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Visualizing Fit and Lack of Fit in Complex Regression Models with Predictor Effect Plots and Partial Residuals

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Abstract

Predictor effect displays, introduced in this article, visualize the response surface of complex regression models by averaging and conditioning, producing a sequence of 2D line graphs, one graph or set of graphs for each predictor in the regression problem. Partial residual plots visualize lack of fit, traditionally in relatively simple additive regression models. We combine partial residuals with effect displays to visualize both fit and lack of fit simultaneously in complex regression models, plotting residuals from a model around 2D slices of the fitted response surface. Employing fundamental results on partial residual plots along with examples for both real and contrived data, we discuss and illustrate both the strengths and limitations of the resulting graphs. The methods described in this paper are implemented in the **effects** package for R.

Keywords: interaction, nonlinearity, model misspecification, component plus residual plot, R, **effects** package.

1. Introduction

Predictor effect displays, a reinterpretation of effect displays introduced by Fox (1987) for generalized linear models, visualize the response surface of complex regression models with a linear predictor that includes main effects and interactions by averaging and conditioning, producing a sequence of 2D line graphs for the predictors in a model. Partial residual plots, also called component plus residual plots, visualize lack of fit, traditionally in relatively simple additive regression models. The properties of partial residuals plots were systematically explored by Cook (1993) and Cook and Croos-Dabrera (1998).

In the first part of this article we describe predictor effect displays, which require one or more 2D line graphs to describe the dependence of a fitted regression surface on each predictor.

This approach corresponds closely to the way most analyses are traditionally summarized based on tests and estimates. We then show how to combine partial residuals with predictor effect displays to visualize both fit and lack of fit simultaneously in complex regression models, plotting residuals from a model around 2D slices of the fitted response surface. Referencing Cook's fundamental results, we discuss and illustrate both the strengths and limitations of the resulting graphs. The extension to predictor effect displays is implemented for linear and generalized linear models of arbitrary complexity in the current version of the **effects** package for R (Fox 2003; Fox, Weisberg, Friendly, and Hong 2017a), which we use to generate the illustrations in the paper. As summarized in Section 5, predictor effect displays have been extended to a wide variety of other models that include a linear predictor in the mean function.

Section 2 of the paper describes the general setting that we address and introduces predictor effect displays. We also discuss the relationship of predictor effect displays to term effect displays, as previously described by Fox (1987). Section 3 reviews partial residual plots, connecting them to predictor effect displays. Section 4 develops a variety of examples, using both real and contrived data, to explore the utility and limitations of adding partial residuals to effect displays. The paper concludes in Section 5 with advice about using partial residuals in effect displays to explore lack of fit in complex regression models, and compares our approach to related work.

2. Predictor effect displays

We address the following situation: There is a response y and a set of p predictors $\mathbf{x} = (x_1, \ldots, x_p)$, along with a regression model for the conditional mean $\mathrm{E}(y|\mathbf{x})$. Predictors in a parametric regression model are represented by regressors. For example, if x_j is a factor with k levels, then a main effect for x_j would be represented by k-1 indicator or contrast regressors. A numeric x_j can be represented by x_j itself, by a transformation such as $\log(x_j)$, by a set of polynomial basis functions, by a spline basis, or perhaps by other regressors. The correspondence between predictors and regressors is not unique, but the methods we discuss are invariant under changes in parameterization. As is conventional, we define an interaction term $x_j:x_{j'}$ to be the set of all pairwise products of the regressors that are derived from x_j with all the those derived from $x_{j'}$. This definition extends straightforwardly to interactions of more than two predictors, such as the three-way interaction $x_j:x_{j'}:x_{j''}$.

We define the linear predictor $h(\beta, \mathbf{x})$ to be a linear combination of regressors in the main effects and interactions created from the predictors \mathbf{x} , with the regression coefficients $\boldsymbol{\beta}$ providing the weights that multiply the regressors. An intercept β_0 is generally included in h with a corresponding constant regressor, that is, a column of ones. We consider only mean functions of the form

$$E(y|\mathbf{x}) = \eta^{-1} [h(\boldsymbol{\beta}, \mathbf{x})]$$
 (1)

for some known invertible link function η . This class of regression models includes linear and generalized linear models, additive and generalized additive models, as well as linear and generalized linear mixed models, among others.

Given a suitable estimate $\widehat{\boldsymbol{\beta}}$ of $\boldsymbol{\beta}$, we write $\widehat{\boldsymbol{y}}(\mathbf{x}) = \eta^{-1}[h(\widehat{\boldsymbol{\beta}}, \mathbf{x})]$ as the estimated mean function. The goal is to visualize the dependence of $h(\widehat{\boldsymbol{\beta}}, \mathbf{x})$ or of $\widehat{\boldsymbol{y}}(\mathbf{x})$ on \mathbf{x} . The most general approach would examine a single high-dimensional display with $h(\widehat{\boldsymbol{\beta}}, \mathbf{x})$ or $\widehat{\boldsymbol{y}}(\mathbf{x})$ on the "vertical" axis and

 \mathbf{x} on the "horizontal" axes. Although concentrating on predictors rather than regressors has reduced the dimension of the visualization problem from approximately the number of linearly independent regressors to approximately the number of linearly independent predictors plus one for the response, this graph is likely to be useful only for $p \leq 2$.

Standard practice in summarizing a regression model is to proceed predictor-by-predictor. Predictors that occur in main effects only are generally summarized by statements or estimates or tests that essentially average over, or conditionally fix, all other predictors. Predictors that occur in interactions require a more complex summary that conditions successively on the combinations of values of the other predictors in the interactions. Predictor effect displays follow this paradigm.

Suppose that we are interested in the visual summary of a particular focal predictor x_f in the set of predictors. We assume that the formula defining the linear predictor is hierarchical, meaning that if an interaction is present in the model, then so are all of its lower-order relatives, equivalent to the principle of marginality (Nelder 1977). For example, the inclusion of $x_j:x_{j'}$ implies that both x_j and $x_{j'}$ are in the formula. We can then partition the set of predictors $\mathbf{x} = (x_f, \mathbf{x}_1, \mathbf{x}_2)$, where $x_j \in \mathbf{x}_1$ if $x_f:x_j$ is in the model formula, and the subvector \mathbf{x}_2 contains all the remaining predictors. Either of \mathbf{x}_1 or \mathbf{x}_2 may be empty.

For a given x_f , we can always fix the values of the predictors in \mathbf{x}_2 , if any, and plot, in linear predictor scale,

$$h\left[\widehat{\boldsymbol{\beta}}, (x_f, \mathbf{x}_1, \mathbf{x}_2^a)\right] \text{ versus } x_f$$
 (2)

where \mathbf{x}_2^a is a fixed value of \mathbf{x}_2 , typically determined by averaging in some meaningful way. In the **effects** package, we use by default the arithmetic average for continuous predictors. For factors, we average by default over the levels of the factor, with weights given by the sample sizes at each level; this procedure is equivalent to averaging the columns of the model matrix encoding a conditionally fixed factor and is therefore invariant with respect to contrast coding. These defaults can be changed, for example to set continuous predictors equal to some meaningful value, or to average a factor over its levels using a different weighting scheme. Then the vertical values in (2) are simply

$$h\left[\widehat{\boldsymbol{\beta}}, (x_f, \mathbf{x}_1, \mathbf{x}_2^a)\right] = C + h\left[\widehat{\boldsymbol{\beta}}, (x_f, \mathbf{x}_1, \mathbf{0})\right]$$
(3)

for some constant C that depends on x_2^a . Thus, choice of \mathbf{x}_2 affects only the *height* of the predictor effect display in linear predictor scale for x_f , but not its *shape*, and \mathbf{x}_2 is therefore generally unimportant for examination of the effect of x_f . In mean scale, conditioning is not entirely benign if the link function is nonlinear, as the shape of the plot can depend on \mathbf{x}_2^a . Understanding these plots is therefore generally simpler in linear predictor scale.

In the important special case of $\mathbf{x}_1 = \varphi$, the empty set, x_f appears in the formula only through a main effect. If the regressor representing x_f is x_f itself, then the predictor effect display in linear predictor scale for x_f is a straight line with slope equal to the estimated coefficient corresponding to x_f , and hence the plot merely displays this estimated slope, along with an essentially arbitrary intercept. If x_f is represented some other way, for example by a transformation such as $\log(x_f)$, a polynomial, a smooth estimated using an additive or generalized additive model, or a spline basis, then the display will visualize the appropriate nonlinear effect of x_f in the linear predictor scale.

If, however, \mathbf{x}_1 is *not* empty, then the plot described by (2) is as a practical matter inadequate because it describes a graph with $1+\dim(\mathbf{x}_1)$ "vertical" axes and one horizontal axis. To reduce

this high-dimensional graph to a sequence of 2D graphs, we invoke *conditioning*: For each $x_j \in \mathbf{x}_1$ define a *grid* of a few values in the range of x_j . If x_j is a factor, then the "grid" typically consists of all factor levels, while for continuous x_j , selected quantiles or values evenly spread over the range of x_j can be used to form the grid. If the *j*th predictor has G_j grid points, there are then $G = \prod G_j$ combinations of grid values of the predictors in \mathbf{x}_1 .

Let \mathbf{x}_1^g be one of the G sets of grid values. Then the corresponding graph in the predictor effect display for x_f is of

$$h\left[\widehat{\boldsymbol{\beta}}, (x_f, \mathbf{x}_1^g, \mathbf{x}_2^a)\right] \text{ versus } x_f$$
 (4)

The predictor effect display in its entirety consists of the sequence of separate 2D line graphs of (4) for each of the G choices of g. Often visualization can be simplified by overlaying some of these 2D line graphs on the same plot, creating a *multi-line* display.

2.1. Example: Infant mortality by per-capita GDP and national group

We begin by loading the **effects** package:

```
R> library("effects")
```

Loading required package: carData

lattice theme set by effectsTheme()
See ?effectsTheme for details.

Loading the **effects** package also loads the **carData** package (Fox, Weisberg, and Price 2017b), which contains a variety of regression data sets, and, if the **lattice** package (Sarkar 2008) isn't loaded, sets a custom theme for lattice graphics. On some platforms, setting the lattice theme may open a trellis graphics device (see ?trellis.device).

To develop a simple example of predictor effect displays, we use the UN data set in the carData package. UN member states and observer states were divided into three groups—African states, OECD states, and other non-African states. The response variable in the example is infantMortality, the infant mortality rate (infant deaths per 1000 live births) for each country, and the predictors are ppgdp, per-person GDP in U.S. dollars, and group. The data are from approximately 2011.

We want to visualize the fit of a model for infant mortality as a function of per person GDP and the three national groups, permitting ppgdp to interact with group:

```
R> m1 <- lm(log(infantMortality) ~ group * log(ppgdp), data = UN,
+ subset = rownames(UN) != "Equatorial Guinea")
R> summary(m1)
```

Call:

```
lm(formula = log(infantMortality) ~ group * log(ppgdp), data = UN,
subset = rownames(UN) != "Equatorial Guinea")
```

```
Residuals:
```

```
Min 1Q Median 3Q Max -1.11823 -0.27109 0.02494 0.28529 1.14925
```

Coefficients:

```
Estimate Std. Error t value
                                                      Pr(>|t|)
(Intercept)
                        6.47641
                                    1.30955
                                              4.946 0.00000169
groupother
                        0.94287
                                    1.34496
                                              0.701
                                                      0.484155
groupafrica
                       -0.04564
                                    1.36583 -0.033
                                                      0.973379
log(ppgdp)
                       -0.48455
                                    0.12617
                                             -3.840
                                                      0.000168
groupother:log(ppgdp)
                       -0.05885
                                    0.13110
                                             -0.449
                                                      0.654028
groupafrica:log(ppgdp)
                       0.14201
                                    0.13766
                                              1.032
                                                      0.303613
```

```
Residual standard error: 0.4413 on 186 degrees of freedom
(20 observations deleted due to missingness)

Multiple R-squared: 0.8391, Adjusted R-squared: 0.8348
F-statistic: 194.1 on 5 and 186 DF, p-value: < 2.2e-16
```

This linear model has two predictors: the factor group, with three levels, and the numeric variable ppgdp. Both the response variable and ppgdp are log-transformed to linearize the partial relationship between the two, a point to which we return in Section 3. The regressors in the model include log(ppgdp) to represent ppgdp, two indicator regressors for the levels of group, and two product regressors for the interactions. Because the linear model uses the identity link function, the mean function and linear predictor are the same. In fitting the model to the data, we removed the African country Equatorial Guinea, for a reason that will become apparent as we further develop this example in Section 3.1.

The interactions and log transformations make it inconvenient to interpret the model directly from the coefficients, and so we turn to predictor effect plots for group and ppgdp, invoking the predictorEffect function in the effects package:

```
R> plot(predictorEffect("group", m1,
             transformation = list(link = log, inverse = exp),
             xlevels = list(ppgdp = 10 ^ (2 : 5))),
         lines = list(multiline = TRUE),
         axes = list(
             x = list(rotate = 45),
             y = list(lab = "Infant Mortality",
                      ticks = list(at = 2 ^ (1 : 8)))
             ),
         confint = list(style = "auto")
         )
R> plot(predictorEffect("ppgdp", m1,
             transformation = list(link = log, inverse = exp)),
         lines = list(multiline = TRUE),
         axes = list(
             x = list(rotate = 45),
```

The objects returned by predictorEffect are graphed by a corresponding plot method. The calls to predictorEffect and plot use several optional arguments to customize the resulting graphs:

- The transformation argument to predictorEffects reverses the log transformation of the response variable, to express the infant-mortality rate as deaths per 1000 births. The effect is plotted on the log(infantMortality) scale, where the structure of the model is linear, but the axis is labelled on the untransformed scale. Adding type = "response" to the y-axis specification list would plot the effect on the scale of the response, producing a less informative graph (try it!).
- The xlevels argument to predictorEffect sets the values to which the predictor ppgdp is conditionally fixed in the predictor effect display for group. The default is to evaluate the numeric predictor ppgdp on a grid of five approximately equally spaced values rounded to "nice" numbers. By supplying the ppgdp grid directly, we can use values that are evenly spaced on the log scale of the regressor log(ppgpd) rather than the default of equally spaced values in the arithmetic scale of the predictor ppgdp.
- The lines argument to plot specifies a multi-line graph for each predictor effect; the default is to draw separate panels for each grid value of the conditioning predictor, or combination of grid values of conditioning predictors when there are more than one.
- The axes argument rotates the horizontal-axis tick-labels, changes the label on the vertical axis to reflect untransformed infant mortality, and customizes the placement of the vertical-axis tick marks.
- The argument confint = list(style = "auto") displays 95-percent pointwise confidence intervals for the fitted effects, using error-bars for factors and bands for numeric predictors. The default in multi-line displays is to suppress confidence intervals.

See ?predictorEffect, ?Effect, and ?plot.eff for details of these and other optional arguments.

The predictor effect displays are shown in Figure 1. The left panel has the focal predictor group on the horizontal axis. The remaining predictor, the numeric predictor ppgdp, interacts with group and hence is evaluated at the supplied grid of four values equally spaced on the log scale, with a separate line drawn for each of the grid values of ppdgp. Because group is a factor, $\widehat{y}(\mathbf{x})$, which is equivalent to the linear predictor because the link function η is the identity link, is computed only at the factor levels, indicated by the plotting symbols, which are slightly displaced horizontally to avoid overplotting. The lines joining the plotting symbols are an aid for viewing the graph, and may be suppressed if desired. We see that, in general, infant mortality at fixed levels of ppgdp is lowest in the oecd group and highest in africa; at the lowest level of ppgdp, however, fitted infantMorality is slightly lower in

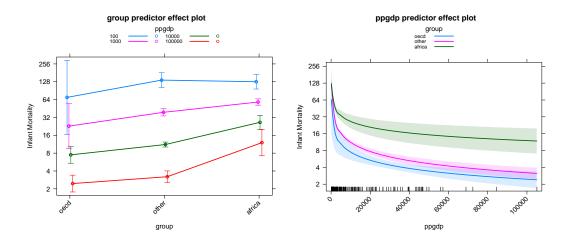


Figure 1: Predictor effect displays for the model for infantMortality fit to the UN data.

africa than in the other group, and the confidence interval for the oecd group is very wide, because there are no oecd countries at this level of ppgdp. In all three groups, infant mortality declines with ppgdp, though less so in africa than in the other groups.

The display in the right panel of Figure 1 is for the effect of ppgdp, with separate lines for the three groups of states overlaid on the same graph. The lines are curved because ppgdp is represented by the regressor log(ppgdp) in the model. By default, a rug plot, showing the marginal distribution of ppgdp, is shown at the bottom of the graph. In this instance the inference is the same from the second plot as it is from the first, namely that infant mortality declines with per-capita GDP in all three groups, though less so in africa than in the other two groups, and that except at the lowest levels of ppgdp, infant mortality is lowest among the oecd states and highest in africa at fixed levels of ppgdp,

2.2. Term effects versus predictor effects

Previous discussions of effect plots (such as Fox 1987), and previous versions of the **effects** package, develop what might be called high-order term effects, or, for short, *term effects*: Term effect displays are drawn for combinations of predictors corresponding to the high-order terms in a model—that is, terms that are not marginal to any terms in the model.

Consider, for example, the model formula $y \sim a*b + a*c$. We adopt the version of the Wilkinson and Rogers (1973) notation for linear models that is used in S and R (Chambers and Hastie 1992). In this notation, \sim separates the left- and right-hand sides of the model and * is the crossing operator, and so, in expanded form, the model is $y \sim 1 + a + b + c + a:b + a:c$, where y is the response, 1 represents the intercept, a, b and c are the main effects of the three predictors, and a:b and a:c are interactions. The high-order terms in the model are a:b and a:c.

The allEffects function applied to a model with this formula produces two plots, one with a and b as the focal predictors, and the other with a and c as the focal predictors. The plot method for more than one focal predictor uses an algorithm to choose which predictor is

plotted on the horizontal axis and which is used as a conditioning variable. If the formula has numeric predictors, then the left-most predictor in the formula is used for the horizontal axis.

For example, if b were the only numeric predictor and a and c were factors, then the term effect plot for a:b would average over c, have b on the horizontal axis, and condition on a. The term effect plot for a:c would average over b, and, for the horizontal axis, would use the factor with the fewest levels or the left-most factor if they have the same number of levels.

Neither of these plots corresponds to a predictor effect plot because they average over, rather than condition on, c in the first plot and b in the second plot, producing a display that is not invariant in shape with respect to the manner in which the levels of the factor c are averaged over in the term effect plot for a:b, or the typical value to which the numeric b is set in the term effect plot for a:c. In contrast, recall that averaging over or fixing the values of predictors in predictor effect plots affects only the height, and not the shape, of the effect. It is largely this invariance property that leads us to prefer predictor effects to term effects.

The most general function in the effects package is Effect, in which the predictors in an effect are specified explicitly. Effect may be used to produce both predictor and term effect displays, including effect displays for terms that don't appear in the model, such as an interaction higher-order to those in the model. For example, a plot equivalent to the predictor effect plot for b could be obtained with the command

where m is the regression-model object. This specification recognizes that b interacts with both a and c, and the x.var argument overrides the default procedure for determining the predictor on the horizontal axis of the graph. Predictor effect plots for the other two predictors are obtained by providing each predictor in turn as the x.var argument.

All predictor effect plots can be producing more conveniently using

R> plot(predictorEffects(m))

The three predictor effect plots in this example are views of the same four-dimensional surface from three different view points. In the preceding infant-mortality example, we used predictorEffect in preference to predictorEffects to exert finer-grain control over the resulting graphs.

3. Partial residual plots

Whereas predictor effect plots are designed to summarize the conditional effects of each predictor given the others in a correctly specified regression model, partial residual plots are used to visualize misspecification of the mean function attributable to continuous predictors. We begin with a working model given by (1) that is potentially misspecified. Suppose that \mathbf{x}_i is the vector of predictors for the *i*th of *n* observations in the data, and y_i is the corresponding value of the response. The estimated working linear predictor for the *i*th observation is $h(\widehat{\boldsymbol{\beta}}, \mathbf{x}_i)$, and the corresponding working residuals are $e(\mathbf{x}_i) = [y_i - \widehat{y}(\mathbf{x}_i)]\eta'(\mathbf{x}_i)$, where $\eta'(\mathbf{x}_i)$ is the first derivative of η with respect to $E(y|\mathbf{x}_i)$ (Cook and Croos-Dabrera 1998), which translates from the mean scale to the linear predictor scale. Partial residual plots are always drawn in the linear predictor scale and only for numeric predictors.

Paralleling the development of predictor effect displays, for a numeric focal predictor x_f , we divide the *i*th vector of observed predictors into $\mathbf{x}_i = (x_{fi}, \mathbf{x}_{1i}, \mathbf{x}_{2i})$. Partial residual plots are traditionally defined only when $\mathbf{x}_1 = \varphi$. In this case, the partial residual plot for a focal predictor x_f is a graph of n points, the *i*th of which is

$$e(\mathbf{x}_i) + \left\{ h[\widehat{\boldsymbol{\beta}}, (x_{fi}, \varphi, \mathbf{0})] - \widehat{\beta}_0 \right\} \text{ versus } \mathbf{x}_{fi}$$
 (5)

where φ has been inserted as a placeholder for the empty value of \mathbf{x}_1 . The term in curly braces in (5) is called a *partial regression function* and it represents the component of the fitted mean function that depends on x_{fi} . The working residuals $e(\mathbf{x}_i)$ appear as random scatter around the partial regression function for a correctly specified model.

In certain circumstances, however, the scatter added by the residuals will be systematic. Suppose that in place of the working linear predictor in (1), the "true" linear predictor is

$$h(\boldsymbol{\beta}, \mathbf{x}) + \{t(x_f) - h\left[\boldsymbol{\beta}, (x_f, \varphi, \mathbf{0})\right]\}$$
(6)

where $t(x_f)$ is a potentially nonlinear function of x_f . If all the regressors (not the predictors) in \mathbf{x} are at least approximately linearly related, and the method used to estimate parameters is Fisher consistent, then a smoother fit to the partial residual plot for x_f provides a visualization of t (Cook 1993, Lemma 2.1) and possible misspecification with respect to x_f . Extension from linear models to generalized linear models is provided by Cook and Croos-Dabrera (1998).

Comparing (5) to (2), we can superimpose the partial residuals on the predictor effect plot simply by adding the constant $\hat{\beta}_0 + C$ to the abscissa of the points in (5). The partial residuals are linearly translated, but nonlinear shapes, the main focus of the partial residuals, are unaffected.

When $\mathbf{x}_1 \neq \varphi$, the predictor effect display consists of G 2D line plots by conditioning on \mathbf{x}_1^g . The points we add to the gth 2D plot are

$$e(\mathbf{x}_i) + h\left[\widehat{\boldsymbol{\beta}}, (x_{fi}, \mathbf{x}_{1i}, \mathbf{x}_2^a)\right] + C \text{ versus } x_f$$
 (7)

for all i such that $|\mathbf{x}_{1i} - \mathbf{x}_1^g|$ is minimized over g for each element of \mathbf{x}_1 , and the constant C is chosen to match the intercept in the predictor effect display. Cook's lemma can then be applied to each grid value separately to diagnose unmodelled curvature with respect to x_f separately for each g.

3.1. Example: Infant mortality revisited

Continuing with the UN infant mortality example in Section 2.1, we start with the response variable infantMortality and predictor ppgdp unlogged. The predictor effect plot for ppgdp with partial residuals is shown in Figure 2. We initially leave Equatorial Guinea in the data set.

ppgdp predictor effect plot

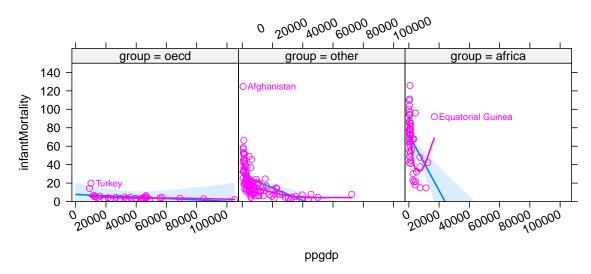


Figure 2: Predictor effect plot with partial residuals for ppgdp when neither it nor the response infantMortality is log-transformed, labeling the most unusual point in each panel.

The effects package suppresses partial residuals for multi-line plots because of the confusion produced by overlapping residuals for different values of a conditioning predictor. Instead, the residuals are plotted with the lines corresponding to different values of the conditioning predictors, here just the predictor group, in separate panels. The blue line in each panel represents the fitted model, with a pointwise 95-percent confidence band shown around the fitted effect. The magenta line in each panel is a loess nonparametric regression smooth (Cleveland, Grosse, and Shyu 1992), using a span of 2/3 by default. The argument id = list(n = 1) to plot identifies the most unusual point in each panel, defined as the point with the largest Mahalanobis distance from the centroid of the points.

The points for other and africa are a clear mismatch for the fitted line, perhaps suggesting the log-transformations of infantMortality and ppgdp used in the initial example in Section 2.1. The right-most point in africa, for Equatorial Guinea, is out of line with the rest of the African states, pairing a large value of ppgdp with a large value of infantMortality. The most unusual points in the other panels, Turkey in the oecd group and Afghanistan in the other group, are not out of line with the other points in their groups to the same degree. While extreme in their values of ppgdp and infantMortality, these two countries follow the general pattern of the data. Recall that we removed Equatorial Guinea, but not Turkey or Afghanistan, in the model fit in Section 2.1.

The partial residuals have the added benefit of highlighting that while ppgdp is both relatively high and highly variable in the oecd group, it has relatively small variation in africa, where it is concentrated in very low values. The other group is intermediate. When both the response variable and ppgdp are log-transformed, as in model m1 in Section 2.1, the partial-residual plots are much more satisfactory (see Figure 3):

```
R> plot(predictorEffects(m1, ~ ppgdp, partial.residuals = TRUE),
+ axes = list(x = list(rotate = 25)))
```

ppgdp predictor effect plot

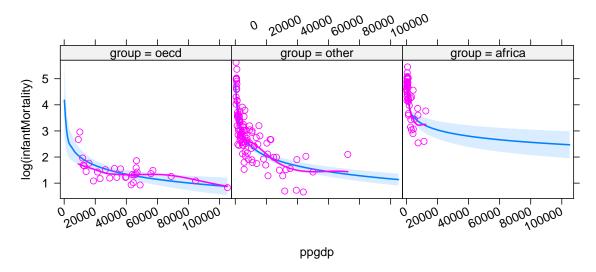


Figure 3: Predictor effect plot with partial residuals for ppgdp in the model with ppgdp and the response infantMortality log-transformed.

3.2. Conditioning on continuous predictors

When \mathbf{x}_1 includes continuous numeric predictors, as in the first example in the next section, the assignment of partial residuals to one of the grid of conditioning values introduces additional variation, because the linear predictor is evaluated at $(x_{fi}, \mathbf{x}_{1i}, \mathbf{x}_2^a)$ rather than at the grid value $(x_{fi}, \mathbf{x}_1^g, \mathbf{x}_2^a)$. That is, there is a potential extra source of variability in the plot due to conditioning. If we assume that the value of this difference has a symmetric distribution about zero, then, from Cook (1993, Lemma 2.1), the unadjusted partial residual plot (7) visualizes $t(x_f)$ with extra variation. If the difference is not symmetrically distributed, as is likely, for example, for extreme values of the continuous predictors in \mathbf{x}_1 , then bias may be introduced.

A predictor effect display in linear predictor scale with partial residuals adjusted for conditioning includes the points given for the gth plot by

$$e(\mathbf{x}_i) + h\left[\widehat{\boldsymbol{\beta}}, (x_{fi}, \mathbf{x}_1^g, \mathbf{x}_2^a)\right] + C \text{ versus } x_f$$
 (8)

substituting the grid values \mathbf{x}_1^g for the data values \mathbf{x}_{1i} of the conditioning predictors. This plot also visualizes $t(x_f)$ for each g under the same conditions as the unadjusted version, but the visualization may be sharper. The adjusted version is implemented in the **effects** package.

The requirement of linearly related regressors for the usefulness of partial residual plots may be restrictive on its face, particularly in problems with $\mathbf{x}_1 \neq \varphi$. Because we are conditioning on $\mathbf{x}_1 = \mathbf{x}_1^g$, however, linearly related regressors are only required within a fixed value of \mathbf{x}_1 . Moreover, experience suggests that only fairly strong nonlinear relationships among the regressors prove to be problematic.

4. More examples

4.1. Volunteering for a psychological experiment

Cowles and Davis (1987) conducted a study on volunteering for a psychological experiment, in which the subjects were students in an introductory psychology course. The authors of the study collected data on the students' gender, on the personality dimensions extraversion and neuroticism, each of which ranges potentially from zero to 24, and on the students' willingness to volunteer for an experiment. Of the 1421 students for whom data were collected, 597 were willing to serve as volunteers. The data are in the Cowles data frame in the carData package:

R> summary(Cowles)

(Intercept)

neuroticism

extraversion

neuroticism:extraversion -0.008552

sexmale

```
neuroticism
                 extraversion
                                              volunteer
                                     sex
       : 0.00
                       : 2.00
                                female:780
                                              no:824
1st Qu.: 8.00
                                male :641
                1st Qu.:10.00
                                              yes:597
Median :11.00
                Median :13.00
Mean
       :11.47
                Mean
                      :12.37
3rd Qu.:15.00
                3rd Qu.:15.00
       :24.00
                       :23.00
Max.
                Max.
```

Cowles and Davis expected extraversion and neuroticism to interact in affecting volunteering, leading to the following logistic regression model:

```
R> library("car")
R> mod.cowles.1 <- glm(volunteer ~ sex + neuroticism * extraversion,</pre>
         data = Cowles, family = binomial)
R> summary(mod.cowles.1)
Call:
glm(formula = volunteer ~ sex + neuroticism * extraversion, family = binomial,
    data = Cowles)
Deviance Residuals:
    Min
              1Q
                   Median
                                 30
                                         Max
-1.4749
        -1.0602 -0.8934
                             1.2609
                                      1.9978
Coefficients:
                           Estimate Std. Error z value
                                                          Pr(>|z|)
```

0.501320 -4.704 0.00000255

2.942

0.02683

0.00326

0.00355

4.423 0.00000975

0.111631 -2.214

0.002934 - 2.915

0.037648

0.037719

-2.358207

-0.247152

0.110777

0.166816

```
(Dispersion parameter for binomial family taken to be 1)
    Null deviance: 1933.5 on 1420
                                    degrees of freedom
                                    degrees of freedom
Residual deviance: 1897.4 on 1416
AIC: 1907.4
Number of Fisher Scoring iterations: 4
R> Anova(mod.cowles.1)
Analysis of Deviance Table (Type II tests)
Response: volunteer
                         LR Chisq Df Pr(>Chisq)
sex
                           4.9184
                                        0.026572
neuroticism
                           0.3139
                                  1
                                        0.575316
                          22.1372 1 0.000002538
extraversion
neuroticism:extraversion
                           8.6213 1
                                        0.003323
```

We use the Anova function in the car package (Fox and Weisberg 2011) to obtain Type II tests for the terms in the model. As expected, the interaction between neuroticism and extraversion has a small p value, and some evidence for a difference between the sexes. is also apparent.

The predictor effect displays in mean scale (i.e., the probability scale) can all be drawn simultaneously by the predictorEffects function, as shown in Figure 4:

The lines in the predictor effect plots for neuroticism and extroversion are not straight because of the conversion from linear predictor (logit) to mean (probability) scale, obtained by specifying the argument axes = list(y = list(type = "response")) to plot. As before, we obtain multi-line plots for the continuous predictors by lines = list(multiline = TRUE). We use the xlevels argument to predictorEffects to exert control over the values of these predictors. The rows and cols arguments to plot specify that the meta-array of effect displays should be arranged horizontally. By default, confidence intervals around the estimated effects are suppressed in multi-line plots; as before, they could be turned on by confint = list(style = "auto"). The predictorEffects function can also be used for a subset of predictors; see the function's help page.

The effect plot for sex is little more than a visualization of the regression coefficient for this factor, with females somewhat more likely than males to volunteer, and because the difference

Figure 4: Predictor effect displays for Cowles and Davis's logistic regression for volunteering for a psychological experiment.

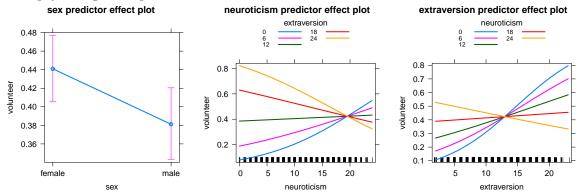
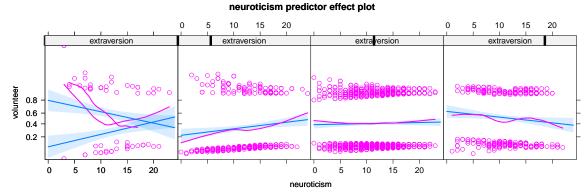


Figure 5: Predictor effect display for neuroticism showing partial residuals.



in estimated probabilities is small, the change to mean scale suggests that this visualization would apply for any meaningful averaging over the remaining predictors. The other two displays are two views of the same 3D surface, because both have $\mathbf{x}_2 = (\mathtt{sex})$ fixed in the same way. The second display suggests clearly that as neuroticism increases, the probability of volunteering increases for subjects with low extraversion, but decreases for subjects with high extraversion. The third display, with extraversion on the horizontal axis, shows that the probability of volunteering generally increases with extraversion, at a very high rate when extraversion is low, and a much lower rate when neuroticism is high; at the highest level of neuroticism, the relationship becomes negative. In this instance, both displays of the interactions can be useful, as they emphasize somewhat different stories.

Figure 5 is the predictor effect plot for neuroticism in linear predictor (logit) scale with the partial residuals shown:

The lattice argument to plot sets the lattice package layout argument, producing a plot with four panels arranged in one row (with the unusual column, row order standard for the

lattice layout argument). The conditionally fixed values of extraversion increase from left to right across the range of this predictor, as indicated by the black line in the strip at the top of each panel.

For this logistic regression, the vertical axis is on the logit scale, and the default in the effects package is to label tick-marks on this axis with values of the inverse link function applied to the logits—that is, with corresponding probabilities. Because this is a diagnostic plot, we haven't bothered to customize the location of the tick-marks on the vertical axis. The partial residuals are given by the magenta open circles, and the magenta line is the loess smooth of the partial residuals, with default span of 2/3. As before, the blue lines, which are straight on the logit scale, represent the fitted model, with the 95-percent point-wise confidence envelope around the fit superimposed. Robust smooths for non-Gaussian GLMs can result in substantial bias in the fitted curve (Landwehr, Pregibon, and Shoemaker 1980), and so a non-robust loess smoother is used. The general agreement of the smooths with the fitted effect suggests that the model reasonably represents the data.

As an additional check, we fit an alternative model to Cowles and Davis's data, in which each of neuroticism and extraversion is represented by a five-degree-of-freedom natural regression spline. The resulting model uses 25 df for the interaction, along with five df for each of the neuroticism and extraversion main effects, and is consequently much more flexible than the original model with a linear-by-linear interaction. A likelihood-ratio test comparing the new model to the original one fails to reveal significant lack of fit in the original model, and the original model is strongly preferred by both the AIC and BIC:

```
R> library("splines")
R> mod.cowles.2 <- glm(volunteer ~
             sex + ns(neuroticism, 5) * ns(extraversion, 5),
         data = Cowles, family = binomial)
R> anova(mod.cowles.1, mod.cowles.2, test = "Chisq")
Analysis of Deviance Table
Model 1: volunteer ~ sex + neuroticism * extraversion
Model 2: volunteer ~ sex + ns(neuroticism, 5) * ns(extraversion, 5)
  Resid. Df Resid. Dev Df Deviance Pr(>Chi)
1
       1416
                1897.4
2
       1384
                1857.0 32
                            40.468
                                      0.1448
R> cbind(AIC(mod.cowles.1, mod.cowles.2),
           BIC(mod.cowles.1, mod.cowles.2))
             df
                     AIC df
                                 BTC
mod.cowles.1 5 1907.440 5 1933.736
mod.cowles.2 37 1930.972 37 2125.560
```

4.2. Canadian occupational prestige data

Blishen and McRoberts (1976) assembled data on the prestige, income level, and education level of males in 102 Canadian occupations, with the purpose of developing a prediction equation for occupational prestige based on income and education. We analyze similar data here, although the income and education scores in our data set are for all occupational incumbents, rather than just for men. These data were also analyzed by Fox and Suschnigg (1989). The prestige scores are average ratings for the occupations in a national survey conducted in the mid-1960s (Pineo and Porter 1967). The income and education scores are averages from the 1971 Canadian census. We classified 98 of the occupations by type: blue collar, white collar, and professional or managerial. Four of the occupations — "athletes," "newsboys," "babysitters," and "farmers" — did not fit into this classification and are dropped from our analysis. The Canadian occupational prestige data are in the data frame Prestige in the carData package:

R> summary(Prestige)

```
education
                      income
                                       women
                                                        prestige
       : 6.380
                                          : 0.000
                                                            :14.80
                  Min.
                         :
                            611
                                   Min.
1st Qu.: 8.445
                  1st Qu.: 4106
                                   1st Qu.: 3.592
                                                     1st Qu.:35.23
Median :10.540
                                   Median :13.600
                                                     Median :43.60
                  Median : 5930
Mean
       :10.738
                  Mean
                         : 6798
                                   Mean
                                          :28.979
                                                     Mean
                                                            :46.83
3rd Qu.:12.648
                  3rd Qu.: 8187
                                   3rd Qu.:52.203
                                                     3rd Qu.:59.27
                                          :97.510
Max.
       :15.970
                  Max.
                         :25879
                                   Max.
                                                     Max.
                                                            :87.20
    census
                  type
Min.
       :1113
                bc :44
1st Qu.:3120
                prof:31
Median:5135
                wc :23
Mean
       :5402
                NA's: 4
3rd Qu.:8312
Max.
       :9517
```

Similar to the analysis by Blishen and McRoberts, we will begin by fitting an additive linear model with continuous numeric predictors income and education, and factor predictor type. Blishen and McRoberts's original analysis did not, however, include the predictor type. We reorder the levels of type from their default alphabetical ordering to their natural ordering:

```
Residuals:
```

```
Min 1Q Median 3Q Max -14.9529 -4.4486 0.1678 5.0566 18.6320
```

Coefficients:

```
Estimate Std. Error t value
                                             Pr(>|t|)
(Intercept) -0.6229292 5.2275255 -0.119
                                                0.905
income
            0.0010132 0.0002209
                                   4.586 0.000014049
education
            3.6731661 0.6405016
                                   5.735 0.000000121
typewc
            -2.7372307 2.5139324 -1.089
                                                0.279
            6.0389707 3.8668551
                                    1.562
                                                0.122
typeprof
```

Residual standard error: 7.095 on 93 degrees of freedom (4 observations deleted due to missingness)

Multiple R-squared: 0.8349, Adjusted R-squared: 0.8278

F-statistic: 117.5 on 4 and 93 DF, p-value: < 2.2e-16

```
R> Anova(mod.prestige.1)
```

```
Anova Table (Type II tests)
```

```
Response: prestige
```

Sum Sq Df F value Pr(>F)
income 1058.8 1 21.0339 0.0000140492
education 1655.5 1 32.8882 0.0000001205
type 591.2 2 5.8721 0.003966

Residuals 4681.3 93

The ANOVA table for the model reveals that all three terms have very small p values, suggesting that all three predictors may be useful.

An effect plot with partial residuals for income in this additive model is, except for the scaling of the vertical axis, a traditional partial residual plot:

The resulting graph, shown in Figure 6, reveals apparent nonlinearity in the partial regression of prestige on income.

An alternative story, however, is told by the term effect plot for income and type of occupation, which is higher-order than the terms actually in the model, and which can be computed using the Effect function in the effects package, producing Figure 7:

Figure 6: Predictor effect display with partial residuals for income in the additive regression of prestige on income, education, and type of occupation.

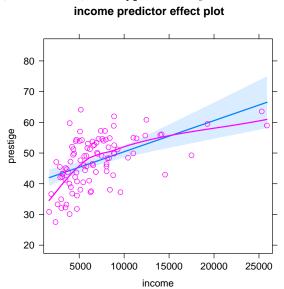
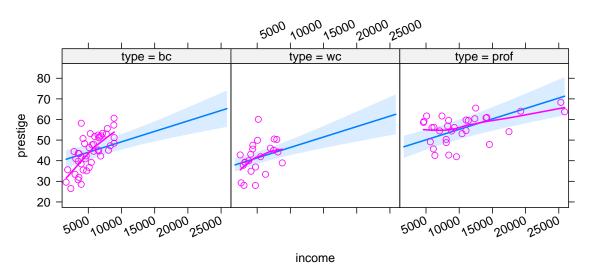


Figure 7: Term effect display with partial residuals for the predictors income and type in the additive regression of prestige on income, education, and type of occupation.

income*type effect plot



We use a large span of 0.9 for the loess smoothers in this graph because dividing the data by the levels of the factor type leaves relatively few cases in each panel of the graph. Although the relationship between prestige and income in each panel appears positive and reasonably linear, the assumption that the slopes are equal in the panels is questionable, with an apparently larger slope for blue-collar occupations, a smaller slope for professional and managerial occupations, and an intermediate slope for white-collar occupations.

Adding the linear income-by-type interaction to the model, as suggested by Figure 7, confirms this impression:

Of course, the test for the interaction needs to be taken with a grain of salt, in that we added the interaction to the model after examining the data.

Figure 8 is the term effect plot for income and type (equivalent to the predictor effect plot for income) in the model that includes the income-by-type interaction:

The nonlinearity apparent in the partial residual plot for income in the additive model in Figure 6 was induced by the relationship between income and occupational type, together with the unmodelled income-by-type interaction: Blue-collar occupations, for which the income slope is steep, are clustered at lower incomes, while professional occupations, for which the income slope is smaller, tend to have higher incomes. In addition to supporting the respecified regression, Figure 8 makes a useful pedagogical point about precision of estimation of the regression surface: The confidence envelopes show that the fitted regression is sensibly imprecisely estimated where there are no data.

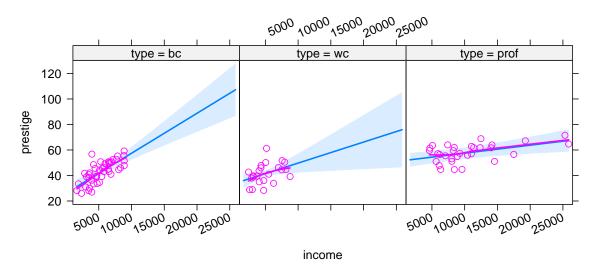
4.3. Contrived regression data

We will analyze contrived data generated according to the following setup:

• We sample n = 5000 observations from a trivariate distribution for predictors x_1 , x_2 , and x_3 , with uniform margins on the interval [-2, 2], and with a prespecified bivariate correlation ρ between each pair of predictors. The method employed, described by

Figure 8: Term effect display with partial residuals for income and type in the model incorporating the income: type interaction.

income*type effect plot



Schumann (2009) and traceable to results reported by Pearson (1907), produces predictors that are nearly linearly related. Using 5000 observations allows us to focus on essentially asymptotic behavior of partial residuals in effect plots while still being able to discern individual points in the resulting graphs.

• We then generate the response y according to the model

$$y = \beta_0 + h\left(\beta, \{x_1, x_2, x_3\}\right) + \varepsilon \tag{9}$$

where $\varepsilon \sim N(0, 1.5^2)$. The regression function $h(\cdot)$ varies from example to example.

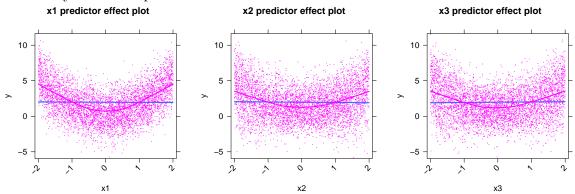
A variety of contrived examples generated in this manner, along with R functions for flexibly generating simulated data, are included in a vignette in the **effects** package.

In a sense, the example developed in this section and the examples in the vignette are unnecessary, because the results obtained are generally predictable from Cook's theoretical analysis of partial-residual plots, discussed in Section 3. We nevertheless think that these examples are useful for illustrating the application of Cook's analysis to partial-residual effect plots and for cultivating judgment about how to interpret these plots.

We consider a true model that combines nonlinearity and interaction, $E(y|\mathbf{x}) = x_1^2 + x_2x_3$; the predictors are moderately correlated, with $\rho = 0.5$. We then fit the incorrect working model $y \sim x_1 + x_2 + x_3$ to the data, producing the predictor effect displays with partial residuals in Figure 9, for the predictors x_1 , x_2 , and x_3 , which appear additively in the working model, and the term effect displays in Figure 10 for $\{x_2, x_3\}$ and $\{x_1, x_2\}$, corresponding respectively to the incorrectly excluded x_2 : x_3 term and the correctly excluded x_1 : x_2 interaction.

The nonlinearity in the partial relationship of y to x_1 shows up clearly. The nonlinearity apparent in the plots for x_2 and x_3 is partly due to contamination with x_1 , but largely to the unmodelled interaction between x_2 and x_3 , coupled with the correlation between these

Figure 9: Effect displays with partial residuals for the predictors x_1 , x_2 , and x_3 in the incorrect model $y \sim x_1 + x_2 + x_3$ fit to data generated with the mean function $E(y|\mathbf{x}) = x_1^2 + x_2x_3$, with moderately correlated predictors.



predictors. A similar phenomenon was noted in our analysis of the Canadian occupational prestige data in Section 4.2, where the unmodelled interaction between type and income induced nonlinearity in the partial relationship of prestige to income. The plot corresponding to the missing $x_2:x_3$ term (in the top panel of Figure 10) does a good job of detecting the unmodelled interaction, and curvature in this plot is slight. The plot for the $x_1:x_2$ term (in the bottom panel of Figure 10), a term neither in the true model nor in the working model, primarily reveals the unmodelled nonlinearity in the partial relationship of y to x_1 .

If we fit the correct model, $y \sim x_1^2 + x_2 * x_3$, to the data, we obtain the plots shown in Figure 11. As theory suggests, the partial residuals in these effect displays validate the model, supporting the exclusion of the $x_1:x_2$ interaction, the linear-by-linear interaction between x_2 and x_3 , and the quadratic partial relationship of y to x_1 .

5. Discussion

Graphical methods play a central role in many aspects of statistical data analysis. Their use roughly divides into three phases: an *exploratory phase*, in which an analyst examines data graphically for expected and unexpected structure (Tukey 1977); an *analysis phase*, in which graphs are used as an aid in formulating and assessing the adequacy of statistical models fit to the data; and a *presentation phase*, in which graphs provide summaries of an analysis that may be shared with others. Predictor effect plots are straightforward summary graphs for each predictor in a regression model. These plots are analogous to the usual numeric summaries of a fitted model, providing a separate explanation of the role of each predictor in a regression model after conditioning on all other relevant predictors.

The contribution of this article and the associated software in the effects package is two-fold:

- 1. We introduce predictor effect displays as an alternative to term effect displays. Predictor effect displays correspond more naturally to how researchers interpret the results of complex regression models, are simpler to describe formally, and have improved invariance properties relative to term effect displays.
- 2. Although effect displays, including effect plots with partial residuals, are related to

Figure 10: Term effect displays with partial residuals for $\{x_2, x_3\}$ (top) and for $\{x_1, x_2\}$ (bottom), the first of which corresponds to the missing $x_2:x_3$ interaction in the model generating the data.

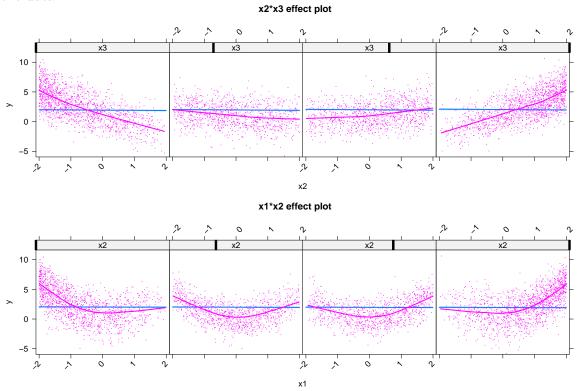
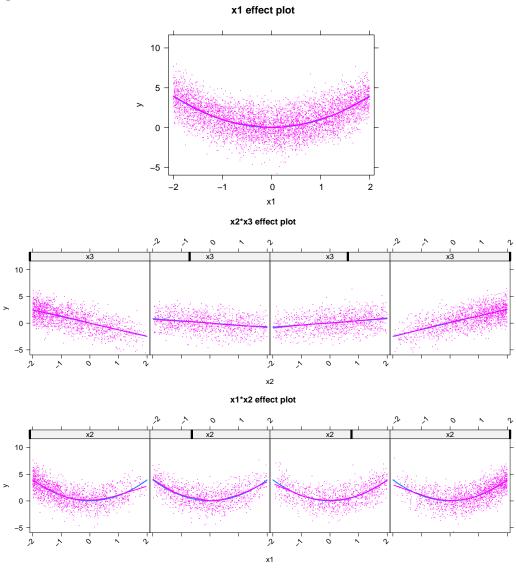


Figure 11: Effect displays with partial residuals for x_1 and $\{x_2, x_3\}$, which correspond to the terms in the model generating and fitted to the data, $y \sim x_1^2 + x_2 * x_3$, and for $\{x_1, x_2\}$, which corresponds to an interaction that is not in the model.



other approaches for interpreting complex regression models, and although the general scheme employed using two-dimensional conditioning plots is not entirely original (see below for both of these points), the conceptualization described in this paper and its implementation in the **effects** package are novel in certain respects and more general than alternative approaches.

Partial residuals in effect plots can help to detect incorrectly specified models and point toward their improvement. If the model is correctly specified, then partial residuals for predictor effects, for the high-order terms of the model, and for effects higher-order to those included in the model, should confirm the correctness of the model. On the other hand, if the model is incorrectly specified, then partial residual plots should not be interpreted naïvely, because a failure in one part of the model can contaminate plots for other combinations of predictors. For example, as we have shown, failure to model an interaction can appear as nonlinearity in a partial residual plot for one of the predictors entering the unmodelled interaction; and unmodelled nonlinearity in one predictor can also appear in the partial residuals for other predictors that are correlated with it. Awareness of these potential artifacts increases the utility of partial residual effect plots in improving complex regression models. For example, if multiple issues are detected in partial residual plots, it is generally sensible to address them one at a time, rechecking at each step.

Displays similar to effect plots are also available in a number of other implementations.

- In R, the **visreg** (Breheny and Burchett 2016) package is most similar to **effects**, but it provides only for conditioning on *specific levels* of a factor rather than *averaging over* them, as is done in the **effects** package. The **visreg** package also seems to be limited to two-factor interactions, excluding the possibility of plotting higher-order terms, so problems with more than one interaction may not be properly displayed.
- The margins and marginsplot programs in Stata (Stata Corp. 2015) create displays that are similar to effect plots, except averaging or conditioning is over the empirical distribution of the regressors rather than the predictors, which can lead to invariance problems. As far was we can see, partial residuals cannot be added to a margins plot.
- Least-squares means (a generalization of adjusted means in analysis of covariance, introduced by Fisher 1936), as implemented in SAS (SAS Institute Inc. 2012) and the **Ismeans** package for R (Lenth 2016; Lenth and Hervé 2015), are capable of displaying interactions among factors, and in certain instances least-squares means coincide with effect displays. Partial residuals are not relevant to displays of least-squares means, however.

For a linear predictor with only main effects, adding partial residuals to an effect plot is straightforward, and provides little that is new. For example, the plots produced by the gam functions in the mgcv (Wood 2017) and gam (Hastie 2015) packages are effect plots with partial residuals added. In an early general article on Trellis displays, Becker, Cleveland, and Shyu (1996) include a graph (their Figure 6) that they describe as a partial residual plot. Rather than fitting an explicit model to the data, however, they subtract marginal means for one factor from the data in a three-way classification with one case per cell, and then plot the resulting values against the other two factors. This procedure works because the data are balanced, and is equivalent to fitting a one-way ANOVA for one of the three factors. The

procedure is not general, however, and the plotted values wouldn't typically be termed partial residuals.

The functions in the **effects** package rely on the presence of a linear predictor in a regression model, and are therefore not suitable for less structured approaches to regression, such as regression trees. For this case, Friedman (2001) suggested plots obtained by averaging the estimate of $\hat{y}(\mathbf{x})$ over the empirical distribution of the predictors. Goldstein, Kapelner, Bleich, and Pitkin (2015) call these *individual conditional expectation* or *ICE* plots, and have implemented them in the **ICEbox** package (Goldstein *et al.* 2015) for R. These plots don't use a linear predictor and are therefore likely to be harder to interpret than predictor effect plots in problems for which the latter are appropriate.

The new ideas and software described in this article were not developed in a vacuum. In particular, we owe a debt to the general notion of conditioning plots (Cleveland 1993, 1994) and to their implementation in Trellis graphics (Becker and Cleveland 1996). In particular, the manner in which we handle the computation and display of partial residuals is loosely inspired by "shingles" in Trellis graphics, although it doesn't use shingles (overlapping sub-ranges for a continuous variable) in the literal sense. We also clearly lean heavily on the theoretical results concerning partial residuals developed by Cook (1993) and Cook and Croos-Dabrera (1998).

Predictor effect plots are reasonably easy to apply to a variety of modeling frameworks that use a linear predictor. In the effects package for R, we have included methods for linear, multivariate linear, and generalized linear models fit by the standard 1m and glm functions and by the svyglm function in the survey package (Lumley 2004); linear models fit by generalized least squares using the gls function in the nlme package (Pinheiro, Bates, DebRoy, Sarkar, and R Core Team 2016); multinomial regression models fit by multinom in the nnet package (Venables and Ripley 2002); ordinal regression models using polr from the MASS package (Venables and Ripley 2002) and clm and clm2 from the ordinal package (Christensen 2015); linear and generalized linear mixed models using the lme function in the nlme package (Pinheiro et al. 2016) and the 1mer and glmer functions in the lme4 package (Bates, Mächler, Bolker, and Walker 2015); and latent class models fit by poLCA in the poLCA package (Linzer and Lewis 2011). We also include a generic method that may work with models fit by other functions that employ a linear predictor. Partial residuals, however, are not available, or even useful, for many of these classes of models. At present, we provide partial residuals for models of arbitrary complexity fit by 1m, glm, 1mer, glmer, and 1me.

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