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Synthesizing the classical and inverse methods in linear calibration

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Synthesizing the classical and inverse methods in linear calibration

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Abstract

This paper considers the problem of linear calibration and presents two estimators arising from a synthesis of classical and inverse calibration approaches. Their performance properties are analyzed employing the small error asymptotic theory. Using the criteria of bias and mean squared error, the proposed estimators along with the traditional classical and inverse calibration are compared. Finally, some remarks related to future work are placed.

1 Introduction

The technique of statistical calibration plays an important role in improving the precision of an instrument or some measuring device. It essentially involves relating the readings obtained from two different instruments or measuring devices and then employing the estimation relationship for the prediction of measurements of one instrument or device on the basis of readings obtained from the other instrument or device. Generally, one instrument or device provides measurements that are accurate but with one or more limitations like highly expensive, time consuming, irksome, complex and destructive. Such limitations are usually either not present or not so pronounced in the other instrument or device, and taking observations is relatively cheaper, quicker, not so irksome and easier but less accurate. Thus one instrument or device is taken as standard and the observations obtained from it are popularly referred as true values while the observations arising from the other instrument or device are known as readings. Such a framework of calibration has been used in numerous applications in physical, social, medical and engineering sciences. At the same time, it has posed several challenging issues in statistical inference; see, e.g., Osborne (1991) for an interesting review of statistical developments.

As an illustration, let us consider the example of a simple bathroom scale used for finding the body weights of human beings. The circular scale on this

instrument is constructed by putting marks on the scale corresponding to some known weights and then calibrating it. Now a person with unknown body weight stands on it and his/her estimated weight is determined from the reading on scale. This kind of measurement technique is based on controlled calibration. Recording temperature, determining the power of eye-sight, analyzing the chemical compositions of substances, finding the level of blood sugar are some other simple examples of controlled calibration.

In this paper, attention is restricted to the problem of controlled calibration in which the true values and readings are linearly related. Further, only the problem of point estimation of the true value corresponding to a given reading is considered though the problem of interval estimation is no less important. In Section 2, we describe the two basic approaches stemming from classical and inverse regression methods and present two estimators arising from a synthesis of the two approaches. In Section 3, the relevance of small error asymptotic (SEA) theory is discussed and SEA approximations for the biases and mean squared errors are derived. Comparison of estimators is presented in Section 4. Finally, some concluding remarks are placed in Section 5.

2 The Proposed Procedures

Suppose that y_1, y_2, \dots, y_n are the readings corresponding to n true values x_1, x_2, \dots, x_n assumed to be fixed and known. These observations are used for the purpose of calibration.

Assuming a linear relationship the readings and true values, we can write

$$y_i = \alpha + \beta x_i + \sigma u_i, \quad i = 1, 2, \dots, n \quad (2.1)$$

where α , β and σ are unknown parameters and u_i denotes the error term.

Next, let Y be the reading on the calibrated scale corresponding to an unknown value X . Thus we can express

$$Y = \alpha + \beta X + \sigma U \quad (2.2)$$

Where U is the error term in the regression relationship.

The errors u_1, u_2, \dots, u_n are assumed to be independently and identically distributed following a normal probability law with mean zero and variance unity.

For the point estimation of X , there are basically two approaches, viz., classical and inverse. In the classical approach, the parameters α and β are estimated from (2.1) by the method of least squares and the resulting estimators are used in (2.2) to get the following classical calibration estimator of X :

$$X_C = \bar{x} + \frac{s_{xx}}{s_{xy}}(Y - \bar{y}) \quad (2.3)$$

where

$$\begin{aligned} \bar{x} &= \frac{1}{n} \sum x_i, & s_{xx} &= \frac{1}{n} \sum (x_i - \bar{x})^2 \\ \bar{y} &= \frac{1}{n} \sum y_i, & s_{xy} &= \frac{1}{n} \sum (x_i - \bar{x})(y_i - \bar{y}) \end{aligned} \quad (2.4)$$

In the inverse approach, the regression of x_i on y_i is run using n observations and the estimated relationship is employed to get the following inverse calibration estimator:

$$X_I = \bar{x} + \frac{s_{xy}}{s_{yy}}(Y - \bar{y}) \quad (2.5)$$

where

$$s_{yy} = \frac{1}{n} \sum (y_i - \bar{y})^2. \quad (2.6)$$

It may be noticed that the classical calibration approach utilizes the regression of readings on the true values for predicting a true value, outside the sample, corresponding to a given reading. Obviously it is inappropriate, and one should predict the true value corresponding to a reading by considering the regression of the true value on the readings. This is followed in inverse calibration approach but then the regression of true values on readings is not meaningful because true values influence the readings and not vice-versa. Thus both the approaches are not very appealing as such.

Various types of interpretations, justifications and modifications to the two basic approaches have appeared in the literature; see Osborne (1991) for an interesting summary. If we look at the distributional properties of classical and inverse calibration estimators, both are found to possess some qualification and some limitations; see Osborne (1991) for details and also Kubokawa and Robert (1994) regarding the issue of admissibility from a decision theoretic perspective.

In both the classical and inverse calibration methods, it may be observed that the parameters are first estimated from n observations and the thus obtained estimated relationship is then used to develop an estimator of unknown X . Alternatively, we may employ all the $(n + 1)$ observations assuming X to be known for a moment and run the regression of true values on the readings in the spirit of inverse calibration. This provides the following regression equation of x on y :

$$x^* = \frac{n\bar{x} + X}{n + 1} + \left[\frac{s_{xy} + \frac{(X - \bar{x})(Y - \bar{y})}{n+1}}{s_{yy} + \frac{(Y - \bar{y})^2}{n+1}} \right] \left(y^* - \frac{n\bar{y} + Y}{n + 1} \right). \quad (2.7)$$

Using to predict X corresponding to the reading Y (i.e., $y^* = Y$), we obtain the following expression:

$$x^* = \frac{n\bar{x} + X}{n + 1} + \left[\frac{s_{xy} + \frac{(X - \bar{x})(Y - \bar{y})}{n+1}}{s_{yy} + \frac{(Y - \bar{y})^2}{n+1}} \right] \left(\frac{n}{n + 1} \right) (Y - \bar{y}). \quad (2.8)$$

Obviously, the expression for x^* as a predictor or estimator of X has no utility owing to involvement of unknown X on the right hand side. However, we can deduce feasible versions of it as follows. Relax the specification that X is known and replace X on the right hand side of (2.8) by some estimate for which there are two natural choices, viz., X_I and X_c . If we set $X = X_I$ in (2.8), the resulting expression of X^* reduces to X_I , on the other hand, if we put $X = X_c$ we get the following expression for a feasible calibration estimator of X :

$$I_c = \frac{n\bar{x} + X_c}{n + 1} + \left[\frac{s_{xy} + \frac{(X_c - \bar{x})(Y - \bar{y})}{n+1}}{s_{yy} + \frac{(Y - \bar{y})^2}{n+1}} \right] \left(\frac{n}{n + 1} \right) (Y - \bar{y}). \quad (2.9)$$

Similarly, if we follow the classical calibration approach and accordingly run the regression of readings on the true values assuming X to be known and thus employing all the $(n + 1)$ observations, we find the regression relationship of y on x as follows:

$$y^{**} = \frac{n\bar{y} + Y}{n + 1} + \left[\frac{s_{xy} + \frac{(X - \bar{x})(Y - \bar{y})}{n+1}}{s_{xx} + \frac{(X - \bar{x})^2}{n+1}} \right] \left(x^{**} - \frac{n\bar{x} + X}{n + 1} \right). \quad (2.10)$$

Now if we put $y^{**} = y$ and invert the relationship, we find

$$X^{**} = \frac{n\bar{x} + X}{n + 1} + \left[\frac{s_{xx} + \frac{(X - \bar{x})^2}{n+1}}{s_{xy} + \frac{(X - \bar{x})(Y - \bar{y})}{n+1}} \right] \left(\frac{n}{n + 1} \right) (Y - \bar{y}) \quad (2.11)$$

which has again no utility like (2.8). Now if we relax the assumption of known X and put $X = X_c$ on the right hand side of (2.11), we find the resulting feasible estimator as identically equal to X_c . If we employ the inverse calibration estimator X_I for replacing X , we get the feasible calibration estimator as follows:

$$C_I = \frac{n\bar{x} + X_I}{n + 1} + \left[\frac{s_{xx} + \frac{(X_I - \bar{x})^2}{n+1}}{s_{xy} + \frac{(X_I - \bar{x})(Y - \bar{y})}{n+1}} \right] \left(\frac{n}{n + 1} \right) (Y - \bar{y}). \quad (2.12)$$

It may be noticed that the estimators defined by (2.9) and (2.12) arise from a synthesis of classical and inverse calibration approaches.

3 Asymptotic Properties:

In order to study the performance properties of calibration estimators, we employ the small error asymptotic (SEA) theory in preference to large sample asymptotic theory. The main reason for such a choice is that the application of SEA theory places no constraint on the number of observations in the calibration experiment. Owing to considerations like cost and practical difficulties in execution, the number of observations may not be sufficiently large to warrant the application of large sample asymptotic theory. In fact, small sample size is a rule rather an exception in many calibration experiments. In such circumstance, the inferences drawn from the results based on large sample asymptotic theory may be invalid and often misleading. On the other hand, the SEA theory contends that errors are not 'meant to be large' and accordingly requires errors to be small. This is ensured by assuming that standard deviation σ is small and tends to zero. Such a specification is reasonable and tenable because calibration experiments are generally conducted under controlled protocol and identical conditions, and every care is taken to reduce the errors as far as possible in order to attain a high level of accuracy and precision. Thus SEA theory in comparison to traditional large sample asymptotic theory for studying the properties of calibration estimators appears to be more relevant as well as appealing; see Srivastava and Singh (1989). Let us now introduce the following notation:

$$\theta = \frac{s_{xx}}{s_{xx} + (n + 1)^{-1}(X - \bar{x})^2},$$

$$\begin{aligned}
d &= (X - \bar{x}), \\
v_1 &= \frac{1}{ns_{xx}\beta} \sum (x_i - \bar{x})u_i, \\
v_2 &= \frac{(U - \bar{u})}{\beta}, \\
v_3 &= \frac{1}{ns_{xx}\beta^2} \sum (u_i - \bar{u})^2 - v_1^2.
\end{aligned} \tag{3.1}$$

By virtue of normality of errors u_1, u_2, \dots, u_n, U we observe that v_1, v_2 and v_3 are stochastically independent. Further v_1 and v_2 are normally distributed with same mean zero but variances $(1/(ns_{xx}\beta^2))$ and $(n+1)/n\beta^2$ respectively. Similarly, $ns_{xx}\beta^2v_3$ has χ^2 - distribution with $(n-2)$ degrees of freedom. From (2.1) and (2.2), we observe that

$$\begin{aligned}
(y - \bar{y}) &= (d + \sigma v_2)\beta \\
s_{xy} &= (1 + \sigma v_1)\beta s_{xx} \\
s_{yy} &= [1 + 2\sigma v_1 + \sigma^2(v_1^2 + v_3)]\beta^2 s_{xx}.
\end{aligned} \tag{3.2}$$

Using these in (2.3) and (2.5), we have

$$X_c = \bar{x} + (d + \sigma v_2)(1 + \sigma v_1)^{-1} \tag{3.3}$$

$$X_I = \bar{x} + (d + \sigma v_2)(1 + \sigma v_1)[1 + 2\sigma v_1 + \sigma^2(v_1^2 + v_3)]. \tag{3.4}$$

When errors are small, i.e., σ is small and tends to zero, we can expect the quantities on the extreme right of the equations (3.3) and (3.4) in increasing powers of σ . This provides the following expressions:

$$(X_c - X) = \sigma(v_2 - dv_1) + O_p(\sigma^2) \tag{3.5}$$

$$(X_I - X) = \sigma(v_2 - dv_1) + O_p(\sigma^2) \tag{3.6}$$

Similarly, using (3.2) in (2.9) and (2.12), we get

$$\begin{aligned}
I_c &= \frac{n\bar{x} + X_c}{n+1} + \left(\frac{n}{n+1}\right) (d + \sigma v_2) \left[1 + \sigma v_1 + \frac{(X_c - X)(d + \sigma v_2)}{(n+1)s_{xx}}\right] \\
&\quad \left[1 + 2\sigma v_1 + \sigma^2(v_1^2 + v_3) + \frac{(d + \sigma v_2)^2}{(n+1)s_{xx}}\right]^{-1}
\end{aligned} \tag{3.7}$$

$$\begin{aligned}
C_I &= \frac{n\bar{x} + X_I}{n+1} + \left(\frac{n}{n+1}\right) (d + \sigma v_2) \left[1 + \frac{(X_I - \bar{x})^2}{(n+1)s_{xx}}\right] \\
&\quad \left[1 + \sigma v_1 + \frac{(X_I - \bar{x})(d + \sigma v_2)}{(n+1)s_{xx}}\right]^{-1}.
\end{aligned} \tag{3.8}$$

Substituting (3.5) and (3.6) in the above expressions and expanding in increasing powers of σ , we find

$$(I_c - X) = (C_I - X) = \sigma(v_2 - dv_1) + O_p(\sigma^2). \tag{3.9}$$

We thus observe from (3.5), (3.6) and (3.9) that all the four calibration estimators X_c, X_I, I_c and C_I are asymptotically equivalent according to SEA

theory in the sense that they share the same asymptotic properties. They are all consistent when σ is small. Further, if we consider σ^{-1} times the estimation error, the asymptotic distribution in each case is normal with mean 0 and variance

$$E(v_2 - dv_1)^2 = \frac{n+1}{n\theta\beta^2}. \quad (3.10)$$

We thus need to consider higher order approximations for studying the superiority of one estimator over the other. Proceeding in the same way and retaining terms up to order $O_p(\sigma^3)$, we obtain the following expressions from (3.3), (3.4), (3.7) and (3.8):

$$(X_c - X) = \sigma(v_2 - dv_1) - \sigma^2(v_2 - dv_1)v_1 + \sigma^3(v_2 - dv_1)v_1^2 + O_p(\sigma^4) \quad (3.11)$$

$$(X_I - X) = \sigma(v_2 - dv_1) - \sigma^2[(v_2 - dv_1)v_1 + dv_3] + \sigma^3[(v_2 - dv_1)v_1^2 - (v_2 - 3dv_1)v_3] + O_p(\sigma^4) \quad (3.12)$$

$$(I_c - X) = \sigma(v_2 - dv_1) - \sigma^2 \left[(v_2 - dv_1)v_1 + \frac{n\theta d}{n+1}v_3 \right] + \sigma^3 \left[(v_2 - dv_1)v_1^2 + \frac{n\theta(1-2\theta)}{n+1}v_2v_3 + \frac{n\theta(1+2\theta)d}{n+1}v_1v_3 \right] + O_p(\sigma^4) \quad (3.13)$$

$$(C_I - X) = \sigma(v_2 - dv_1) - \sigma^2 \left[(v_2 - dv_1)v_1 + \left(1 - \frac{n\theta}{n+1}\right)dv_3 \right] + \sigma^3 \left[(v_2 - dv_1)v_1^2 + \left(1 - \frac{n\theta(1-2\theta)}{n+1}\right)v_2v_3 - \left(3 + \frac{2n\theta^2}{n+1}\right)dv_1v_3 \right] + O_p(\sigma^4). \quad (3.14)$$

Employing the distributional properties of v_1, v_2 and v_3 , it is easy to see from (3.11) that the expression for bias of X_c to order $O(\sigma^2)$ is given by:

$$\begin{aligned} B(X_c) &= E(X_c - X) \\ &= \sigma E(v_2 - dv_1) - \sigma^2 E(v_1v_2 - dv_1^2) \\ &= \sigma^2 \left(\frac{d}{ns_{xx}\beta^2} \right) \end{aligned} \quad (3.15)$$

while its mean squared error to order $O(\sigma^4)$ is

$$\begin{aligned} M(X_c) &= E(X_c - X)^2 \\ &= \sigma^2 E(v_2 - dv_1)^2 - 2\sigma^3 E(v_2 - dv_1)^2 v_1 \\ &\quad + 3\sigma^4 E(v_2 - dv_1)^2 v_1^2 \\ &= \sigma^2 \left(\frac{n+1}{n\theta\beta^2} \right) + 3\sigma^4 \frac{(n+1)(3-2\theta)}{n\theta s_{xx}\beta^4}. \end{aligned} \quad (3.16)$$

In a similar manner, we can obtain the expressions of bias to order $O(\sigma^2)$ and mean squared error to order $O(\sigma^4)$ for the remaining three estimators. The

results for bias are as follows:

$$B(X_I) = -\sigma^2 \frac{(n-3)d}{ns_{xx}\beta^2} \quad (3.17)$$

$$B(I_c) = \sigma^2 \left[1 - \frac{n(n-2)\theta}{n+1} \right] \frac{d}{ns_{xx}\beta^2} \quad (3.18)$$

$$B(C_I) = \sigma^2 \left[n-3 - \frac{n(n-2)\theta}{n+1} \right] \frac{d}{ns_{xx}\beta^2}. \quad (3.19)$$

Similarly, the mean squared error differences to order $O(\sigma^4)$ are given by

$$\begin{aligned} D(X_I, X_c) &= E(X_c - X)^2 - E(X_I - X)^2 \quad (3.20) \\ &= \sigma^4 \frac{(n+1)(n-2)}{n^2\theta s_{xx}\beta^4} [(n-6)\theta - (n-8)] \end{aligned}$$

$$\begin{aligned} D(I_c, X_c) &= E(X_c - X)^2 - E(I_c - X)^2 \quad (3.21) \\ &= \sigma^4 \frac{(n-2)}{ns_{xx}\beta^4} \left[2(2-\theta) - \frac{n^2\theta(1-\theta)}{n+1} \right] \end{aligned}$$

$$\begin{aligned} D(C_I, X_c) &= E(X_c - X)^2 - E(C_I - X)^2 \quad (3.22) \\ &= -\sigma^4 \frac{(n+1)(n-2)}{n^2\theta s_{xx}\beta^4} \left[2 \left(2 - \frac{\theta}{n+1} \right) + \right. \\ &\quad \left. n \left(1 - \frac{n\theta}{n+1} \right)^2 (1-\theta) \right]. \end{aligned}$$

It may be remarked that the results (3.15), (3.16) and (3.20) have been obtained by Srivastava and Singh (1989) but their expression for the mean squared error on X_I is incorrect and consequently the inferences based on it are wrong. Moreover, our derivation is comparatively more simple and straight forward than their derivation.

4 Comparison of Estimators

From the expressions for bias to the order of our approximation, we observe that the sign of bias crucially depends upon the sign of d , i.e. whether X is above or below \bar{x} . Comparing the estimators with respect to magnitude of bias, we see from (3.15) and (3.17) that $[B(X_c)]^2$ is less than $[B(X_I)]^2$ when n exceeds 4. Similarly, it follows from (3.15), (3.17) and (3.18) that the estimator I_C has invariably smaller magnitude of bias than X_I so long as n exceeds 4. Further, I_C has smaller bias in magnitude than X_c when

$$\theta < \frac{2(n+1)}{n(n-2)}. \quad (4.1)$$

Similarly, comparing C_I with X_c and X_I with respect to magnitude of bias, we find that C_I is better than X_c when

$$\theta < \frac{(n+1)(n-4)}{n(n-2)}. \quad (4.2)$$

and C_I is better than X_I when

$$\theta < \frac{2(n+1)(n-3)}{n(n-2)}. \quad (4.3)$$

From (4.2) and (4.3), it thus follows that C_I has smaller magnitude of bias than both the estimators X_c and X_I so long as (4.2) is satisfied.

If we compare (3.18) and (3.19), it is seen that I_C has smaller magnitude of bias than C_I for n exceeding 4.

Thus the estimator I_C emerges out to be superior to the remaining three estimators with respect to the criterion of absolute bias when n is greater than 4 and (4.2) holds true. Notice that this condition reduces, for instance, to $\theta < 0.4$ for $n = 5$ and $\theta < 0.9$ for $n = 15$, and is likely to be satisfied when X is away from \bar{x} in either direction. Further, if n is sufficiently large, the inequality (4.2) will always be satisfied. Next, let us compare the four estimators with respect to the criterion of mean squared error to order $O(\sigma^4)$.

From (3.20), we see that X_I is better than X_c when n does not exceed 8, when n exceeds 8, this result continues to remain true provided that

$$\theta > \left(\frac{n-8}{n-6} \right). \quad (4.4)$$

The reverse is true, i.e., X_c is better than X_I when the inequality (4.4) holds true with a reverse sign (i.e., $\theta < 0.5$ if $n = 10$ and $\theta < 0.85$ if $n = 20$, for example). Notice that θ lies between 0 and 1.

Looking at the expression (3.21), we find that the estimator I_c is superior to the traditional classical calibration estimator X_c when

$$\frac{n^2}{n+1} < \frac{2(2-\theta)}{\theta(1-\theta)} \quad (4.5)$$

which is satisfied for all values of θ provided that n does not exceed 12. For $n > 12$, the range of θ is constrained. As an illustration, the condition (4.5) holds true for $n = 20$ when $\theta < 0.25$ or $\theta > 0.86$.

Similarly, using (3.20), the estimator I_c is superior to the inverse calibration estimator X_I when

$$\left[n^2 - 7n - 6 + \left(2 - \frac{n^2\theta}{n+1} \right) n\theta \right] (1-\theta) > 2. \quad (4.6)$$

which is likely to happen for large values of n and small values of θ . For example, this holds true when at least as long as $\theta \leq 0.5$ for $n = 10$, $\theta \leq 0.8$ for $n = 20$ and $\theta \leq 0.9$ for $n = 30$.

From (3.22) we observe that the estimator C_I is inferior to the classical calibration estimator X_c for all values of n and θ . It thus follows that I_c will be superior to C_I at least so long as I_c is better than X_c meaning thereby that as long as (4.5) is satisfied.

5 Some Remarks

Synthesizing the classical and inverse calibration approaches, we have presented two estimators I_c and C_I , and have analyzed their performance properties employing the SEA theory. Our investigations have revealed that the estimator I_c

is superior to C_I as well as X_c and X_I with respect to the criterion of absolute bias when n exceeds 4 and the condition (4.2) holds. Interestingly enough, this condition always holds true when n is sufficiently large.

If the performance criterion is mean squared error (to the order of our approximation), the estimator I_c is found to be superior to X_c and C_I at least so long as (4.5) holds true. Similarly, it is superior to X_I when the condition (4.6) is satisfied.

Our technique of synthesizing the classical and inverse calibration approach suggests two iterative estimators also. For instance, consider the estimator I_c . Now if we replace X on the right hand side of (2.8) by I_c , we get another feasible estimator. This, in turn, can be used in (2.8) for replacing X so as to formulate yet another feasible estimator. This process may be continued till the estimates stabilize. A similar iterative estimator can be defined using (2.11). It will be interesting to find conditions of convergence and to compare the speed of convergence of the two iterative procedures. Analyzing the bias and mean squared error properties of estimators in successive iterations will be an exercise that may provide some useful guidance to practitioners.

We have studied the performance of calibration estimators under the assumption that errors are normally distributed. Such a specification can be relaxed and asymptotic approximations for the bias and mean squared error can be derived following Lwin and Maritz (1982, Appendix).

We have assumed that merely one reading is taken for estimating X . Our investigation can be easily extended when two or more readings corresponding to X are recorded.

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