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1. INTRODUCTION

A variety of methods exist for modeling a nonlinear relationship between two variables. Probably the most common way of doing this, in practice, is to use linear regression analysis. The data are first linearized by making a suitable transformation of either the dependent variable, the independent variable, or both. A linear regression model is then fitted, and its validity is tested, provided that the necessary assumptions regarding residuals apply *after* transformation. This process is described in most statistics textbooks (e.g., Draper and Smith 1981) and is also treated extensively in the literature. The focus is generally upon the choice of an appropriate transformation for achieving linearity and properly behaving residuals (e.g., Box and Cox 1964). The Box-Cox equations and the "ladder of re-expressions" (Mosteller and Tukey 1977) are designed to guide the choice of a transformation. A variety of curves, with their transformed linear counterparts, are described by Daniel and Wood (1971) and Draper and Smith.

In many applications, however, the real interest lies in the nonlinear relationship between the original variables—that is, in specifying a representative curve. When the dependent variable has been transformed, this means that some sort of reverse transformation is required after the linearized model has been fitted. There are several common practices in this regard. One may simply detransform the fitted linear model (i.e., apply the inverse transformation). This results in a model of the median response in the original variable space, as will be discussed later. Confidence intervals and prediction intervals can easily be obtained by detransforming their counterparts from the transformed data. Sometimes, however, it is desired to develop a model of the mean response given a value of the independent variable. When used for this purpose, the detransformed fitted linear model sometimes produces a severely biased model.

The purposes of this paper are to call this problem to the attention of teachers and practitioners and to suggest simple remedies for a set of commonly applied transformations.

An example is presented in Section 2 that illustrates the need for an estimator of mean response in the original variable space. Section 3 provides an explanation of the underlying reason for the bias. The specific biases and appropriate remedies are given in Section 4, for a variety of transformations. (For another approach to this problem, see Duan, 1983.) Concluding remarks are given in Section 5.

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2. AN EXAMPLE

The following example illustrates the occasional need to estimate the mean response in terms of the original variables, as well as the magnitude of the problem that can occur. Suppose that a market planner of a company wishes to use market research data to model the relationship between the volume of sales to customer establishments (Y) and an indicator of sales volume (X) such as the number of employees of the establishments. The model will be used to estimate total sales volumes for market segments corresponding to representative values of X. To do this, a model for the mean of Y, rather than the median, is needed, because it can be multiplied by the number of establishments in the segment to provide a valid estimate of total sales.

The data of this example were taken from an actual market research study. A logarithmic transformation was applied to both variables, and a linear least squares fit resulted in the model

$$\ln(Y) = 7.3 + .5\ln(X), \qquad (2.1)$$

with a satisfactory set of residuals. Exponentiating (the inverse transformation) results in the estimated curve

$$Y = 1500X^{.5}, \qquad (2.2)$$

which is graphed in Figure 1 (the lower curve), along with the original data points. Note that this curve is representative in the sense that approximately half the data points lie above it and half below it. However, as an estimator of the mean response, it appears to be heavily biased to the low side. This is in fact the case: The true mean response is approximately 50% higher

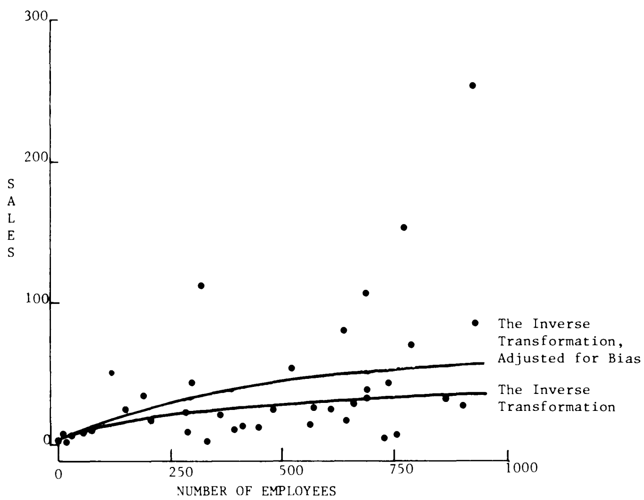

Figure 1. Scatter diagram and curve resulting from inverse transformation, for sales (Y) vs. number of employees (X).

than the curve. When a bias-reducing adjustment (developed in Section 4) is applied, the approximately unbiased upper curve is obtained.

3. THE UNDERLYING REASON FOR THE BIAS

It can be shown (see Hald 1952) that for any transformation that is a monotonic function, the transformation of the median of the original distribution becomes the median of the transformed distribution. Since the residuals for the linear model are presumably normally distributed, the fitted straight line represents the median of the transformed response variable, given X, as well as its mean. Consequently, the curve that results from applying the inverse transformation to the fitted linear model, with the error term set to zero, represents the median value of Y given X, rather than the mean. Its bias for estimating the mean response therefore has the same theoretical basis as results from using the sample median from a skewed univariate data set as an estimator of the population mean.

4. TRANSFORMATION BIAS AND REMEDIES

Results are given for a simple set of transformations that provide satisfactory linearization for a large number of applications. The set consists of the logarithmic transformation $\ln(Y)$ and all fractional power transformations of the form $Y^{1/N}$ and $Y^{-1/N}$, where N is a positive integer. This set includes most of the transformations in the ladder of re-expressions, referenced in Section 1. It includes as special cases the square root ($Y^{1/2}$) and the inverse (Y^{-1}) as well as the logarithm—all common transformations. It is assumed that in each of these transformations, we are dealing with entirely positive data sets. (Thus, for the power transformations, the residuals of the linearized model can only be approximately normal.) The development for the logarithm is given in some detail. For the others, a brief summary is given. For a more complete development, see Miller (1983).

The Logarithm

When a logarithmic transformation is appropriate, the fitted linear model will be of the form

$$\ln(\hat{Y}) = \hat{\beta}_0 + \hat{\beta}_1 X, \tag{4.1}$$

where $\hat{\beta}_0$ and $\hat{\beta}_1$ are the least squares estimators of the linear model coefficients. Detransforming yields the model

$$\hat{Y} = \hat{\beta}_0{}^* e^{\hat{\beta}_1 X} \tag{4.2}$$

where $\hat{\beta}_0^* = e^{\hat{\beta}_0}$. To demonstrate the bias of this detransformed model, we first consider the presumed true underlying model

$$\ln(Y) = \beta_0 + \beta_1 X + \epsilon, \tag{4.3}$$

which, upon detransforming, leads to the multiplicative model

$$Y = \beta_0^* e^{\beta_1 X} \cdot \epsilon^* \tag{4.4}$$

where $\beta_0^* = e^{\beta_0}$, and $\epsilon^* = e^{\epsilon}$ is lognormally distributed. The mean of Y is simply

$$\begin{aligned} E(Y) &= \beta_0^* e^{\beta_1 X} E(\epsilon^*) \\ &= \beta_0^* e^{\beta_1 X} \cdot e^{1/2\sigma^2}. \end{aligned} \tag{4.5}$$

(For the mean of a lognormal random variable, see Hald 1952.) However, the *median* response is given by

$$\begin{aligned} \mathrm{MD}(Y) &= \beta_0^* e^{\beta_1 X} \mathrm{MD}(\epsilon^*) \\ &= \beta_0^* e^{\beta_1 X}, \end{aligned} \tag{4.6}$$

since the median of ϵ^* equals 1 in this case (Hald 1952). Now, $\ln(\hat{Y})$ is easily shown to have a normal distribution with mean $\beta_0 + \beta_1 X$ and variance

$$\sigma^2\left\{\frac{1}{n} + \left[(x - \bar{x})^2 / \sum_{i=1}^{n} (X_i - \bar{X})^2\right]\right\}.$$

Hence $\hat{Y}$ has lognormal distribution with mean

$$E(\hat{Y}) = \exp\left[(\beta_0 + \beta_1 X + \tfrac{1}{2}\sigma^2)\left\{\frac{1}{n} + \frac{(X - \bar{X})^2}{\sum_{i=1}^{n} (X_i - \bar{X})^2}\right\}\right].$$

As the sample size n increases, this expectation approaches (4.6). Therefore, the detransformed estimator (4.2) provides a consistent estimator of median response, but systematically underestimates the mean response (4.5). Note that the biasing factor, $e^{1/2\sigma^2}$, is multiplicative and grows exponentially with σ^2. A simple remedy is to apply an estimator of this factor to the detransformed estimator (4.2),

$$\hat{E}(Y) = \hat{\beta}_0^* e^{\hat{\beta}_1 X} e^{1/2\hat{\sigma}^2}, \tag{4.7}$$

where $\hat{\beta}_0$, $\hat{\beta}_1$, and $\hat{\sigma}^2$ are the least squares estimators for the linearized model (4.3). This model remains somewhat biased, since $\hat{\beta}_0^*$ and $\exp(\hat{\beta}_1)$ are biased estimators for β_0^* and $\exp(\beta_1)$, respectively. Nevertheless, applying the adjustment factor eliminates the major portion of bias.

The Square Root and Other Positive Fractional Powers

For the positive fractional power transformations $Y^{1/N}$, detransforming the assumed underlying model leads to the model

$$Y = (\beta_0 + \beta_1 X + \epsilon)^N. \tag{4.8}$$

If ϵ is distributed normal $(0, \sigma^2)$, then $E(Y)$ is the nth moment of a normal random variable with mean $\beta_0 + \beta_1 X$ and variance σ^2. The moments of the normal distribution are well known (Kendall and Stuart 1969) and provide the expected value of Y, given X, for any value N. (Note that (a) Y being positive ensures that (4.8) is monotonic, and (b) the moments are approximate since ϵ can only be approximately normal.) For the square root transformation, $N = 2$, we have

$$E(Y) = (\beta_0 + \beta_1 X) + \sigma^2. \tag{4.9}$$

Therefore, the low-bias estimator is obtained by substituting $\hat{\beta}_0$, $\hat{\beta}_1$, and $\hat{\sigma}^2$ from the fitted linear model:

$$\hat{E}(Y) = (\hat{\beta}_0 + \hat{\beta}_1 X)^2 + \hat{\sigma}^2. \tag{4.10}$$

Note that the first term is the detransformed fitted model, and the second term is the bias-reducing adjustment factor.

The Inverse

If the inverse transformation $1/Y$ is appropriate, the underlying model is

$$1/Y = \beta_0 + \beta_1 X + \epsilon. \tag{4.11}$$

Note that Y being always positive ensures that $E(Y)$ exists. To find $E(Y)$, we invoke the identity

$$1/W = 1/E(W)\{1 + [W - E(W)]/E(W)\}^{-1}. \tag{4.12}$$

By expressing the bracketed expression as a geometric progression and truncating after three terms, we obtain the approximate result

$$E(Y) = \frac{1}{\beta_0 + \beta_1 X}\left\{1 + \frac{\sigma^2}{(\beta_0 + \beta_1 X)^2}\right\}. \tag{4.13}$$

A low-bias estimator is obtained by substituting $\hat{\beta}_0$, $\hat{\beta}_1$, and $\hat{\sigma}^2$. The first factor will then be the detransformed fitted model, while the bracketed factor is the adjustment.

Inverse Fractional Powers

When any inverse fractional power transformation $Y^{-1/N}$ is appropriate, the mean of Y can be found by combining the methods used for the inverse and the positive fractional powers. For the inverse square root, we have

$$\hat{E}(Y) = \frac{1}{(\hat{\beta}_0 + \hat{\beta}_1 X)^2 + \hat{\sigma}^2} \times \left\{1 + \frac{2\hat{\sigma}^4 + 4(\hat{\beta}_0 + \hat{\beta}_1 X)^2 \hat{\sigma}^2}{[(\hat{\beta}_0 + \hat{\beta}_1 X)^2 + \hat{\sigma}^2]^2}\right\}. \tag{4.14}$$

For the more general result, see Miller (1983).

Unbiased Estimation

The estimators suggested reduce the bias of the estimated inverse transformation by simply including an additional term or factor to compensate for the understated (or overstated) expected values. They are still biased to a small degree, because they consist of nonlinear functions of the least squares estimators (Hald 1952).

Neyman and Scott (1960) give unbiased, uniformly minimum variance estimators for the expectation of estimated inverse transformations that are recursive functions. Of those mentioned here, the square root, cube root, and logarithmic transformations have recursive inverse transformations. It can be shown (see Miller 1983) that their unbiased formulations differ only slightly from the low-bias models presented here and are more complex. The differences become negligible for larger sample sizes. Neyman and Scott, Hoyle (1975), Schmetterer (1960), and Granger and Newbold (1976) also give more general solutions applying to a broader class of inverse transformations. However, these results are based on complex generating functions that have little chance of finding their way into the mainstream of statistical practice.

5. CONCLUSION

A substantial bias occurs when, in estimating the mean response, one simply detransforms the least squares model fitted after transforming the data to normality. This bias has been approximated for a widely applicable set of transformations. Low-bias alternatives have been suggested that are simple enough to be used by practitioners, computed with the output of standard statistical packages, and covered in an applied statistics course.

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