Large–Sample Comparisons of Calibration Procedures When Both Measurements Are Subject to Error †

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Abstract

A predictive functional relationship model is presented for the calibration problem in which the standard as well as the nonstandard measurements are subject to error. For the estimation of the relationship between the two measurements, the ordinary least squares and maximum likelihood estimation methods are considered, while for the prediction of unknown standard measurements we consider direct and inverse approaches. Relative performances of those calibration procedures are compared in terms of the asymptotic mean square error of prediction.

1. Introduction

The statistical calibration of a nonstandard instrument or method involves two distinct but related activities: first, the determination of the relationship between the nonstandard and standard measurements by performing a calibration experiment, and second, the estimation (prediction) of the standard measurement in the future based upon the estimated relationship and future nonstandard observations.

The fundamental assumption in the classical theory of calibration is that the standard method measures a certain characteristic without error. Although this assumption is convenient and necessary for utilizing elegant

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theories of linear regression, its validity is questionable in many real world applications.

Recently several authors investigated the calibration problem when the standard as well as the nonstandard measurement is subject to error. Mandel (1984), in discussing applicability of the ordinary least squares (OLS) procedure when both variables are subject to error, proposed a new estimation method based upon transformation of the original, error-contaminated data. Carroll and Spiegelman (1986) examined the effect of ignoring small measurement errors on the performance of the OLS procedure. Based upon large-sample approximation, they identified critical quantities which affect the confidence limits of the unknown standard measurement and the average behavior of the OLS estimators of the unknown parameters. Lwin and Spiegelman (1986) considered a situation where imprecise measurements are calibrated against working standards which are rarely exact. They also constructed confidence limits of the unknown exact values assuming that errors in the working standards are bounded. Fuller (1987, p.177) considered a calibration problem when the error variance of the standard measurement is known. He proposed a modification of the maximum likelihood (ML) estimator for the slope parameter of the functional relationship model, and gave an estimate of the asymptotic mean square error of the predictor.

The present investigation takes an error–in–variables approach to the proposed calibration problem, and compares several competing calibration procedures. That is, procedures based the OLS and ML estimation, combined with "direct" and "inverse" prediction, are compared in terms of the asymptotic mean square error (AMSE) of predicton.

2. The model and estimators

The following model is proposed for the calibration experiment.

$$x_i = \xi_i + u_i \tag{1}$$

$$y_i = \eta_i + v_i \qquad i = 1, 2, \ldots, n \tag{2}$$

$$\eta_i = \alpha + \beta\xi_i \tag{3}$$

where unobservables ξ_i and η_i respectively represent the true standard and nonstandard measurement, and α and β are unknown constants. Random measurement error vectors are assumed to be independently, identically distributed as

$$\begin{bmatrix} u_i \\ v_i \end{bmatrix} \overset{iid}{\sim} \text{BVN}\left\{0, \begin{bmatrix} \sigma_u^2 & \rho\sigma_u\sigma_v \\ \rho\sigma_u\sigma_v & \sigma_v^2 \end{bmatrix}\right\} \tag{4}$$

where BVN reads 'bivariate normal distribution'.

By symmetry, relationship (3) can be rewritten as

$$\xi_i = \gamma + \delta\eta_i, \quad i = 1, 2, \ldots, n \tag{5}$$

where $\gamma = -\alpha/\beta$ and $\delta = 1/\beta$.

The model in Eqs. (1), (2), and (3), or (1), (2), and (5) is commonly called an errors-in-variables model (EVM) in the literature. The EVM is further classified into the functional or structural model depending upon the nature of the variables involved. That is, it is called functional if variables involved are fixed, and structural if random (Kendall and Stuart, 1979).

In this paper ξ and η are assumed to be fixed, and the OLS and ML methods are considered for the estimation of relationships (3) and (5).

The OLS estimators of β, α, δ, and γ are respectively given by

$$b_{OLS} = S_{xy}/S_{xx} \tag{6}$$

$$a_{OLS} = \bar{y} - b_{OLS}\bar{x} \tag{7}$$

$$d_{OLS} = S_{xy}/S_{yy} \tag{8}$$

$$c_{OLS} = \bar{x} - d_{OLS}\bar{y} \tag{9}$$

For the ML estimation, further information on error varinaces is needed to avoid the indentifiability problem. In this paper we assume that the ratio of error variances, $\lambda = \sigma_v^2/\sigma_u^2$, and ρ are known. Then, the ML estimators of β and α are respectively given by (e.g., see Kendall and Stuart, 1979)

$$b_M = \{P + (P^2 - Q)^{\frac{1}{2}}\}/R \tag{10}$$

$$a_M = \bar{y} - b_M\bar{x} \tag{11}$$

where $P = S_{yy} - \lambda S_{xx}$, $Q = 4(S_{xy} - \theta S_{xx})(\theta S_{yy} - \lambda S_{xy})$, $R = 2(S_{xy} - \theta S_{xx})$, $\theta = \rho\sigma_u/\sigma_v = \rho\lambda^{-\frac{1}{2}}$

Similary, the ML estimators of δ and γ are respectively given by

$$d_M = \{P^* + (P^{*2} - Q^*)^{\frac{1}{2}}\}/R^* \tag{12}$$

$$c_M = \bar{x} - d_M\bar{y} \tag{13}$$

where $P^* = \lambda S_{xx} - S_{yy}$, $Q^* = 4(\lambda S_{xy} - \theta S_{yy})(\theta S_{xx} - S_{xy})$, $R^* = 2(\lambda S_{xy} - \theta S_{yy})$

In the future, suppose nonstandard measurement y_f is obtained where

$$\begin{aligned} y_f &= \eta_f + v_f \\ &= (\alpha + \beta\xi_f) + v_f, \quad v_f \sim \mathrm{N}(0, \sigma_v^2) \end{aligned} \tag{14}$$

Then, based upon relationship (3), the corresponding ξ_f is estimated as

$$\hat{\xi}_{fD} = (y_f - a)/b \tag{15}$$

where a and b are either the OLS or ML estimators of α and β, respectively. If relationship (5) is used, ξ_f is predicted as

$$\hat{\xi}_{fI} = c + dy_f \tag{16}$$

where c and d are either the OLS or ML estimators of γ and δ, respectively. Following Mandel (1984), we will subsequently call (15) and (16) "direct" and "inverse" predictor, respectively.

The ML estimation method has the interesting property that it yields the same estimate of ξ_f regardless of the prediction method adopted. To show this, note that $b_M = 1/d_M$. Then,

$$\begin{aligned} \hat{\xi}_{fD} &= (y_f - a_M)/b_M = (y_f - \bar{y})/b_M + \bar{x} = (y_f - \bar{y})d_M + \bar{x} \\ &= d_M y_f + (\bar{x} - d_M\bar{y}) = d_M y_f + c_M = \hat{\xi}_{fI} \end{aligned}$$

Therefore, in this paper the following three procedures are compared in terms of the mean square error of prediction, $\mathrm{E}(\hat{\xi}_f - \xi_f)^2$, based upon large-sample approximation.

Procedure 1 :	direct prediction, OLS estimation
Procedure 2 :	direct prediction, ML estimation
Procedure 3 :	inverse prediction, OLS estimation

3. Asymptotic mean square error of prediction

For simplicity, AMSE's for estimators in Eqs. (15) and (16) are determined when the true value for ρ in Eq. (4) is 0.

After some algebraic manipulation, Eqs. (15) and (16) can be respectively rewritten as

$$\hat{\xi}_{fD} - \xi_f = (\xi_f - \bar{\xi})(\beta/b - 1) + \bar{u} - \bar{v}/b + v_f/b \tag{17}$$

$$\hat{\xi}_{fI} - \xi_f = (\eta_f - \bar{\eta})(d - \delta) + \bar{u} - d\bar{v} + dv_f \tag{18}$$

where b and d are either the OLS or ML estimators of β and δ, respectively.

It is well known (e.g., see Davies and Hutton, 1975) that b_{OLS} is asymptotically normally distributed with asymptotic bias (ABIAS) and variance (AVAR) as

$$\mathrm{ABIAS}(b_{OLS}) = -\beta/(1 + \tau_\xi) \tag{19}$$

$$\mathrm{AVAR}(b_{OLS}) = n^{-1}\{\lambda/(1 + \tau_\xi) + \beta^2\tau_\xi(1 + \tau_\xi^2)/(1 + \tau_\xi)^4\} \tag{20}$$

where

$$\tau_\xi = \lim_{n\to\infty} \sum_{i=1}^{n} (\xi_i - \bar{\xi})^2/(n\sigma_u^2) \tag{21}$$

For the ML estimator b_M, it is asymptotically unbiased, and its asymptotic variance is given by (e.g., see Gleser, 1981)

$$\mathrm{AVAR}(b_M) = n^{-1}\{\sigma_v^2/(\tau_\xi^2\sigma_u^2) + \sigma_v^2/(\tau_\xi\sigma_u^2) + \beta^2/\tau_\xi\} \tag{22}$$

Then, the results on the asymptotic properties of b can be used to characterize the asymptotic behavior of $\hat{\xi}_{fD} - \xi_f$ It can be shown that $\hat{\xi}_{fD} - \xi_f$ is asymptotically normal, and

$$\begin{aligned}\mathrm{AMSE1} = {} & n^{-1}[\{(\xi_f - \bar{\xi})^2 + \psi\sigma_u^2\}\{\psi(1 + \tau_\xi)^3/\tau_\xi^4 + (1 + \tau_\xi^2)/\tau_\xi^3\}] \\ & + n^{-1}\sigma_u^2 + (n^{-1} + 1)\psi\sigma_u^2(1 + \tau_\xi)^2/\tau_\xi^2 + (\xi_f - \bar{\xi})^2/\tau_\xi^2 \end{aligned} \tag{22}$$

$$\begin{aligned}\mathrm{AMSE2} = {} & n^{-1}[\{(\xi_f - \bar{\xi})^2 + \psi\sigma_u^2\}\{\psi/\tau_\xi^2 + \psi/\tau_\xi + 1/\tau_\xi\}] \\ & + n^{-1}\sigma_u^2 + (n^{-1} + 1)\psi\sigma_u^2 \end{aligned} \tag{23}$$

where

$$\psi = \sigma_v^2/(\beta^2\sigma_u^2) \tag{24}$$

Similary, the AMSE of $\hat{\xi}_{fI}$ for Procedure 3 is given by

$$\begin{aligned}\text{AMSE3} = n^{-1}[\{(\xi_f-\bar{\xi})^2+\psi\sigma_u^2\}\{1/\psi(1+\tau_\eta)+\tau_\eta(1+\tau_\eta^2)/(1+\tau_\eta)^4\}] \\ +n^{-1}\sigma_u^2+(n^{-1}+1)\psi\sigma_u^2\tau_\eta^2/(1+\tau_\eta)^2+(\xi_f-\bar{\xi})^2/(1+\tau_\eta)^2\end{aligned} \tag{25}$$

where

$$\tau_\eta = \lim_{n\to\infty}\sum_{i=1}^{n}(\eta_i-\bar{\eta})^2/(n\sigma_v^2) = \tau_\xi/\psi \tag{26}$$

4. AMSE comparisons

It can be easily shown that AMSE1 > AMSE2. To compare Procedures 2 and 3, we reexpress AMSE2 in terms of τ_η as follows.

$$\begin{aligned}\text{AMSE2} =& n^{-1}[\{(\xi_f-\bar{\xi})^2+\psi\sigma_u^2\}\{1/(\tau_\eta^2\psi)+1/\tau_\eta+1/(\tau_\eta\psi)\}] \\ &+n^{-1}\sigma_u^2+(n^{-1}+1)\psi\sigma_u^2\end{aligned} \tag{27}$$

Then, it can be shown that AMSE2 - AMSE3 < 0 if and only if

$$n^{-1}\{(h+p)q+r\}-(h-r)<0 \tag{28}$$

where $h=(\xi_f-\bar{\xi})^2$, $p=\psi\sigma_u^2$, $q=(1+2\tau_\eta)(1+\tau_\eta)/(\tau_\eta^2\psi)+(1+4\tau_\eta+5\tau_\eta^2+4\tau_\eta^3)/\{\tau_\eta(1+\tau_\eta)^2\}$, and $r=\psi\sigma_u^2(1+2\tau_\eta)$. Solving inequality (28) with respect to n and h we obtain the following.

1. If $0<n\le q$, then no $h>0$ exists to satisfy (28). In other words, AMSE2 > AMSE3 in this case.
2. If $n>q$, then (28) is equivalent to

$$h>h^*=(pq+r+nr)/(n-q) \tag{29}$$

For some selected parameter values, Figures 1 and 2 illustrate $\sqrt{h^*}$ versus n by the contours which fix the boundaries of preference between Procedures 2 and 3.

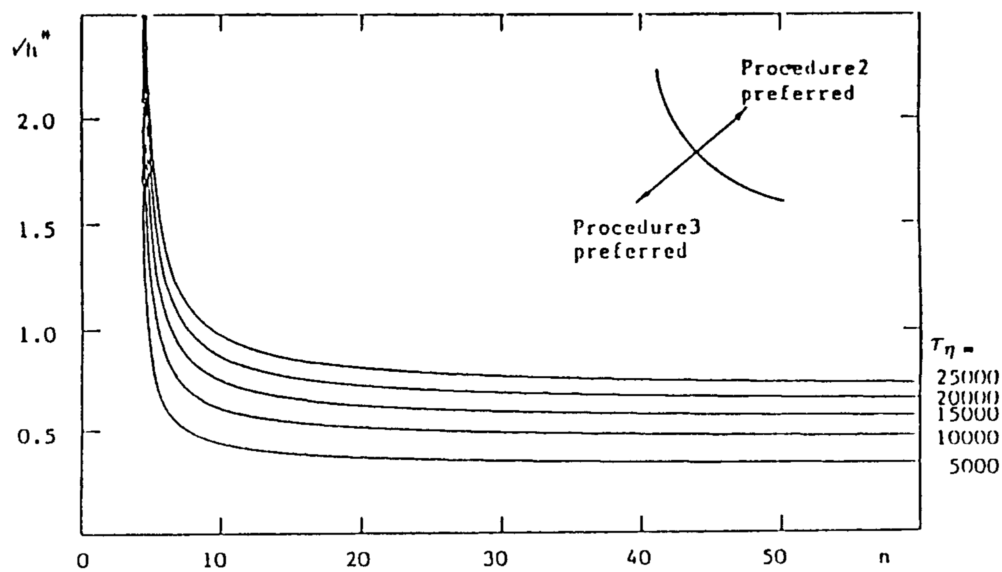

Figure 1. Contours of $\sqrt{h^*}$ versus n (σ_u = 0.001, ψ = 10).

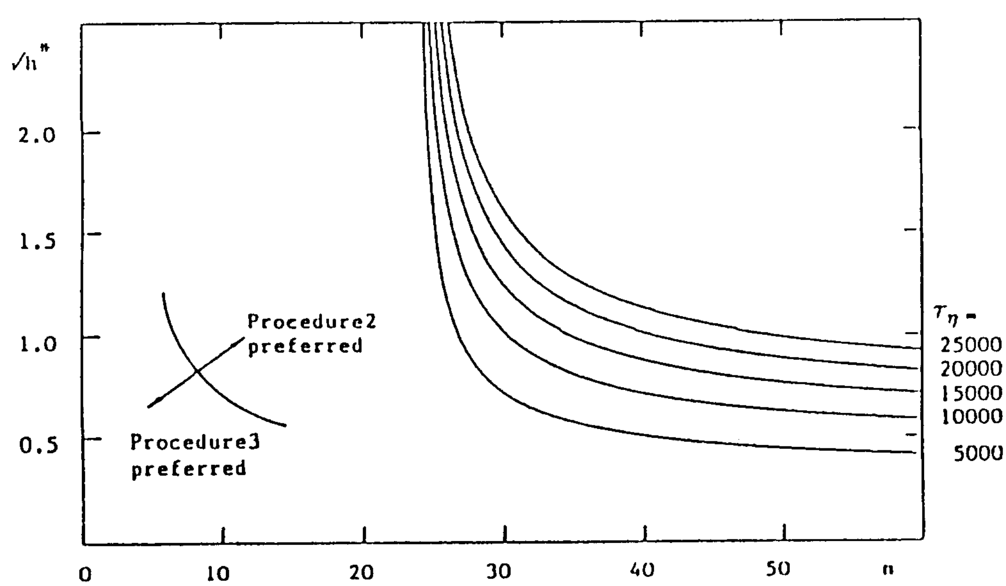

Figure 2. Contours of $\sqrt{h^*}$ versus n (σ_u = 0.01, ψ = 0.1).

We note that h^* is a decreasing funtion of n since

$$\frac{\partial h^*}{\partial n} \equiv -(qr + pq + r)/(n-q)^2 < 0$$

Furthermore, as σ_u^2 increases h^* also increases. To show this, note that as σ_u^2 increases ψ decreases, and consequently, q increases. However, h^* is an increasing function of q since

$$\frac{\partial h^*}{\partial q} \equiv \{p(n-q) + (pq + r + nr)\}/(n-q)^2 > 0$$

Therefore, h^* increases as σ_u^2 increases. This behavior of h^* can be also observed in Figures 1 and 2. We also found that h^* is not necessarily an increasing funtion of τ_η for a given n, σ_u^2, and ψ (although it is so for the cases in Figures 1 and 2).

5. Conclusion

For the calibration problem when both measurements are subject to error, a predictive functional relationship model is proposed and three estimation/prediction procedures were compared in terms of the asymptotic mean square error of prediction.

It is found that AMSE values for Procedure 1 (OLS estimation and direct prediction) are always larger than those of Procedure 2 (ML estimation). The choice between Procedures 2 and 3 (OLS estimation and inverse prediction) depends upon the values of parameters involved. In general, the superiority of Procedure 3 tends to be restricted to the region where ξ_f is close to $\bar{\xi}$ (i.e., where $h = (\xi_f - \bar{\xi})^2$ is small). This trend becomes more prominent as n increases and/or σ_u^2 decreases.

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