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Dynamic Added Variable Plots[1)]

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Abstract

Partial residual plots, augmented partial residual plots and CERES plots are basic diagnostic tools for dealing with curvature as a function of specific predictors in regression problem. However, it is known that these plots can miss a curve or show a false curve in some cases such as predictors are related each other. Dynamic display of these plots is developed and applied. Examples demonstrate that dynamic plots are useful for obtaining additional information on the curvature.

Keywords : ARES plot, Augmented partial residual plots, CERES plots, Partial residual plots, Dynamic graphics.

1. Added variable plots

Consider a regression model:

$$Y = \beta_0 + X\beta_1 + f(Z) + \varepsilon \tag{1.1}$$

where β_1 is an unknown $(p-1)\times 1$ vector, Z is an explanatory variable, ε is independent of X and Z, and f is unknown function. Then a model in which a new explanatory variable W is included to the Eq. (1.1) is defined as

$$Y = \alpha_0 + X\alpha_1 + g(Z) + \gamma W + \varepsilon. \tag{1.2}$$

As a variable W is added to the model (1.1), the function of Z is affected. From Eq. (1.1) and (1.2) conditional expected values are calculated as $E(Y \mid X, Z, W) = \alpha_0 + X\alpha_1 + g(Z) + \gamma W$, $E(Y \mid X, Z) = \beta_0 + X\beta_1 + f(Z)$ and $E(Y \mid X, Z) = \alpha_0 + X\alpha_1 + g(Z) + \gamma E(W \mid X, Z)$. If, given Z, W is independent of X then

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$\beta_0 = \alpha_0$, $\beta_1 = \alpha_1$ and $f(Z) = g(Z) + \gamma E(W|Z)$. This article concerns a development and a comparison of dynamic plots of various graphical methods, displaying the impact caused by smooth transition between the fit of (1.1) and the fit of (1.2).

For visualizing f in (1.1) several graphical methods including partial residual plots, augmented partial residual plots and CERES plots are suggested. Partial residual plots (Larsen and McLeary, 1972) are constructed based on the model

$$Y = a_0 + Xa_1 + Zb + error \tag{1.3}$$

and obtain coefficient estimates by minimizing a convex objective function :

$$(\hat{a_0}, \hat{a_1}, \hat{b}) = \arg\min L_n(a_0, a_1, b) \tag{1.4}$$

where $L_n(a_0, a_1, b) = \frac{1}{n}\sum_{i=1}^{n} L(y_i - a_0 - x_i a_1 - z_i b)$ and L is a convex objective function. A partial residual plot for Z is described as the plot of $e + Z\hat{b}$ versus Z and is expected to depict f correctly only with variability caused by error when f is linear or $E(X \mid Z)$ is linear in Z. But to have a firm information indicating that f is linear when a partial residual plot is linear, the condition that $E(X \mid Z)$ is linear in Z is always required. When conditional expectations $E(X \mid Z)$ are all linear, partial residual plots would be enough to examine the curvature in regression problem. Partial residual plots are especially good for detecting curve, even if there is substantial collinearity. But it does not work well if there are nonlinear relationships among the predictors.

Augmented partial residual plots are another diagnostic plot, suggested by Mallows (1986), to improve the ability of partial residual plots. Augmented partial residual plots replace the model (1.3) with a model containing a quadratic term in Z :

$$Y = \rho_0 + X\rho_1 + \phi_1 Z + \phi_2 Z^2 + error. \tag{1.5}$$

An augmented partial residual plot for Z is construct as the plot of $e + \hat{\phi_1} Z + \hat{\phi_2} Z^2$ versus Z where coefficient estimates are obtained by minimizing a convex objective function defined in (1.4). Evidently augmented partial residual plots can depict f better than partial residual plots if $\phi_1 Z + \phi_2 Z^2$ provides a better approximation of $f(Z)$. If f is exactly quadratic or $E(X \mid Z)$ is a quadratic in Z then augmented partial residual plots reflect the form of f accurately with random variation. Whatever the form of f is, an augmented partial residual plot can display f better than a partial residual plot.

CERES plots, an abbreviated acronym for "Combining Conditional Expectations and

RESiduals" were suggested by Cook(1993). To depict f accurately it is required that $E(X \mid Z)$ should be included in the function of Z as a special case. If we let the model be

$$Y = a_0 + Xa_1 + E(X \mid Z)b + error \tag{1.6}$$

then estimate $\widehat{a_1}$ in (1.4) converges almost surely to β_1 in (1.1), and consequently $e_i + E(X \mid Z_i)\hat{b}$ converges to $constant + f(Z_i) + \varepsilon_i$. CERES plots use $e + E(X \mid Z)\hat{b}$ on the vertical axis and Z on the horizontal axis. $E(X \mid Z)$ can be modeled either parametrically or nonparametrically. If $E(X \mid Z)$ is linear in Z CERES plots are same as partial residual plots. And if $E(X \mid Z)$ is quadratic in Z CERES plots are same as augmented partial residual plots. CERES plots are designed to work well even when predictors are arbitrary noise function of each other or when $E(X \mid Z)$ are neither linear nor quadratic. But Many examples show that the efficiency of CERES plots depends sensitively on the accuracy of the estimated value of $E(X \mid Z)$.

Johnson and McCulloch(1987) compared partial residual plots and augmented partial residual plots. They suggested another plot based on locally linear approximation method. Berk and Booth(1995) also compared nine graphical methods including added variable plot, partial residual plots, augmented partial residual plots and CERES plots. Cook(1993) extended the residual plot to three dimensions and showed how 3-D partial residual plots can be applied (Cook and Weisberg, 1994). Berk(1998) showed that 2-D add variable plots, partial residual plots, augmented partial residual plots are included as views in the 3-D plots.

In section 2 dynamic plots are constructed using partial residual plots and augmented partial residual plots for the specification of function f at each plot in the animation. Section 3 includes examples which were selected to show that the dynamic display of these plots, including animated CERES plots (Seo, 1999), can give us a warning against detecting false curve or missing a curve. Section 4 contains concluding remarks.

2. Dynamic plots

The effects of adding a variable W to the model (1.1) can be identified by displaying smooth transition between the fit of (1.1) and the fit of (1.2). For this purpose the idea of ARES plot, proposed by Cook and Weisberg(1989, 1994), can be applied. ARES plot is designed to show the impact of a set of added predictors between two models,

$$Y = \beta_0 + X\beta_1 + \varepsilon \tag{2.1}$$

and

$$Y=\beta_0+X\beta_1+\psi W+\varepsilon. \tag{2.2}$$

ARES plot begins with a smaller linear model then smoothly add a predictor W according to some control parameter $\lambda\in[0,1]$ so that λ=0 corresponds to fitting (2.1) and when λ=1 full model (2.2) is fit. The plot consists of some specific aspect of the fitted, such as a plot of $\hat{\eta}_\lambda$ versus e_λ, where $\hat{\eta}_\lambda, e_\lambda$ are, respectively, the fitted values and residuals obtained when the control parameter is equal to λ.

Now we use partial residual plots instead of using residual plots in the ARES plot procedure which begins with model (1.1) and then smoothly adds W, ending with fit of the full model (1.2). Consider the following model:

$$\begin{aligned} Y&=X^*a+Zb+\gamma W+\varepsilon \\ &=U\delta+\gamma W+\varepsilon \end{aligned} \tag{2.3}$$

where $X^*=(1_n:X)$ is n by p fixed known matrix , $a=(a_0:a_1^T)^T$ is p by 1 vector, b is a scalar and W is n by 1 known vector, γ is an unknown scalar and $U=(X^*:z)$ $\delta=(a^T b)^T$. Let Q_u be the projection operator on the orthogonal complement of the space spanned by the columns of U. Then modified version of (2.3) is

$$Y=U\delta^*+\gamma^*\tilde{W}+\varepsilon \tag{2.4}$$

where $\tilde{W}=Q_uW/\|Q_uW\|$, $\delta^*=\delta+\gamma(U^TU)^{-1}U^TW$. For each $0<\lambda\leq 1$ we estimate $a=(\delta^*\ \gamma^*)^T$ by

$$\hat{a}_\lambda=(V^TV+\frac{1-\lambda}{\lambda}cc^T)^{-1}V^TY \tag{2.5}$$

where c is a $2p$ by 1 vector of zeros except for a single 1 corresponding to W, and . $V=(U:\tilde{W})$. And for each λ and $\hat{a}_\lambda$, we denote the corresponding estimators as $\hat{\delta}_\lambda$, $\hat{\gamma}_\lambda$, $\hat{a}_\lambda$, $\hat{b}_\lambda$. $\hat{a}_\lambda$ is a ridge estimator. The ordinary ridge regression estimator of Hoerl and Kennard (1970) is based on kI rather than $\frac{1-\lambda}{\lambda}cc^T$ in (2.5) to portray the sensitivity of the estimates to the particular set of data being used. $\hat{a}_\lambda$, with $\frac{1-\lambda}{\lambda}cc^T$ represents the effect of adding variable W. For a particular value of λ the residuals and fitted values from the fit of (2.4) are respectively

$$\hat{Y}_\lambda=U(U^TU)^{-1}U^TY+\lambda\tilde{W}(\tilde{W}^T\tilde{W})^{-1}\tilde{W}^TY$$

$$e_\lambda=e+(1-\lambda)\tilde{W}(\tilde{W}^T\tilde{W})^{-1}\tilde{W}^TY$$

where e is residual from the fit of model (2.4). At $\lambda=1$ $\widehat{\alpha_\lambda}$ is the ordinary least squares regression of Y on U and W. When $\lambda=0$ $\widehat{\alpha_\lambda}$ corresponds to the estimate in the fit of the regression model of Y on U. As λ increases from 0 to 1, $\widehat{\alpha_\lambda}$ becomes a sequence of estimators that represent the effect of adding W smoothly to the smaller model. Thus an animated plot of $e_\lambda+Z\widehat{b_\lambda}$ versus Z, where $e_\lambda = Y-U\widehat{\delta_\lambda}-\widehat{\gamma_\lambda}W$, gives a dynamic view of the effects of adding W to the model which already includes X and Z.

For an animated augmented partial residual plot the following model is considered:

$$\begin{aligned} Y &= \rho_0+X\rho_1+\phi_1 Z+\phi_2 Z^2+\gamma W+\varepsilon \\ Y &= X^* a+Db+\gamma W+\varepsilon \\ &= U\delta+\gamma W+\varepsilon \end{aligned} \tag{2.6}$$

where $X^*=(1_n:X)$, $D=(Z:Z^2)$, n by p and n by 2 fixed known matrix respectively, $a=(a_0:a_1^T)^T$ is p by 1 vector, b is 2 by 1 vector and $U=(X^*:D)$ $\delta=(a^T b^T)^T$. Following the expressions in the model (2.4) and estimators in (2.5) an animated augmented partial residual plot can be constructed as a plot of $e_\lambda+(E(X\mid Z)-E(Z))\widehat{b_\lambda}$ versus Z, where $e_\lambda = Y-U\widehat{\delta_\lambda}-\widehat{\gamma_\lambda}W$. Animated CERES plots were constructed by letting $D=E(X\mid Z)-E(Z)$ in the model (2.6) and defined as $e_\lambda+(E(X\mid Z)-E(Z))\widehat{b_\lambda}$ versus Z, where $e_\lambda = Y-U\widehat{\delta_\lambda}-\widehat{\gamma_\lambda}W$ (Seo, 1999).

3. Examples

It is known that diagnostic plots fail to detect a curve correctly for some cases (Berk and Booth, 1995; Cook, 1996). For example, CERES plots and augmented partial residual plots could give false curve when a curve really does belong to another variable. We apply dynamic plots developed in section 2 to the cases that usual diagnostic plots do not work well. Customized animation plots displayed throughout the examples are coded by using Xlisp-stat. (Tierney, 1990).

Examples are considering the problem of hidden variable with four predictors x_1, x_2 , x_3 and x_4. Assume that x_4 is defined by $x_4\approx h(x_3)$ and dependent variable y is related with predictors by one of following models:

$$y = x_1+x_2+h(x_3)+N(0\,,0.1^2), \tag{3.1}$$

$$y = x_1 + x_2 + x_4 + N(0, 0.1^2). \tag{3.2}$$

Then diagnostic plots for x_3 with predictors x_1, x_2 may give same image for both of model (3.1) and (3.2). To determine the true model between (3.1) and (3.2), animated plots of x_3 with adding variable x_4 are applied. Several cases are considered according to the different form of $h(x_3)$ which is assumed to be either linear or quadratic or cubic.

Data for examples are artificially created. x_3 is consist of 100 values spaced evenly between -1 and 1 including values -1 and 1. Then x_4 is defined by $x_4 = h(x_3) + N(0, 0.1^2)$. x_1 and x_2 are two independent normal random variables with mean 1 and variance 5^2.

Case A : $h(x_3) = x_3$

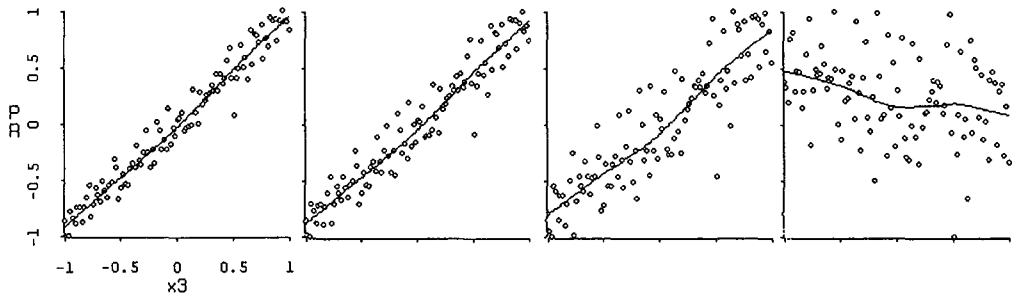
Dependent variable y was generated according to the model (3.1) with $h(x_3) = x_3$. With adding variable x_4, Figure 1 shows animated plots of partial residual plots, augmented partial residual plots and CERES plots for x_3 of independent variables x_1, x_2 and x_3. Loewss smooths are superimposed. Four frames of animated plots in Figure 1 correspond to λ = 0, 0.3 0.6 1 respectively. The first frames of three diagnostic plots show a substantial linearity. As λ moves from 0 to 1 partial residual plots and augmented partial residual plots still imply a linear relationship, but CERES plots do not show any trend.

With the same data of x_1, x_2, x_3 and x_4, dependent variable y is defined by the model (3.2). Animated plots with these data are shown at Figure 2. The first frames of three diagnostic plots show a linear trend. But as λ moves from 0 to 1 neither of them shows a perceptible line. When λ=1 that is, x_4 is fully included, CERES plot does not show any trend with or without x_3 in the model. This is partly because of indeterminacy of CERES plots (Cook, 1995) caused by the fact that x_4 is nearly a function of x_3. But it is mainly because the estimated values of expectation of predictors given x_3 are not certain.

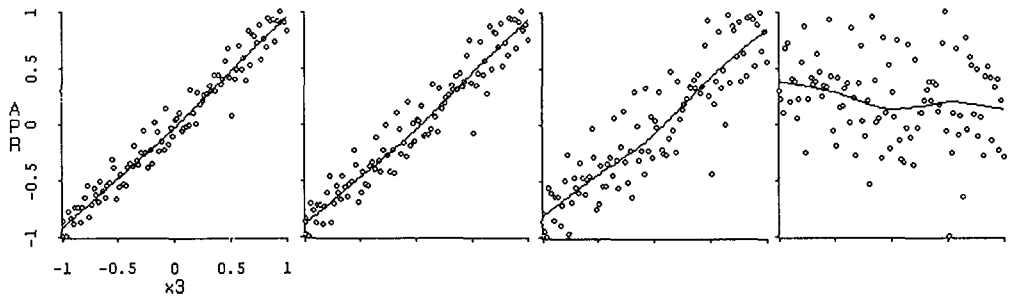
As we can see at Figure 1, Figure 2, diagnostic plots for x_3 with predictors x_1, x_2, x_3 draw a straight line regardless of inclusion of x_3 to the model. But we can get a clue to find a true model from animated plots. If partial residual plots and augmented partial residual plots for x_3 show a linearity both with and without predictor x_4, then we do have information indicating that the function of x_3 is truly linear. But if partial residual plots and augmented partial residual plots for x_3 do not show any trend with adding variable x_4 then the linearity of x_3 implied by partial residual plots and augmented partial residual plots with predictors

x_1, x_2 and x_3 is wrong and the correct model does not involve x_3.

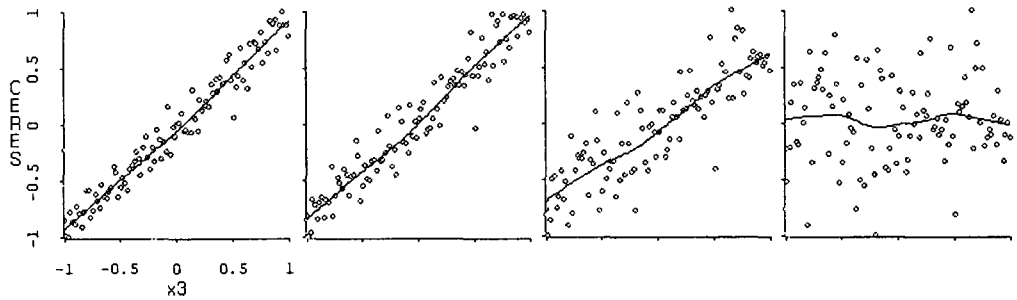
Now we consider a case that the behaviors of partial residual plots and those of augmented partial plots are different.



(a) Animated Partial Residual Plots

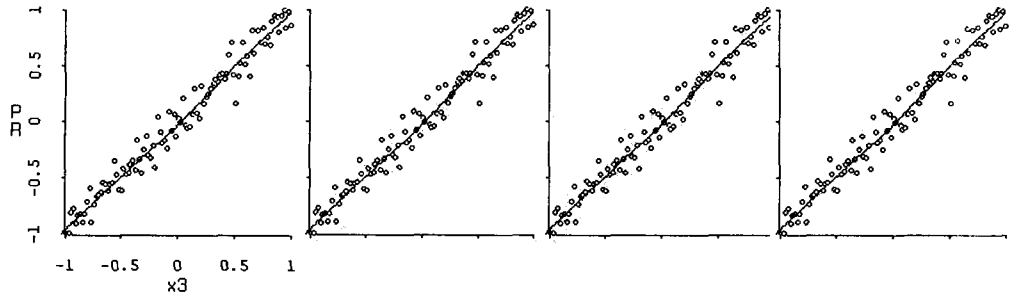


(b) Animated Augmented Partial Residual Plots

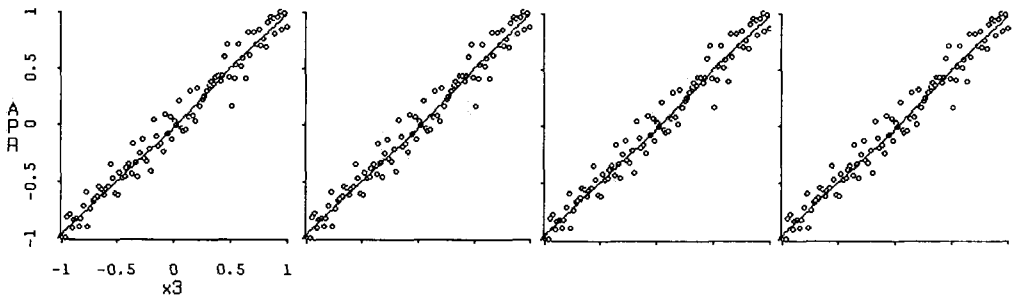


(c) Animated CERES Plots

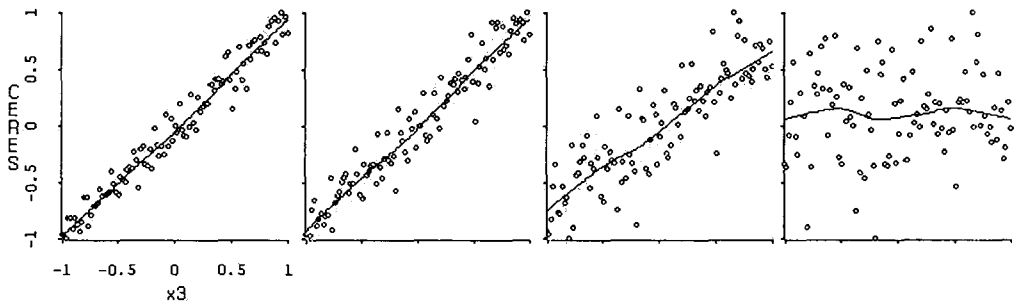
Figure 1. Animated plots under model (3.1) for Case A. λ = 0, 0.3, 0.6, 1.



(a) Animated Partial Residual Plots



(b) Animated Augmented Partial Residual Plots



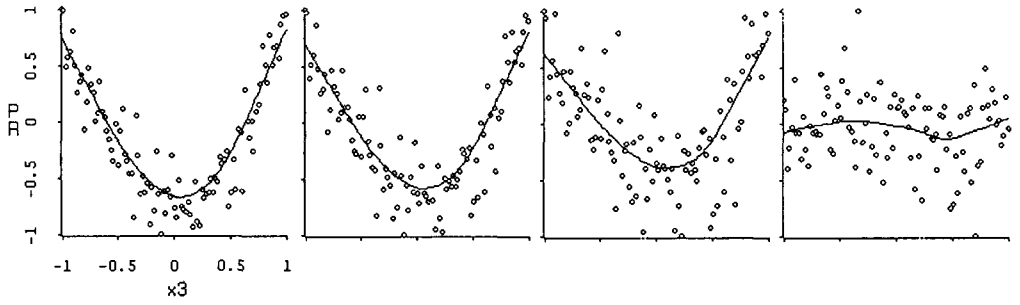
(c) Animated CERES Plots

Figure 2. Animated plots under model (3.2) for Case A. λ = 0, 0.3, 0.6, 1.

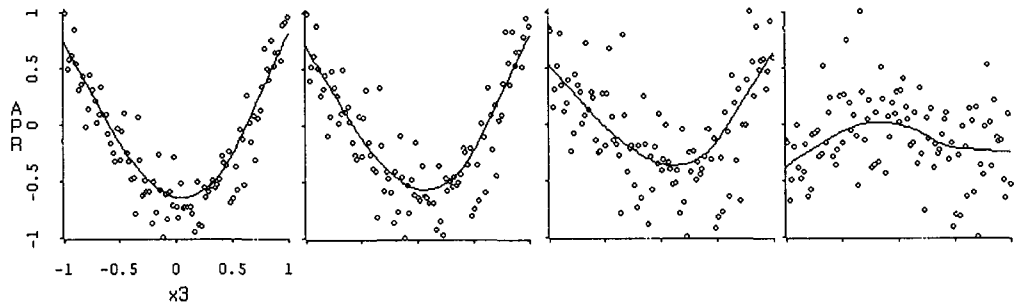
Case B : $h(x_3) = x_3^2$

Because of the quadratic terms in x_3 and the quadratic relationship between x_3 and x_4, augmented partial residual plots can retrieve a curve in this case. Animated plots for x_3 with adding variable x_4 are displayed at Figure 3 and Figure 4, in which dependent variable y is defined by the model (3.1) and (3.2) respectively. When $\lambda = 0$, three diagnostic plots at Figure 3 and Figure 4 show a curve. As λ moves from 0 to 1 only augmented partial residual plots at Figure 3 keep showing a curvature but none of diagnostic plots at Figure 4

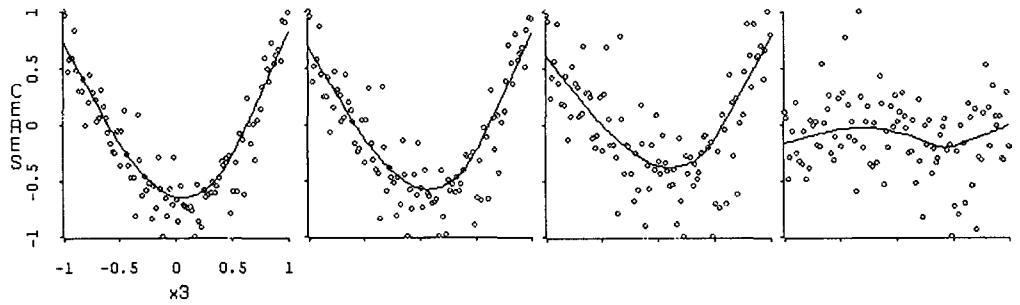
shows a clear curve. So if an augmented partial residual plot with predictors x_1, x_2 and x_3 shows a curve in x_3, and keeps showing a curvature throughout the display of animation, it indicates that the function of x_3 is really quadratic. But if augmented partial residual plots do not show any trend with adding variable x_4 then augmented partial residual plots showing a curve in x_3 with predictors x_1, x_2 and x_3 give false alarm about the need for transforming x_3. CERES plots may show a curve in this case with $\lambda = 1$ as in Berk and Booth(1995). But as mentioned early, because of the uncertainty of estimation of conditional expectation it does not show any trend.



(a) Animated Partial Residual Plots

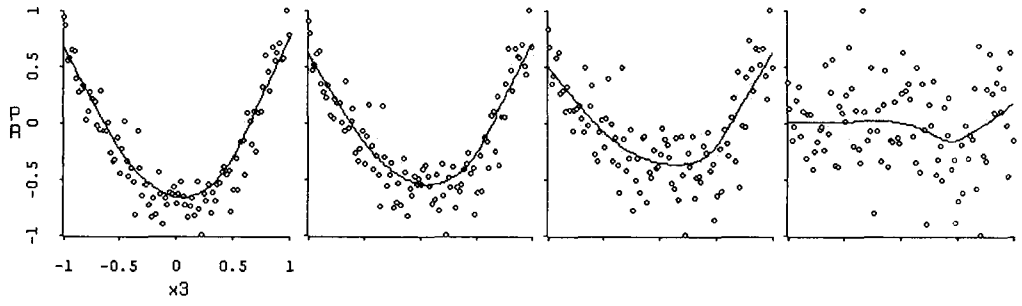


(b) Animated Augmented Partial Residual Plots

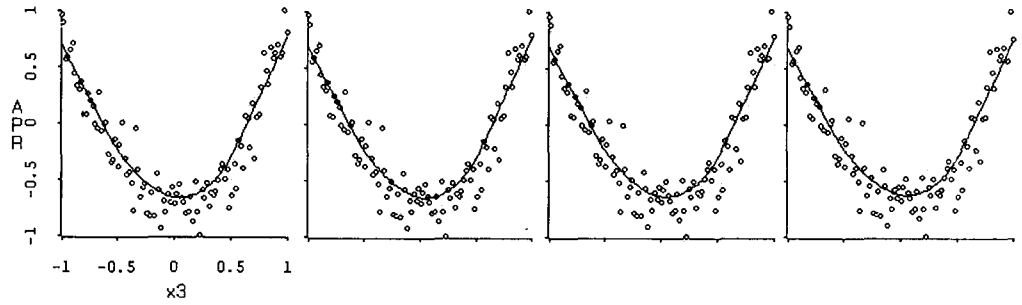


(c) Animated CERES Plots

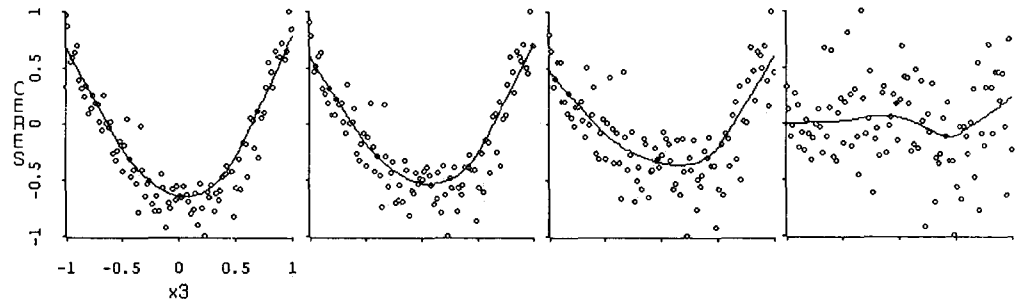
Figure 3. Animated plots under model (3.1) for Case B. λ = 0, 0.3, 0.6, 1.



(a) Animated Partial Residual Plots



(b) Animated Augmented Partial Residual Plots



(c) Animated CERES Plots

Figure 4. Animated plots under model (3.2) for Case B. λ = 0, 0.3, 0.6, 1.

Case C : $h(x_3) = x_3^3$

When cubic relationship is involved in the model or in the relationship between predictors, unlike in case A and case B, neither of partial residual plots nor augmented partial residual plots work well. Under the model (3.1) and (3.2) the behaviors of plots are nearly same. When $\lambda = 0$, plots show a cubic but as λ moves from 0 to 1 none of diagnostic plots shows a curve. So when an augmented partial residual plot with predictors x_1, x_2 and x_3 shows a cubic in x_3, it is not easy to know the inclusion of x_3 in the correct model from the

animation. CERES plots in this case do not look useful either. We skip the figures of this case.

4. Concluding remarks

Though partial residual plots, augmented partial residual plots and CERES plots are used widely for detecting a curve, for some cases they may give an uncorrect curve or a false curve of a predictor which is not involved in the model. Useful information regarding these problems can be obtained by animating plots. Especially when a visualized image is linear or quadratic, animated augmented partial residual plots can be helpful to discern between two specific models. Behaviors of animated CERES plots heavily depend on the accuracy of estimated values of conditional expectations and indeterminancy caused by a functional relationship among predictors.

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