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TWO BOOKS ON REGRESSION DIAGNOSTICS

D. A. BELSLEY, E. KUH AND R. E. WELSCH, *Regression Diagnostics: Identifying Influential Data and Sources of Collinearity.* John Wiley and Sons, New York, 1980, xv + 292 pages, $32.95.

R. D. COOK AND SANFORD WEISBERG, *Residuals and Influence in Regression.* Chapman and Hall, New York and London, 1982, x + 230 pages, $25.00.

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My brief in writing this article was not only to review the two books but also to provide a survey of the field of regression diagnostics, including some mention of unsolved problems; these suggestions for research come at the end of the article. In the major part of the article the methods of regression diagnostics are developed with reference to the material in the two books. But first the material must be put in context.

Diagnostic methods are directed at the building and criticism of statistical models. Traditional statistical procedures, such as model fitting and hypothesis testing, are not adequate for this task. For example, rejection of a model does not, *per se*, give guidance as to a more suitable model. Similarly, failure to reject a model does not guarantee that all important aspects of the fit have been adequately examined. One effect of the almost ubiquitous use of the computer in statistics has been the relative ease with which graphs may be produced and used to test models. At the level of text books on regression, the increase in the use of graphical material can be seen by comparing the books of Brownlee (Second edition, 1965), Draper and Smith (1966) and Box, Hunter and Hunter (1978). This trend may be partly due to the increased impact in our society of television as against the printed word. But one of the achievements of diagnostic regression analysis is to provide a framework within which to produce graphs which illustrate both the effect of individual observations on aspects of the fitted model and also ways in which the model is systematically inadequate.

A second consequence of the computer is that complicated statistical analyses can now be routinely performed by scientists with little statistical training or expertise. A major use of diagnostic methods, especially plots, is to call attention to important features of the data which may have been overlooked. The combination of computer and the diagnostic approach may then serve as a substitute for the insight and guile of an experienced statistician. For this combination to be effective the methods have to be easy to program, so that they can readily be added to, or incorporated in, a statistical package. They must also be cheap to compute and the results must be easily intelligible.

The product of a diagnostic analysis may be the identification of an inadequate

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model, in which case the model can be elaborated and the cycle of fitting and diagnosis repeated. Or the analysis may lead to the identification of inexplicable features in the data, such as apparent outliers. Such features should, in turn, lead to further experimentation or data collection. Cook and Weisberg (1983) contrast this emphasis on identification with robust methods where the emphasis is on accomodation. By this they are calling attention to the use of robust methods to fit a model to the data in the knowledge that a small, but unidentified, fraction of the observations comes from some other process.

There is nothing in these general remarks which is specific to regression models and least squares. Box (1980) provides a discussion of model building and criticism from a Bayesian point of view. Several of the diagnostic measures which he derives are close to those discussed in the two books. There is also no restriction to linear models: diagnostic measures can readily be developed for all members of the family of generalized linear models (McCullagh and Nelder, 1983). But we begin where the books begin, with the least squares analysis of linear regression models.

A regression model and the data to which it is fitted may disagree for several reasons. These include:

1. There may be gross errors in either response or explanatory variables, which could arise, for example, from errors in key punching or data entry;
2. The linear model may be inadequate to describe the systematic structure of the data;
3. It may be that the data would be better analysed in another scale, for example after a logarithmic or other transformation;
4. The error distribution for the response variable may be appreciably longer tailed than the normal distribution. As a result, least squares may be far from the best method of fitting the model.

These departures are not all equally easy to identify. The methods of diagnostic regression analysis are concerned with detection of the first three kinds of departure. The main purpose of robust regression is estimation in the presence of the fourth departure, that of error distributions other than normal. We return to this topic at the end of the article where unsolved problems are discussed.

To detect departures which are hidden by the fitting process, the methods of diagnostic regression rely on the effect on the fitted model and its residuals of the deletion of one, or a group, of observations. We begin by considering the linear regression model $E(Y) = X\beta$, where X is an $n \times p$ matrix of known carriers, which are functions of the explanatory variables: as usual, $\text{var}(Y) = \sigma^2 I$. The deletion of only one observation at a time will be considered. The deletion of a group of observations introduces few new ideas, although it can lead to appreciable difficulties in interpretation of the mass of material which results.

For the linear model, the least squares estimate of β is $\hat{\beta} = (X^TX)^{-1}X^Ty$ and the predicted values are given by

$$\hat{y} = X\hat{\beta} = X(X^TX)^{-1}X^Ty = Hy, \tag{1}$$

where H, with diagonal elements h_i, is the "hat" matrix. The ordinary residuals

$$r = y - \hat{y} = (I - H)y \tag{2}$$

have variance $\mathrm{var}(r) = \sigma^2(I - H)$, so that the standardized residuals

$$r_i' = r_i/\sqrt{s^2(1 - h_i)} \tag{3}$$

all have the same variance. In (3) s^2 is the usual residual mean square estimate of σ^2.

The agreement of the ith observation with the fit from the remaining $n - 1$ observations can be checked by comparing the prediction

$$\hat{y}_{(i)} = x_i^T\hat{\beta}_{(i)}, \tag{4}$$

where the subscripted i in parentheses is to be read as "with observation i deleted", with the observed value y_i. The t test for this comparison reduces to the "deletion" residual

$$r_i^* = r_i/\sqrt{s_{(i)}^2(1 - h_i)}, \tag{5}$$

which can be shown to be a monotone function of the standardized residual r_i'.

How do these quantities relate to the departures mentioned at the beginning of this article, and how are they to be used? The quantity h_i, often called a "leverage" measure, indicates how remote, in the space of the carriers, the ith observation is from the other $n - 1$ observations. For a balanced experimental design, such as a D-optimum design, all $h_i = p/n$. For a point with high leverage, $h_i \rightarrow 1$ and the prediction at x_i will be almost solely determined by y_i, the rest of the data being irrelevent. The ordinary residual r_i will therefore have very small variance. Points with high leverage are often created by errors in entering the values of the explanatory variables. Investigation of the values of h_i and of the deletion residuals r_i^* is therefore one way of checking for such a departure. For the r_i^*, which, unlike the h_i, are random variables, it is possible to conduct a formal t test for departure from the model, allowance for selection being made by use of the Bonferroni inequality. It is usual, and more helpful, to give plots of the values. Both Belsley, Kuh and Welsch (1980) and Cook and Weisberg (1982) give normal probability plots of residuals: r_i^* in the former case and r_i' in the latter. Both sets of authors also give plots of the residuals against observation number, that is, index plots. Cook and Weisberg also give examples of index plots of the h_i.

The nomenclature in the two books is not the same. Cook and Weisberg call (3) an internally studentized residual, with (5) called externally studentized. In the analysis of examples (3) is used and is called studentized, the name which Belsley et al. reserve for (5). In view of the potential for confusion which this introduces, it seems prudent to avoid the term studentized, as has been done here, where (5) is called a deletion residual. The notation of Belsley *et al.* for this residual is RSTUDENT, one of many examples in their book of the rebarbative effect of Fortran on notation and variable names. Although the two residuals are monotone functions of each other, the use of (5) is slightly to be preferred for normal plotting. Obviously there can be no difference for hypothesis testing, although it is easier to refer (5) to tables of the t distribution than to refer the square of (3) to the scaled beta distribution.

Perhaps more important than the identification of outliers is the use of diagnostic methods to identify influential observations, that is, observations which significantly affect the inferences drawn from the data. Methods for assessing influence are based on the change in the vector of parameter estimates when observations are deleted, given by

$$\hat{\beta} - \hat{\beta}_{(i)} = (X^T X)^{-1} x_i r_i / (1 - h_i). \tag{6}$$

The individual components of this p vector can be used to determine the effect of observation i on the estimation of β_j. The change can also be scaled by the estimated standard error of $\hat{\beta}_j$. When σ^2 is estimated by $s^2_{(i)}$ this procedure yields the quantity which Belsley *et al.* call DFBETAS_{ij}.

If particular components of (6) are of interest, the sensitivity of the parameter estimate to individual observations can be displayed in an index plot. If instead the vector of estimates is of interest, Cook's distance measure, a version of the sample influence curve, is found by considering the position of $\hat{\beta}_{(i)}$ relative to the confidence region for β derived from all the data. Then

$$D_i = (\hat{\beta}_{(i)} - \hat{\beta})^T X^T X (\hat{\beta}_{(i)} - \hat{\beta})/ps^2 = (1/p) r_i'^2 \{h_i/(1 - h_i)\}. \tag{7}$$

Cook and Weisberg give index plots of (7). Modifications of the square root of (7) lead to quantities which are multiples of residuals, which can therefore meaningfully be plotted in ways similar to those used for residuals. For example, in Atkinson (1981) I suggested the use of half normal plots, with a simulation envelope, of the modified Cook statistic

$$C_i = \left\{ \frac{n - p}{p} \cdot \frac{h_i}{1 - h_i} \right\}^{1/2} | r_i^* |. \tag{8}$$

Examples of the use of this quantity, which Belsley et al. call DFFITS_i, are given by Cook and Weisberg.

These are some of the basic diagnostic quantities which are becoming available in computer packages. Use of them can lead to detection of the first of the four kinds of departure with which I began this article. For the detection of systematic departures another tool is needed. Suppose that the model with carriers X has been fitted and it is desired to determine whether a new carrier w should be added to the model. The augmented model is

$$E(Y) = X\beta + w\gamma. \tag{9}$$

Although a plot of residuals against w may indicate the need to include the new carrier, this plot will not, in general, have slope $\hat{\gamma}$. Plots with this desirable property can be derived from least squares estimation in the partitioned model (9) which yields

$$\hat{\gamma} = \frac{w^T \{I - X(X^T X)^{-1} X^T\} y}{w^T \{I - X(X^T X)^{-1} X^T\} w} = \frac{w^T (I - H) y}{w^T (I - H) w} = \frac{w^T A y}{w^T A w}, \tag{10}$$

a result familiar from the analysis of covariance. Since A is idempotent, $\hat{\gamma}$ is the coefficient of regression of the residuals r on the residual variable

$$\overset{*}{w} = Aw. \tag{11}$$

A plot of r against $\overset{*}{w}$ is called an added variable plot. It provides a means of assessing the effect of individual observations on the estimated coefficient $\hat{\gamma}$.

With these basic ideas and definitions established, it is time to begin the review of the two books. One important basic difference is that the work described in Belsley *et al.* arose in economics, whereas Cook and Weisberg take their examples from the natural and engineering sciences. The ethos of the latter book will therefore be familiar to readers of *Biometrika* or of *Technometrics.* Perhaps because of this difference in applications, Belsley *et al.* stay much closer to least squares than do Cook and Weisberg.

Both books open with a brief first chapter. Chapter 2 of Belsley *et al.* lists the diagnostic tools described above, together with some others that are closely related. To my mind, a defect of this section is that the writing does not distinguish sufficiently between those tools that are important and those that are not. The second section of the chapter applies the methods to an analysis of data on personal savings in 50 countries. The results presented in the book do not entirely avoid the sensation of being the uncritical reproduction of tables produced by computer. The ability to produce an indigestible amount of numerical information by the application of even a few single deletion diagnostics to a handful of models is the main hazard of diagnostic regression. The solution is the use of graphical methods to highlight informative results. For their example Belsley *et al.* give one normal plot of residuals and five added variable plots. Because these are calculated to show the effect of dropping variables from the model, the calculations, but not the plots, are different. To stress the difference, the name partial regression leverage plots is used.

The basic material on diagnostic quantities is spread over two chapters in Cook and Weisberg. Chapter 2, "Diagnostic Methods using Residuals", describes the residuals mentioned above as well as BLUS and recursive residuals. Examples are given of the use of plots in the analysis of five data sets. The plots include normal plots, index plots and added variable plots. Chapter 3, "Assessment of Influence", begins with a general theoretical discussion of influence, from which Cook's distance measure emerges as one of several related possibilities. Further examples are analysed and plots given, including half normal plots of the modified Cook statistic (8) with a simulation envelope as an aid to interpretation.

One kind of departure not mentioned since the beginning of this review is the third in the initial list. That is, a transformation of the response may be needed to reconcile the data and a simple linear model. Experience suggests that lack of a transformation is a frequent cause of apparent outliers. The subject is fully covered by Cook and Weisberg, perhaps rather surprisingly in their second chapter on methods using residuals. Belsley *et al.* accord the topic the penultimate half page of their book.

As the start for a diagnostic approach to transformations, consider the standardized transformation $z(\lambda)$ introduced by Box and Cox (1964), which is such that the log likelihood maximized over all parameters except λ is proportional to the residual sum of squares of $z(\lambda)$. The approximate model is that, for some λ and to a sufficient degree of approximation,

$$z(\lambda) = X\beta + \varepsilon.$$

This model can be expanded about a hypothesized value λ_0 to yield the linearized model

$$z(\lambda_0) = X\beta - (\lambda - \lambda_0)w(\lambda_0) + \varepsilon, \tag{12}$$

where the derivative $w(\lambda_0) = \partial z(\lambda)/\partial\lambda \mid \lambda = \lambda_0$ is what Box (1980) calls a constructed variable. Often in diagnostic work $\lambda_0 = 1$, corresponding to the hypothesis of no transformation.

Comparison of (12) with (9) shows that testing the significance of regression on the constructed variable $w(\lambda_0)$ is locally equivalent to testing the hypothesis $\lambda = \lambda_0$. This t test is an easily calculated approximation to the score test based on the slope of the partially maximized log likelihood.

One diagnostic tool which can be used to detect the effect of individual observations on the evidence for a transformation is an added variable plot for the constructed variable. In their Section 2.4, Cook and Weisberg give plots of partially maximized log likelihoods and added variable plots for the parametric family of power transformations. Other constructed variables include those formed by series expansion of the constructed variable for the power transformation and by substitution of predicted values for observations, which yields an exact test. The combination of these two procedures provides one derivation of Tukey's one degree of freedom for nonadditivity. A measure of the up-to-date nature of the book is that some of this material is taken from Atkinson (1982) which was not yet printed when the book was delivered to the publisher.

The material so far reviewed in this article is fast becoming standard. Less standard material is covered in the 107-page third chapter of Belsley *et al.*, "Detecting and Assessing Collinearity". The problem of collinearity is not acute in the data from the natural and engineering sciences with which I have been concerned. But it does arise in economic modelling where there is an understandable reluctance to exclude from models variables which economic theory suggests are important.

The fourth and last major chapter of Belsley *et al.*, "Applications and Remedies", describes cures for collinearity which include "Bayesian-type Techniques" divided into "Pure Bayes", "Mixed Estimation" and "Ridge Regression". The fruitful relationships between these three are not explored. The chapter includes analyses of several economic series using both regression diagnostics and the cures for collinearity.

Less standard material of a very different type is also to be found in Chapter 4 of Cook and Weisberg, "Alternative Approaches to Influence". These approaches include the effect of deletion on the volume of confidence regions and on the volume of ellipsoids generated in the combined space of the carriers and of the response. The third approach is via predictive influence. A comparison of these and more conventional measures of influence shows that all are functions of the basic building blocks r_i' and h_i.

My personal opinion is that this material is unlikely to lead to interesting future developments. The same is not true of the material in Cook and Weisberg's fifth chapter, "Assessment of Influence in Other Problems". The first section applies diagnostic procedures to the maximum likelihood residuals of Cox and Snell (1968). The most important new developments are likely to come from work of the kind contained in Sections 5.2–5.4. The first of these, "A General Approach to Influence", widens the scope to maximum likelihood estimation of the vector parameter θ. Influence curves can be derived from the distance $\hat{\theta} - \hat{\theta}_{(i)}$, which will in general require the possibly iterative calculation of $n + 1$ sets of maximum likelihood estimates. Approximations to this distance can be found from the quadratic approximation to the log likelihood at $\hat{\theta}$, which yields the "one-step" estimates $\hat{\theta}^1_{(i)}$. Assessment of influence is then based on the likelihood distance

$$\mathrm{LD}_i = 2\{L(\hat{\theta}) - L(\hat{\theta}_{(i)})\} \tag{13}$$

where $L(\theta)$ is the log likelihood at θ, or on the one-step approximation in which $\hat{\theta}^1_{(i)}$ replaces $\hat{\theta}_{(i)}$ in (13). One special case of this theory is "Nonlinear Least Squares", Section 5.3, when the one-step estimates of the parameters are found from the model linearised at $\hat{\theta}$. Using this linearised model, residuals and influence measures are constructed as for the linear model which has been the main subject of this review. If these approximations are not sufficiently accurate, the nonlinear model can be used combined with the one step parameter estimates.

The choice of one-step or fully iterated estimates arises also in Section 5.4 of Cook and Weisberg "Logistic Regression and Generalized Linear Models", which is based on Pregibon's trailblazing paper published in this journal in 1981. In this work linear regression diagnostics are elegantly expanded to cover the range of generalized linear models through the use of diagnostics obtained by down-weighting observations. Application of these results to the iterative weighted least squares fitting method used in GLIM provides easily calculated diagnostics for generalized linear models. Cook and Weisberg illustrate these methods with an extensive analysis of a set of data on leukemia.

The last major section of Cook and Weisberg covers robust regression. Both here and in Belsley *et al.*, where the technique is also used, the method employed can be inelegantly described as the Huberization of the residuals. Thus, very surprisingly, both sets of authors fail to allow for the effect of leverage on robust estimation, the difficulties with which are considered by Huber (1981, Section 7.9).

The fifth chapter of Belsley *et al.*, "Research Issues and Directions for Extensions", is little more than a 15-page list of possibilities for further work. Amongst these is the extension of diagnostic methods to sets of simultaneous equations and also to nonlinear least squares. The two year gap between the two books is shown by the absence from the chapter of numerical examples.

With these comments my comparative review of the two books is complete. What of future developmens in this area? It seems clear that linear regression diagnostics will become increasingly available in regression packages. It is to be hoped that increasing use of the methods will lead to improved statistical analyses rather than to an explosion of indigestible tables and graphs. One readily available source of such overkill is the use of multiple deletion diagnostics. The description in this review, although not in the two books, has been in terms of deletion measures for a single observation. Are there real, rather than didactic, examples in which important features of the data would be missed in the absence of multiple deletion diagnostics? If so how do we deal with the resultant explosion of calculated quantities?

A broader problem is to improve our understanding of diagnostics for the generalized linear model. For the practitioner there will be a series of decisions to be made. What diagnostic measures should be calculated? What definition of residuals will yield greatest insight? Should fully iterated estimates be used, or are one-step approximations adequate? Given enough time, these questions can be resolved, example by example, perhaps through the use of simulation. But the diagnostic measures lose much of their appeal if they are not both easy to calculate and easy to interpret. A valuable contribution from theoretical statisticians would be to provide signposts with would make it possible, in a particular case, to put bounds on the accuracy of the approximations. Perhaps the ideas of differential geometry might be helpful.

A class of problems of a different order of magnitude arises when consideration is given to the next logical stage in the development of these methods. At the beginning of this review there was the image of a nonexpert statistician being guided in the analysis of data by diagnostic plots for features of the data which might have been overlooked. The next stage is an expert or intelligent knowledge based system in which decisions about the structure and direction of the analysis are made with minimal human intervention. Whether such a system is desirable or possible, and at least one start has already been made on linear regression, the attempt at implementation will require a thorough understanding of diagnostic techniques.

At a more conventional level of statistical research, the role of robust regression needs further definition. Huber (1983, page 66) repeats his assertion mentioned above that robust regression is not "concerned with gross errors in the independent variables". This comment comes in a paper which has as its starting point the bounded influence regression of Krasker and Welsch (1982), a preliminary version of which is mentioned on page 274 of Belsley *et al.* In a dissenting comment on Huber's paper, Krasker and Welsch (1983) state that concern for gross errors in the explanatory variables is one of the most important reasons for interest in bounded influence regression. Clearly the dispute requires resolution. One possible role of such a regression analysis would be diagnostic, so that differences between robust and least squares fitting indicate that the data require more thoughtful analysis. But such a use highlights the difference between identification and accomodation mentioned at the beginning of this article. While the careful analysis encouraged by diagnostic methods may be appropriate for a few dozen valuable observations, such care is hardly possible in the semiautomatic analysis of tens of thousands of data points. If robust methods are more appropriate in the latter case, what are the differences in objective and are there situations where both techniques are useful?

These are not anything like all the ideas stimulated by the two books. Many interesting questions remain about the power transformation and related procedures such as the score tests and added varible plots (Bickel and Doksum, 1981; Box and Cox, 1982; Carroll, 1982; Cook, 1982). But the time has come to sum up. It should be clear from what I have written that I prefer Cook and Weisberg's book as clearly written, up-to-date, broad in coverage and illuminated by a wide variety of examples. Statisticians whose interest is in aplications in economics may prefer the book of Belsley *et al.*, however.

The level of the two books is similar. The source of Belsley *et al.* lies in a series of technical reports, co-authored by Welsch, which appeared in the years immediately before publication of the book. The level and style of Cook and Weisberg is much like that of their paper, Cook and Weisberg (1980), and so should present no problems to academic statisticians. However, one of the excitements of the current development of regression diagnostics is that the tools provided by research are being almost immediately made available in computer packages. For scientists and engineers interested in the methods, the level of Cook and Weisberg may be too high. An introduction to the methods may be found in Chapters 5 and 6 of Weisberg (1980). There remains an appreciable distance between this introduction and the more advanced treatment given by Cook and Weisberg. I hope that my forthcoming book (Atkinson, 1985) will help to fill this gap.

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