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INTERVAL ESTIMATION IN CALIBRATION MODELS : AN APPLICATION OF FIELLER'S THEOREM

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ABSTRACT

In this note we demonstrate how Fieller's theorem may be used to provide interval estimates for calibrated data obtained using the classical calibration method. Using a matrix formulation of the general linear model, it is straightforward to incorporate extensions to the univariate, multiple regression setting. The results provided are easily programmed in a matrix-based language such as GAUSS.

1. INTRODUCTION

The so-called 'calibration problem' has a long and checkered history [e.g.: see Berkson (1950,1969), Krutchkoff (1967,1969) and Williams (1969)] and whilst the early controversy has largely been resolved, much work continues to be done on other interesting and

useful applications of calibration models [e.g.: Fox (1989(a))]. It is not the purpose of this note to review the lengthy debate concerning the controversy surrounding the use of "classical" versus "inverse" methods of calibration. The reader interested in these aspects should consult the literature review provided in Fox (1989(b)). However, we shall make mention of these two fundamental strategies for the simple linear calibration model.

In a typical calibration experiment we collect measurements y corresponding to some true state of nature X. For example, the random variable Y may be an instrument reading associated with some physical quantity, X. For calibration purposes, observations are taken on Y for various levels of X so as to estimate the parameters in one of two models.

The 'classical' approach to calibration assumes the linear model:

$$Y_i = \beta_0 + \beta_1 x_i + \varepsilon_i \tag{1.1}$$

where the ε_i are i.i.d. random variables having zero expectation and finite variance. The parameters in equation (1.1) are estimated using OLS to yield $\hat{\beta}_0$ and $\hat{\beta}_1$. The classical estimator, $\hat{X}_{oc}$, of X corresponding to some future value y_0 is

$$\hat{X}_{oc} = \frac{y_0 - \hat{\beta}_0}{\hat{\beta}_1} \tag{1.2}$$

An alternative, and equally appealing approach is to regress x on y directly and so estimate the parameters in the model:

$$X_i = \gamma_0 + \gamma_1 y_i + \xi_i \tag{1.3}$$

where again the ξ_i are i.i.d. random variables having zero expectation and finite variance. (Clearly, equation 1.3 violates the usual assumption that X is measured without error and indeed most of the controversy has centered on appropriateness of this approach).

Again, γ_0 and γ_1 in equation (1.3) are estimated using OLS and thus a calibrated X_0 corresponding to some future reading y_0 is given as:

$$\hat{X}_{oi} = \hat{\gamma}_0 + \hat{\gamma}_1 y_0 \tag{1.4}$$

The use of equation (1.4) is known as the inverse calibration method.

The problem of placing confidence bounds on $\hat{X}_0$ (obtained by either method) has also been investigated [Carroll, Sacks, & Spiegelman (1988), Fox (1989(b)), Graybill (1976),pp 280-282].

For $\hat{X}_{oc}$, a (1-α)100% prediction interval may be obtained as follows. Let $J_0(x)$ be the (1-α)100% prediction interval for response y, i.e.:

$$J_0(x) = \hat{y} \pm t_{n-2,\alpha/2}\, \hat{\sigma}_\varepsilon \left[1 + \frac{1}{n} + \frac{(x - \bar{x})^2}{S_{xx}} \right] \qquad (1.5)$$

where S_{xx} is the usual sum of squares and $\hat{\sigma}^2_\varepsilon$ is the unbiased estimator of the error variance. Then a (1-α)100% prediction interval for X_{oc} is:

$$K_0(y_0) = \left\{ x \,|\, y_0 \in J_0(x) \right\} \qquad (1.6)$$

This procedure is depicted in figure 1 below.

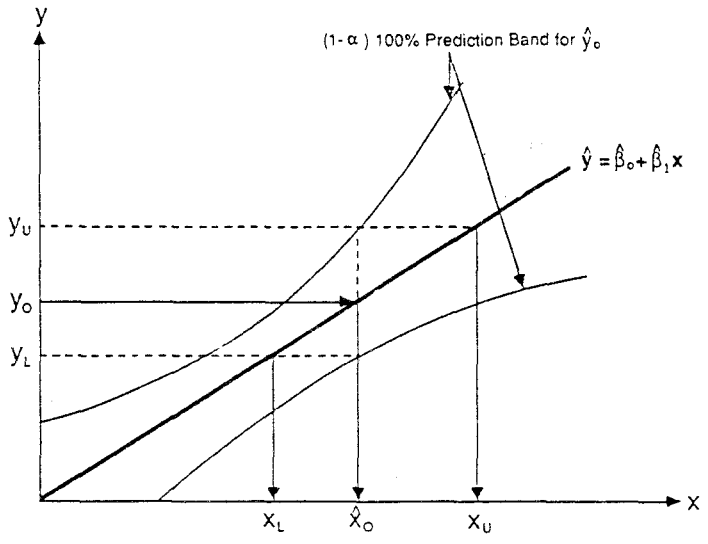

Figure 1. Determination of prediction bands for X_{oc}

(X_U and X_L denote upper and lower limits respectively).

Scheffé (1973) suggested replacing the $J_0(x)$ of equation (1.5) with prediction bounds of the form:

$$J_1(x) = \left\{ y \middle| \hat{y} - \hat{\sigma}_\varepsilon [c_1 + c_2\, s(x)] \le y \le \hat{y} + \hat{\sigma}_\varepsilon [c_1 + c_2\, s(x)] \right\} \qquad (1.7)$$

where $s(x)$ is the expression inside the square brackets of equation (1.5) and c_1 and c_2 are constants chosen such that the interval has $(1-\alpha)100\%$ confidence. This results in a prediction interval of the form:

$$K_1(y_0) = \left\{ x \middle| y_0 \in J_1(x) \right\} \qquad (1.8)$$

The problem with Scheffé's modification is that his own set of tables must be consulted in order to determine c_1 and c_2. Carroll, Sacks, & Spiegelman (1988) provided a modification to the Scheffé procedure which enables c_1 and c_2 to be obtained from percentiles of the T and F distributions respectively. However, the remaining difficulty with both the Scheffé method and that of Carroll et al. is that the confidence level α is conditional and is therefore not directly comparable with other, more straightforward procedures.

In the following sections we illustrate how Fieller's theorem (Fieller, 1944) can be used together with a matrix formulation of the general linear model to provide prediction intervals for X_{oc}. The approach is simple to implement and has the added advantage of generalizing to univariate multiple regression calibration models. A more detailed discussion concerning various strategies for this type of calibration problem is given in Fox (1989(b)).

2. PREDICTION INTERVALS USING FIELLER'S THEOREM

Fieller's theorem provides a general methodology for constructing interval estimates for ratios of random variables.

Zerbe (1978) considered applications of Fieller's theorem to linear combinations of parameter estimates in the general linear model :

$$\underline{Y} = X\underline{\beta} + \underline{\varepsilon} \qquad (2.1)$$

where $\underline{\varepsilon} \sim N(\underline{O}, \sigma_\varepsilon^2 I_n)$

and $\underline{Y}$ is an (n x 1) vector of observable random variables

X is an (n x p) full-rank design matrix

$\underline{\beta}$ is a (p x 1) vector of unknown constants.

By a simple extension we can construct a prediction interval for a calibrated X_0 in the general linear model formulation of equation (2.1).

The OLS estimator of $\underline{\beta}$ is:

$$\hat{\underline{\beta}} = (X^T X)^{-1} X^T Y \tag{2.2}$$

having covariance matrix

$$\text{Cov}[\hat{\underline{\beta}}] = \Sigma = \sigma_\varepsilon^2 (X^T X)^{-1} \tag{2.3}$$

An unbiased estimator of σ_ε^2 is

$$\hat{\sigma}_\varepsilon^2 = \frac{Y^T (I - H) Y}{(n - p)} \tag{2.4}$$

where H is the hat or projection matrix $X(X^T X)^{-1} X^T$.

Let $\hat{\Sigma}$ be the sample estimate obtained by replacing σ_ε^2 in equation (2.3) with the estimate of equation (2.4).

We define a new quantity $\underline{\beta}^*$ as the vector obtained by inserting Y_0 in the first row position of $\underline{\beta}$. That is:

$$\underline{\beta}^{*T} = [Y_0 | \underline{\beta}^T] \tag{2.5}$$

$\hat{\underline{\beta}}^*$ is similarly defined by replacing $\underline{\beta}$ in equation (2.5) with $\hat{\underline{\beta}}$.

Under the assumption that Y_0 is a random variable from the same population as the original calibration data, we have:

$$V = \text{Cov}[\hat{\underline{\beta}}^*] = \left[\begin{array}{c|c} \sigma_\varepsilon^2 & \underline{O} \\ \hline \underline{O}^T & \Sigma \end{array}\right]$$

$$= \sigma_\varepsilon^2 \left[\begin{array}{c|c} 1 & \underline{O} \\ \hline \underline{O}^T & (X^T X)^{-1} \end{array}\right] \tag{2.6}$$

where $\underline{O}$ is a (1 x p) row vector of zeros.

The classical estimator given by equation (1.2) can be written as the ratio of linear combinations of the elements of $\hat{\underline{\beta}}^*$. Specifically,

$$x_{oc} = \frac{K^T\beta^*}{L^T\beta^*} \tag{2.7}$$

where $K^T = [1 \quad -1 \quad 0]$

and $L^T = [0 \quad 0 \quad 1]$

Following Zerbe (1978), we consider the quantity

$$(K^T\underline{\beta}^* - x_{oc}L^T\underline{\beta}^*)$$

which has variance $(KVK^T - 2x_{oc}KVL^T + x_{oc}^2LVL^T)$.

Thus the quantity,

$$T = \frac{K^T\hat{\underline{\beta}}^* - x_{oc}L^T\hat{\underline{\beta}}^*}{[KVK^T - 2x_{oc}KVL^T + x_{oc}^2LVL^T]^{1/2}} \tag{2.8}$$

has a t-distribution with $\nu = (n - p)$ degrees of freedom.

Therefore $P[-t_{\nu,\alpha/2} \leq T \leq t_{\nu,\alpha/2}] = 1 - \alpha$. Using Fieller's argument and dropping the subscripts on $t_{\nu,\alpha/2}$, we set

$$P[-t \leq T \leq t] = P[Ax_{oc}^2 + Bx_{oc} + C \leq 0].$$

It can be shown that the preceding equation is satisfied for the following choices of A, B, and C

$$A = (L^T\hat{\underline{\beta}}^*)^2 - t^2\,L^TVL \tag{2.9}$$

$$B = 2[t^2\,K^TVL - (K^T\hat{\underline{\beta}}^*)(L^T\hat{\underline{\beta}}^*)] \tag{2.10}$$

and $$C = (K^T\hat{\underline{\beta}}^*)^2 - t^2\,K^TVK \tag{2.11}$$

Let a, b, and c be the observed values of the corresponding random variables. Then provided $a > 0$ and $b^2 - 4ac > 0$, the limits of the $(1-\alpha)100\%$ prediction interval for X_{oc} are given as :

$$\frac{-b \pm \sqrt{b^2 - 4ac}}{2a} \tag{2.12}$$

The interval generated by this approach is equivalent to that given by Graybill (1976,p280) when p = 2. The advantage of the present method is that it is applicable for any p.

3. AN EXAMPLE

We illustrate the method using data originally reported by Hader and Grandage (1958) and later used by Atkinson (1985 table 4.5 p53) to illustrate the use of measures of influence. These data relate the percentage yield of gasoline to four other explanatory variables associated with the distillation and fractionation process. For each of 32 observations, measurements were taken on: x_1, crude oil gravity; x_2, crude oil vapor pressure; x_3, the temperature at which 10% of crude is vaporized; x_4, the temperature at which all of the gasoline has vaporized; and y, the % gasoline yield.

For the purpose of illustration, all but the last observation were used to estimate model parameters with the last observation being used for calibration. In this case we assume that variable X_3 is to be calibrated for.

Using a classical regression model we may write:

$$Y_i = \beta_0 + \beta_1 x_{1i} + \beta_2 x_{2i} + \beta_3 x_{3i} + \beta_4 x_{4i} + \varepsilon_i \qquad (3.1)$$

For observation #32 we have the following calibration data:

$y_0 = 45.7,\ x_1 = 50.8,\ x_2 = 8.6,\ x_4 = 407$

(X_3 is also known to be 190).

Applying the method described in this paper, we have:

$$\underline{\beta}^* = [Y_0 | \beta_0\ \beta_1\ \beta_2\ \beta_3\ \beta_4]^T$$

Therefore, $K^T = [1\ \ -1\ \ -x_1\ \ -x_2\ \ 0\ \ -x_4]$

and $L^T = [0\ \ 0\ \ 0\ \ 0\ \ 1\ \ 0]$.

The vector of parameter estimates obtained using the first 31 observations is

$$\hat{\underline{\beta}}^T = [-4.14\ \ 0.1954\ \ 0.4987\ \ -0.1519\ \ 0.1525]$$

resulting in an (unadjusted) R^2 of 0.954.

Application of equation (2.7) gives a calibrated value of

$\hat{X}_3 = 174.164$ for observation 32.

Furthermore, the residual error variance is estimated as

$\hat{\sigma}^2_\varepsilon = 5.02885$, and hence

$$V = \hat{\sigma}^2_\varepsilon \left[\begin{array}{c|c} 1 & \underline{0} \\ \hline \underline{0}^T & (X^TX)^{-1} \end{array}\right]$$

$$= \begin{bmatrix} 5.029 & 0 & 0 & 0 & 0 & 0 \\ 0 & 112.120 & -0.787 & -2.882 & -0.279 & -0.006 \\ 0 & -0.787 & 0.011 & 0.004 & 0.001 & 0.000 \\ 0 & -2.882 & 0.004 & 0.141 & 0.009 & 0.000 \\ 0 & -0.279 & 0.001 & 0.009 & 0.001 & 0.000 \\ 0 & -0.006 & 0.000 & 0.000 & 0.000 & 0.000 \end{bmatrix}$$

Sample values of A, B, and C obtained from equations (2.9), (2.10), and (2.11) respectively are computed to be

$a = 0.0194, \qquad b = -6.7043, \qquad c = 548.5769.$

The critical t-value for a 95% prediction interval is $t_{26,0.025} = 2.056$ and thus the interval given by expression (2.12) is (133.15, 212.28). Note that the true value of $X_3 = 190$ has been captured by the prediction interval.

The calculations associated with this procedure are readily programmed using a matrix-based language such as GAUSS.

4. SUMMARY

In this note we have indicated how, with a simple extension, Fieller's theorem may be used to generate prediction intervals in the univariate, multiple predictor calibration problem. A matrix formulation of the procedure lends itself to easy computation via a programming language such as GAUSS.

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