regression Forests*, 2014. R package, <https://CRAN.R-project.org/package=quantregForest>. Cited on pages 10 and 19.
- [13] David Meyer, Evgenia Dimitriadou, Kurt Hornik, Andreas Weingessel, and Friedrich Leisch. *e1071: Misc Functions of the Department of Statistics, Probability Theory Group (Formerly: E1071), TU Wien*, 2015. R package, <https://CRAN.R-project.org/package=e1071>. Cited on page 10.
- [14] S. Milborrow. *rpart.plot: Plot rpart models. An enhanced version of plot.rpart*, 2011. R package, <http://www.milbo.org/rpart-plot>. Cited on page 10.

- [15] S. Milborrow. *Guidelines for S3 regression models*, 2015. Vignette for R package plotmo, <http://www.milbo.org/doc/modguide.pdf>. Cited on page 24.
- [16] S. Milborrow. *Variance models in earth*, 2015. Vignette for R package earth, <http://www.milbo.org/doc/earth-varmod.pdf>. Cited on page 20.
- [17] S. Milborrow. *plotmo: Plot a Model's Residuals, Response, and Partial Dependence Plots*, 2018. R package, <https://CRAN.R-project.org/package=plotmo>. Cited on page 2.
- [18] S. Milborrow. Derived from mda:mars by T. Hastie and R. Tibshirani. *earth: Multivariate Adaptive Regression Splines*, 2011. R package, <http://www.milbo.users.sonic.net/earth>. Cited on pages 9 and 19.
- [19] Hong Ooi. *glmnetUtils: Utilities for 'Glmnet'*, 2017. R package, <https://CRAN.R-project.org/package=glmnetUtils>. Cited on page 10.
- [20] Greg Ridgeway et al. *gbm: Generalized Boosted Regression Models*, 2014. R package, <https://CRAN.R-project.org/package=gbm>. Cited on pages 3, 9, and 10.
- [21] Terry Therneau and Beth Atkinson. *rpart: Recursive Partitioning and Regression Trees*, 2014. R package, <https://CRAN.R-project.org/package=rpart>. Cited on pages 3, 9, and 10.
- [22] W.N. Venables and B.D. Ripley. *MASS: Support Functions and Datasets for Venables and Ripley's MASS*, 2014. R package, <http://www.stats.ox.ac.uk/pub/MASS4>. Cited on pages 9 and 10.
- [23] W.N. Venables and B.D. Ripley. *nnet: Feed-forward Neural Networks and Multinomial Log-Linear Models*, 2014. R package, <https://CRAN.R-project.org/package=MASS>. Cited on page 3.
- [24] Sanford Weisberg. *Applied Linear Regression (4th Edition)*. Wiley, 2013. Cited on page 20.
- [25] Simon Wood. *mgcv: Mixed GAM Computation Vehicle with GCV/AIC/REML smoothness estimation*, 2014. R package, <https://CRAN.R-project.org/package=mgcv>. Cited on page 19.
- [26] Hao Helen Zhang and Chen-Yen Lin. *cosso: Fit Regularized Nonparametric Regression Models Using COSSO Penalty.*, 2013. R package, <https://CRAN.R-project.org/package=cosso>. Cited on page 10.