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Multivariate Linear Calibration with Univariate Controlled Variable

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ABSTRACT

This paper gives some new results on the multivariate linear calibration problem in the case when the controlled variable is univariate. Firstly, a condition under which one can obtain a finite closed confidence interval of x_0(unknown controlled variable) is suggested. Secondly, this article considers a criterion to find out whether the multivariate calibration significantly shortens the confidence interval of x_0 and supports this criterion by examples. Finally, a multivariate extension of the results in Lwin Maritz(1982) is given.

1. Introduction

Consider the following multivariate linear calibration model;

$$\begin{aligned} \underset{\sim}{y}_i &= \underset{\sim}{\alpha} + B' \underset{\sim}{x}_i + \underset{\sim}{e}_i \quad i=1, \cdots, n \\ \underset{\sim}{y}_{0j} &= \underset{\sim}{\alpha} + B' \underset{\sim}{x}_0 + \underset{\sim}{e}_{0j} \quad j=1, \cdots, k \end{aligned} \tag{1.1}$$

where $\underset{\sim}{y}_i$'s, $\underset{\sim}{y}_{0j}$'s, $\underset{\sim}{e}_i$'s and $\underset{\sim}{e}_{0j}$'s are p-dimensional random variables, $\underset{\sim}{x}_i$'s are q-dimensional known variables, $\underset{\sim}{x}_0$ is a q-dimensional unknown variable, $\underset{\sim}{\alpha}$ is a $p\times 1$ vector of unknown parameters, and B is a $q\times p$ matrix of unknown parameters.

Assume that $\underset{\sim}{e}_i$'s and $\underset{\sim}{e}_{0j}$'s are independent and identically distributed(i.i.d.) $N_p(\underset{\sim}{0}, V)$ random variables. The multivariate calibration problem is to make statistical inferences about $\underset{\sim}{x}_0$ based on $\underset{\sim}{y}_i$'s, $\underset{\sim}{y}_{0j}$'s and $\underset{\sim}{x}_i$'s. The calibration is called controlled(random) calibration when $\underset{\sim}{x}_i$'s and $\underset{\sim}{x}_0$ are controlled(random) variables(see Brown(1982)). In

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random calibration we can make inferences about $\underset{\sim}{x}_0$ based on the following model instead of (1.1).

$$\underset{\sim}{x}_i=\underset{\sim}{\tau}+A\underset{\sim}{y}_i+\underset{\sim}{e}_i,\ i=1,\cdots,n. \tag{1.2}$$

Note that we can predict $\underset{\sim}{x}_0$ by the standard multivariate regression theory in (1.2). Therefore throughout this paper $\underset{\sim}{x}_i$ and $\underset{\sim}{x}_0$ are assumed to be controlled (or fixed) variables.

For $p=q=1$ (univariate calibration) various estimation methods have been proposed by many authors and there are many controversies on which estimation method is desirable (see Hoadley (1970), Brown (1979), Lwin and Maritz (1980, 1982), Hunter and Lamboy (1981), and references listed therein). For the multivariate calibration Draper and Smith (1981, page 125) touch on the case of $p=1$, $q>1$ which is ill-specified case since $\underset{\sim}{x}_0$ can not be completely determined. Recently Brown (1982), Oman and Wax (1984) and Naes (1985) have considered many interesting multivariate calibration problems for $p>1$, $q>1$.

This paper presents some new results for the multivariate linear calibration when the controlled variable is univariate. Section 2 studies a confidence interval of x_0 and provides a condition under which one can derive a finite closed confidence interval of x_0, which is an extension of Graybill (1976, page 282). Section 3 considers the confidence interval of x_0 by assuming that a large calibration experiment has been performed. Section 3 also proposes a condition under which a confidence interval of x_0 with multivariate calibration is significantly shorter than with univariate calibration. Section 4 treats the linear compound estimation which is an extension of the results in Lwin and Maritz (1982). Section 5 gives some examples to back up the results of Section 3.

2. Confidence Interval of x_0

The model (1.1) can be rewritten as follows;

$$\begin{aligned}\underset{\sim}{y}_i&=F'\underset{\sim}{x}_i^*+\underset{\sim}{e}_i,\ i=1,\cdots,n\\ \underset{\sim}{y}_{0j}&=F'\underset{\sim}{x}_0^*+\underset{\sim}{e}_{0j},\ j=1,\cdots,k,\end{aligned} \tag{2.1}$$

where $F'=(\underset{\sim}{\alpha},B')$, $\underset{\sim}{x}_i^*=(1,\underset{\sim}{x}_i')'$, $i=1,\cdots,n$ and $\underset{\sim}{x}_0^*=(1,\underset{\sim}{x}_0')'$. Assume $\underset{\sim}{e}_i$'s and $\underset{\sim}{e}_{0j}$'s are i.i.d. $N_p(\underset{\sim}{0},V)$ random variables. It can be easily shown that $\hat{\underset{\sim}{x}}_0=(\hat{B}S^{-1}\hat{B}')^{-1}\hat{B}S^{-1}(\bar{\underset{\sim}{y}}_0-\hat{\underset{\sim}{\alpha}})$ is the natural maximum likelihood estimator of $\underset{\sim}{x}_0$, where

$$\bar{y}_0=(1/k)\sum_{j=1}^{k} y_{0j},\quad \hat{F}=\begin{pmatrix}\hat{\alpha}'\\ \hat{B}\end{pmatrix}=(Z'Z)^{-1}Z'Y,\quad Z'=(x_1^*,\ \cdots,\ x_n^*),$$

$$Y'=(y_1,\ \cdots,\ y_n),\quad S=(n-q+k-2)^{-1}\Big[(Y-Z\hat{F})'(Y-Z\hat{F})+\sum_{j=1}^{k}(y_{0j}-\bar{y}_0)(y_{0j}-\bar{y}_0)'\Big].$$

Brown(1982) proposed the various estimators for x_0 and compared these by specific examples.

Now, let us consider an interval estimation of x_0. To do this, it can be easily shown that

$$\bar{y}_0-\hat{\alpha}-\hat{B}'x_0\sim N_p(0,\ [k^{-1}+x_0^{*\prime}(Z'Z)^{-1}x_0^*]\,V)$$

and

$$(n-q+k-2)S\sim W_{n-q+k-2}(\cdot\,|\,V),$$

where $W_u(.\,|\,V)$ denotes a Wishart distribution. Without loss of generality, we may assume $\sum_{i=1}^{n} x_i=0$ in this section. Since $\bar{y}_0-\hat{\alpha}-\hat{B}'x_0$ and S are independent,

$$\frac{(\bar{y}_0-\hat{\alpha}-\hat{B}'x_0)'S^{-1}(\bar{y}_0-\hat{\alpha}-\hat{B}'x_0)}{k^{-1}+n^{-1}+x_0'(X'X)^{-1}x_0}\ \frac{n-p-q+k-1}{(n-q+k-2)p}\sim F_{p,n-p-q+k-1} \tag{2.2}$$

by the distribution of Hotelling T^2 statistic, where $X'=(x_1,\ \cdots,\ x_n)$ and $F_{u,v}$ denotes a F distribution with degrees of freedom u and v. From (2.2) we can obtain the following $100(1-r)\%$ confidence region of x_0;

$$[k^{-1}+n^{-1}+x_0'(X'X)^{-1}x_0]^{-1}\frac{n-p-q+k-1}{(n-q+k-2)p}(\bar{y}_0-\hat{\alpha}-\hat{B}'x_0)'S^{-1}(\bar{y}_0-\hat{\alpha}-\hat{B}'x_0)$$
$$\leqq F_{p,n-p-q+k-1;r}, \tag{2.3}$$

where $F_{u,v;r}$ denotes the upper $100r$-th percentiles of $F_{u,v}$. It should be noted that Brown (1982) derived (2.3) in a rather complicated way by introducing a multivariate t distribution. This paper's approach is more comprehensible and shorter than Brown's.

When $p=q=1$, (2.3) reduces to the following;

$$\Big[(\hat{\beta}^2/s^2)-\Big(t^2_{n+k-3,r/2}/\sum_{i=1}^{n}x_i^2\Big)\Big]x_0^2-2(\hat{\beta}/s^2)(\bar{y}_0-\bar{y})x_0+(\bar{y}_0-\bar{y})^2/s^2$$
$$-(n^{-1}+k^{-1})\,t^2_{n+k-3,r/2}\leqq 0, \tag{2.4}$$

where

$$\hat{\beta}=\sum_{i=1}^{n}x_i(y_i-\bar{y})/\sum_{i=1}^{n}x_i^2,\quad \bar{y}=(1/n)\sum_{i=1}^{n}y_i,$$

$s^2=(n+k-3)^{-1}\Big[\sum_{i=1}^{n}(y_i-\bar{y}-\hat{\beta}x_i)^2+\sum_{j=1}^{k}(y_{0j}-\bar{y}_0)^2\Big]$, and $t_{u,r}$ is the upper $100r$-th percentiles of the t-distribution with u degrees of freedom. Graybill(1976, page 282) showed the following;

If $(\hat{\beta}^2/s^2)-t^2_{n+k-3,r/2}/\sum_{i=1}^{n}x_i^2$ *is positive, then* (2.4) *gives a finite closed interval of* x_0. (2.5)

when $q=1$ and $p>1$, (2.3) reduces to

$$(\bar{y}_0-\hat{\alpha}-\hat{\beta}x_0)'S^{-1}(\bar{y}_0-\hat{\alpha}-\hat{\beta}x_0)\leqq(n^{-1}+k^{-1}+x_0^2/\sum_{i=1}^{n}x_i^2)\,T_{0,r}^2, \tag{2.6}$$

where $\hat{\alpha}=\bar{y}=(1/n)\sum_{i=1}^{n}y_i$, $\hat{\beta}=\sum_{i=1}^{n}x_iy_i/\sum_{i=1}^{n}x_i^2$ and $T_{0,r}^2=[(n+k-3)p/(n+k-p-2)]$ $F_{p,n+k-p-2;r}$.

It is easily observed that (2.6) can be written as follows;

$$g(x_0)=a\,x_0^2-2\,bx_0+c\leqq0 \tag{2.7}$$

where $a=\hat{\beta}'S^{-1}\hat{\beta}-T_{0,r}^2\Big/\sum_{i=1}^{n}x_i^2$, $b=(\bar{y}_0-\bar{y})'S^{-1}\hat{\beta}$ and

$$c=(\bar{y}_0-\bar{y})'S^{-1}(\bar{y}_0-\bar{y})-(n^{-1}+k^{-1})\,T_{0,r}^2.$$

It is shown in Appendix that if $a>0$, then (2.7) leads to the following closed interval;

$$a^{-1}[(\bar{y}_0-\bar{y})'S^{-1}\hat{\beta}-\sqrt{D}]\leqq x_0\leqq a^{-1}[(\bar{y}_0-\bar{y})'S^{-1}\hat{\beta}+\sqrt{D}], \tag{2.8}$$

where $D=b^2-ac$. This is an extension of (2.5).

REMARK 2.1 In a size r test of H_0 ; $\beta=0$ versus H_1 ; $\beta\neq0$, we reject H_0 if $a>0$. In practice one would not employ the model if $\beta=0$ and it is unwise to use the data leading to $\beta=0$.

REMARK 2.2 In (2.3) Brown(1982) proved that if $p=q$ and $\hat{B}S^{-1}\hat{B}'-(X'X)^{-1}$ $[(n-q+k-2)p/(n-p-q+k-1)]\,F_{p,n-p-q+k-1;r}$ is positive definite, then the confidence region is a closed ellipsoid. But he did not give any answer when $p\neq q$.

3. Effect of Multivariate Calibration

In this section the effect of multivariate calibration will be considered. For simplicity we treat the case when a large calibration experiment is performed with $p=2$ and $q=1$.

When a large calibration experiment is performed, that is, when n is large, in (1.1), we can use the following model;

$$y_{0j}=\alpha+B'x_0+e_{0j},\quad j=1,\cdots,k, \tag{3.1}$$

where α, B are known, x_0 is an unknown parameter and e_{0j}'s are i.i.d. $N_p(0,\ V)$ (V; known) random variables. Note that $\hat{x}_0=(BV^{-1}B')^{-1}BV^{-1}(\bar{y}_0-\alpha)$ is the usual maximum likelihood estimator of $\underset{\sim}{x}_0$. The following facts about $\underset{\sim}{x}_0$ are useful in our development.

$$\hat{\underset{\sim}{x}}_0 \sim N_q(\underset{\sim}{x}_0,\ k^{-1}(BV^{-1}B')^{-1}) \tag{3.2}$$

$$k(\hat{\underset{\sim}{x}}_0-\underset{\sim}{x}_0)'BV^{-1}B'(\hat{\underset{\sim}{x}}_0-\underset{\sim}{x}_0) \sim \chi_q^2, \tag{3.3}$$

where χ_q^2 denotes a chi-square distribution with q degrees of freedom.

When $q=1$ and $p=2$, $100(1-r)\%$ confidence interval of x_0 can be obtained from

$$k(\hat{x}_0-x_0)^2 \underset{\sim}{\beta}' V^{-1} \underset{\sim}{\beta} \leqq \chi_{1,r}^2 \tag{3.4}$$

where

$$\underset{\sim}{\alpha}'=(\alpha_1,\ \alpha_2),\ \ \underset{\sim}{\beta}'=(\beta_1,\ \beta_2),\ \ \bar{\underset{\sim}{y}}_0'=(\bar{y}_{01},\ \bar{y}_{02})$$

$\hat{x}_0=(\underset{\sim}{\beta}' V^{-1}\underset{\sim}{\beta})^{-1}\underset{\sim}{\beta}' V^{-1}(\bar{\underset{\sim}{y}}_0-\underset{\sim}{\alpha})$ and $\chi_{q,r}^2$ is the upper $100r$-th percentiles of χ_q^2. In (3.4) let

$$V=\begin{pmatrix}\sigma_1^2 & \rho\sigma_1\sigma_2\\ \rho\sigma_1\sigma_2 & \sigma_2^2\end{pmatrix},$$

where ρ is the correlation coefficient of y_{01} and y_{02}. Then $100(1-r)\%$ confidence interval of x_0 is

$$\hat{x}_0-\sqrt{H_r} \leqq x_0 \leqq \hat{x}_0+\sqrt{H_r}\ , \tag{3.5}$$

where $H_r=[\sigma_1^2\sigma_2^2(1-\rho^2)\chi_{1,r}^2]/k(\beta_1^2\sigma_2^2+\beta_2^2\sigma_1^2-2\rho\sigma_1\sigma_2\beta_1\beta_2)$.

If we use y_{01} only, then $100(1-r)\%$ confidence interval of x_0 is

$$\hat{x}_0-(\sigma_1/|\beta_1|)\sqrt{\chi_{1,r}^2/k} \leqq x_0 \leqq \hat{x}_0+(\sigma_1/|\beta_1|)\sqrt{\chi_{1,r}^2/k}\ , \tag{3.6}$$

where $\hat{x}_0=(\bar{y}_{01}-\alpha_1)/\beta_1$. Hence the ratio of the lengths of the above two confidence interval is given by

$$\begin{aligned} K &= \text{length of (3.6)/length of (3.5)}\\ &= \sqrt{1+(1-\rho^2)^{-1}[\rho-(\beta_2\sigma_1/\beta_1\sigma_2)]^2}. \end{aligned}$$

REMARK 3.1 The larger $(1-\rho^2)^{-1}[\rho-(\beta_2\sigma_1/\beta_1\sigma_2)]^2$ is the larger K is and the multivariate calibration is effective. When $\rho=\beta_2\sigma_1/\beta_1\sigma_2$, length of (3.5) = length of (3.6) and there is no reason to employ the multivariate calibration model.

4. Linear Compound Estimation

When $p>1$ and $q=1$, (1.1) becomes

$$\begin{aligned} &\underset{\sim}{y}_i=\underset{\sim}{\alpha}+\underset{\sim}{\beta}x_i+\underset{\sim}{e}_i,\ \ i=1,\ \cdots,\ n\\ &\underset{\sim}{y}_{0j}=\underset{\sim}{\alpha}+\underset{\sim}{\beta}x_0+\underset{\sim}{e}_{0j},\ \ j=1,\ \cdots,\ k, \end{aligned} \tag{4.1}$$

where $\underset{\sim}{y}_{0j}'=(y_{01j},\ \cdots,\ y_{0pj})$, $\underset{\sim}{y}_i'=(y_{1i},\ \cdots,\ y_{pi})$, $\underset{\sim}{\alpha}'=(\alpha_1,\ \cdots,\ \alpha_p)$ and $\underset{\sim}{\beta}'=(\beta_1,\ \cdots,\ \beta_p)$.

Assume that $\underset{\sim}{e}_i$'s and $\underset{\sim}{e}_{0j}$'s are i.i.d. random variables with mean zero and covariance matrix V. Also assume that $\underset{\sim}{\alpha}$ and $\underset{\sim}{\beta}$ are known.

Consider the class of linear estimators $\phi(\underset{\sim}{\bar{y}}_0)=\lambda_0+\underset{\sim}{\lambda}'\underset{\sim}{\bar{y}}_0$ of x_0, where $\underset{\sim}{\lambda}'=(\lambda_1, \cdots, \lambda_p)$. Linear compound estimation is to find $\lambda_0, \lambda_1, \cdots, \lambda_p$ that minimize

$$\Phi_n=\sum_{i=1}^{n} E_F\,[\phi(\underset{\sim}{y}_i)-x_i]^2, \tag{4.2}$$

where E_F denotes the expectation with respect to the distribution function F of $\underset{\sim}{y}_i$ for each fixed x_i. Lwin and Maritz(1982) suggested this method to investigate the controversy existing in the univariate calibration. This section's results are the multivariate extensions of their results.

First rewrite (4.2) as

$$\Phi_n=\sum_{i=1}^{n}(\lambda_0-x_i)^2+n\underset{\sim}{\lambda}'\,V\underset{\sim}{\lambda}+\sum_{i=1}^{n}[\underset{\sim}{\lambda}'(\underset{\sim}{\alpha}+\underset{\sim}{\beta}x_i)]^2+2\sum_{i=1}^{n}(\lambda_0-x_i)\,\underset{\sim}{\lambda}'(\underset{\sim}{\alpha}+\underset{\sim}{\beta}x_i).$$

From $\partial\Phi_n/\partial\lambda_0=0$ and $\partial\Phi_n/\partial\underset{\sim}{\lambda}=0$, one can readily see that

$$\lambda_0=\bar{x}-(\underset{\sim}{\alpha}+\underset{\sim}{\beta}\bar{x})'(V+\underset{\sim}{\beta}\underset{\sim}{\beta}'s_x^2)^{-1}\underset{\sim}{\beta}s_x^2,\quad \underset{\sim}{\lambda}=(V+\underset{\sim}{\beta}\underset{\sim}{\beta}'s_x^2)^{-1}\underset{\sim}{\beta}s_x^2,$$

where $\bar{x}=(1/n)\sum_{i=1}^{n}x_i$ and $s_x^2=(1/n)\sum_{i=1}^{n}(x_i-\bar{x})^2$. Hence we arrive at the optimal estimator given by

$$x^*(\underset{\sim}{\bar{y}}_0)=\bar{x}[1-s_x^2\underset{\sim}{\beta}'(V+\underset{\sim}{\beta}\underset{\sim}{\beta}'s_x^2)^{-1}\underset{\sim}{\beta}]+s_x^2\underset{\sim}{\beta}'(V+s_x^2\underset{\sim}{\beta}\underset{\sim}{\beta}')^{-1}(\underset{\sim}{\bar{y}}_0-\underset{\sim}{\alpha}). \tag{4.3}$$

Using formular (A.2.1) in Cook and Weisberg(1982) we get the following reasonable form;

$$x^*(\underset{\sim}{\bar{y}}_0)=(1+s_x^2\underset{\sim}{\beta}'\,V^{-1}\underset{\sim}{\beta})^{-1}\bar{x}+(1+s_x^2\underset{\sim}{\beta}'\,V^{-1}\underset{\sim}{\beta})^{-1}s_x^2\underset{\sim}{\beta}'\,V^{-1}(\underset{\sim}{\bar{y}}_0-\underset{\sim}{\alpha}). \tag{4.4}$$

Note that $x^*(\underset{\sim}{\bar{y}}_0)$ is a weighted average of $\bar{x}$ and $x^M(\underset{\sim}{\bar{y}}_0)$, where $x^M(\underset{\sim}{\bar{y}}_0)=(\underset{\sim}{\beta}'\,V^{-1}\underset{\sim}{\beta})^{-1}\underset{\sim}{\beta}'\,V^{-1}(\underset{\sim}{\bar{y}}_0-\underset{\sim}{\alpha})$ is the natural maximum likelihood estimator of x_0 when all parameters of (4.1) are known and the errors are normal.

The estimator $x^*(\underset{\sim}{\bar{y}}_0)$ is a biased estimator in general while $x^M(\underset{\sim}{\bar{y}}_0)$ is unbiased. In fact

$$E_F[x^*(\underset{\sim}{\bar{y}}_0)]=x_0+(1+s_x^2\underset{\sim}{\beta}'\,V^{-1}\underset{\sim}{\beta})^{-1}(\bar{x}-x_0).$$

The mean squared errors of $x^*(\underset{\sim}{\bar{y}}_0)$ and $x^M(\underset{\sim}{\bar{y}}_0)$ are

$$MSE[x^*(\underset{\sim}{\bar{y}}_0)]=(k\theta^2)^{-1}[(\theta^2 s_x^2)/(1+s_x^2\theta^2)]^2+[(x_0-\bar{x})/(1+s_x^2\theta^2)]^2,$$

$$MSE[x^M(\underset{\sim}{\bar{y}}_0)]=(k\theta^2)^{-1},\ \text{respectively,}$$

where $\theta^2=\underset{\sim}{\beta}'\,V^{-1}\underset{\sim}{\beta}$. Hence the mean squared error of $x^*(\underset{\sim}{\bar{y}}_0)$ is less than that of $x^M(\underset{\sim}{\bar{y}}_0)$ if

$$(x_0-\bar{x})^2<k^{-1}s_x^2(2+\theta^{-2}s_x^{-2}).$$

As Lwin and Maritz(1982) pointed out, if $\theta^2 s_x^2$ is small and if the estimation is restricted to the calibration range, then $x^*(\bar{y}_0)$ is likely to be preferable to $x^M(\bar{y}_0)$.

In the remainder of this section, the inverse estimator will be compared with the linear compound estimation. The wrong inverse regression model is

$$x_i=\tau_0+\tau_1 y_{1i}+\cdots+\tau_p y_{pi}+e_i,\quad i=1,\ \cdots,\ n$$

and the inverse estimator of x_0 is

$$x^I(\bar{y}_0)=\hat{\tau}'\bar{y}_0=\bar{x}+\sum_{i=1}^{n}(x_i-\bar{x})\,y_i'\left[\sum_{i=1}^{n}(y_i-\bar{y})\,y_i'\right]^{-1}(\bar{y}_0-\bar{y}),$$

where $\hat{\tau}'=(\hat{\tau}_0,\ \hat{\tau}_1,\ \cdots,\ \hat{\tau}_p)$ is the least squares estimator of τ'. The maximum likelihood estimators of β and V are, assuming normality,

$$b=(ns_x^2)^{-1}\sum_{i=1}^{n}(x_i-\bar{x})\,y_i$$

$$S^*=(1/n)\sum_{i=1}^{n}(y_i-\bar{y})\,y_i'-s_x^2\,bb'.$$

Replacing β and V by b and S^* in (4.3), $x^*(\bar{y}_0)$ coincides with $x^I(\bar{y}_0)$. Therefore, though $x^I(\bar{y}_0)$ is derived from the wrong model, it is supported by the compound estimation approach. However one can not find a confidence interval of x_0 from $x^I(\bar{y}_0)$, which seems a major demerit of the inverse estimator.

5. Examples

This section introduces two examples to back up Remark 3.1 of Section 3. The data in Table 1 are a part of the wheat quality data in Brown(1982). y_1 and y_2 are infrared reflectance measurements and w is the percentages of protein content for a wheat of size 21.

The relationship between $y'=(y_1,\ y_2)$ and $x=w-\bar{w}$ is estimated from observations 1 to 17. Then treat each x_i, $i=18, 19, 20, 21$ as the unknown x_0 and use the corresponding y_i as the current observation y_0. It should be noted that $k=1$. The scatter diagram of the above data suggests a linear calibration model (4.1) and a normal error distribution. The maximum likelihood estimates of α, β and an unbiased estimate S of V are given as follows;

$$\hat{\alpha}=\begin{pmatrix}\hat{\alpha}_1\\ \hat{\alpha}_2\end{pmatrix}=\begin{pmatrix}103.94118\\ 358.64697\end{pmatrix},\qquad \hat{\beta}=\begin{pmatrix}\hat{\beta}_1\\ \hat{\beta}_2\end{pmatrix}=\begin{pmatrix}-4.4975\\ -2.73327\end{pmatrix}$$

Table 1. Wheat Quality Data

observation number	y_1	y_2	w	$x=w-\bar{w}$ $\left(\bar{w}=(1/17)\sum_{i=1}^{17} w_i\right)$
1	108	361	10.73	−0.54177
2	107	361	11.05	−0.22177
3	110	362	9.86	−1.41177
4	105	362	11.41	0.13823
5	104	362	11.57	0.29823
6	113	367	9.42	−1.85177
7	113	362	8.82	−2.45177
8	103	360	11.81	0.53823
9	97	351	12.33	1.05823
10	95	353	12.93	1.65823
11	97	352	12.69	1.41823
12	96	355	13.13	1.85823
13	106	357	10.41	−0.86177
14	93	351	13.57	2.29823
15	113	363	9.26	−2.01177
16	110	363	9.82	−1.45177
17	97	355	12.81	1.53823
18	108	366	10.93	−0.34177
19	104	360	11.61	0.33823
20	114	366	9.46	−1.81177
21	96	355	12.85	1.57823

$$S=\begin{pmatrix} s_1^2 & s_{12} \\ s_{12} & s_2^2 \end{pmatrix}=\begin{pmatrix} 1.97901 & 3.50096 \\ 3.50096 & 7.9075 \end{pmatrix}.$$

$$(\hat{\rho}=s_{12}/s_1 s_2=0.8850)$$

Note that we can reject the null hypothesis of $\underset{\sim}{\beta}=0$ at a level of 5%. When both y_1 and y_2 are used, the confidence interval length of x_0 is by (2.8)

$$L_1=2a^{-1}\sqrt{D},$$

where a and D were defined in Section 2. When only y_1 is used, the confidence interval length of x_0 is by Graybill(1976)

$$L_2=2h^{-1}\sqrt{\left(t^2_{15,r/2}\Big/\sum_{i=1}^{n}x_i^2\right)(\bar{y}_{01}-\bar{y}_1)^2+h(n^{-1}+k^{-1})\,t^2_{15,r/2}}$$

where $h=(\hat{\beta}_1^2/s_1^2)-\left(t^2_{15,r/2}\Big/\sum_{i=1}^{n}x_i^2\right)$. Table 2 gives the values of L_1, L_2 and $R=L_2/L_1$ for $r=0.05$ and for each $\underset{\sim}{y_0}$. Table 2 shows that the multivariate calibration is very effective in this example.

It should be remarked that since $\hat{K}=\sqrt{1+(1-\hat{\rho}^2)^{-1}[\hat{\rho}-(\hat{\beta}_2 s_1/\hat{\beta}_1 s_2)]^2}\doteqdot 2.1$, one can

Table 2. Confidence Interval Lenths and Their Ratios

$\underset{\sim}{y}_0'$	L_1	L_2	$R=L_2/L_1$
(108, 336)	0.68764	1.97487	2.87194
(104, 360)	1.11777	1.95363	1.74779
(114, 366)	1.18621	2.08069	1.75406
(96, 350)	0.92521	2.03375	2.19814

expect $R\doteqdot 2.1$ which nearly agrees with Table 2.

Now compare the actual predictions. Let $\hat{x}_i$ be the maximum likelihood estimates of x_i, $i=18, 19, 20, 21$. A natural criterion for prediction accuracy is

$$PA=100\sum_{i=18}^{21}(x_i-\hat{x}_i)^2 \Big/ \sum_{i=18}^{21} x_i^2,$$

the percentage of unexplained variation. When both y_1 and y_2 are used $PA=3.6$, where as $PA=12.8$ if we use y_1 only. In this respect the multivariate prediction is much better than the univariate prediction.

Table 3. Changed Wheat Quality Data

observation number	y_1	y_2	w	$x=w-\bar{w}$ $\left(\bar{w}=(1/17)\sum_{i=1}^{17} w_i\right)$
1	108	361	10.73	−0.54177
2	107	361	11.05	−0.22177
3	110	362	9.86	−1.41177
4	105	362	11.41	0.13823
5	104	361	11.57	0.29823
6	113	370	9.42	−1.85177
7	113	368	8.82	−2.45177
8	103	360	11.81	0.53823
9	97	350	12.33	1.05823
10	95	353	12.93	1.65823
11	97	352	12.69	1.41823
12	96	351	13.13	1.85823
13	106	360	10.41	−0.86177
14	93	350	13.57	2.29823
15	113	366	9.26	−2.01177
16	110	369	9.82	−1.45177
17	97	355	12.81	1.53823
18	108	363	10.93	−0.34177
19	104	360	11.61	0.33823
20	114	366	9.46	−1.81177
21	96	350	12.85	1.57823

The above example is a case when the multivariate calibration is highly effective. Next consider an example in which the multivariate calibration can hardly shorten the confidence interval length. First change the data of Table 1 artificially to get a small $\hat{K}$. The modified data are given in Table 3.

By similar computation one can get $\hat{K}=1.01427$, $\hat{\rho}=0.61544$ and Table 4. Since $\hat{K}$ is near to 1, one can primarily expect that the multivariate calibration does not shorten the length of the confidence interval. In fact the multivariate calibration can not significantly shorten the length of the confidence interval when compared with the confidence interval length of the univariate calibration as Table 4 shows. In the actual predictions by using the maximum likelihood estimates $PA=12.8$ when both y_1 and y_2 are used, while $PA=13.6$ when only y_1 is used. Therefore the multivariate prediction is not much better than the univariate prediction in this example.

Table 4. Confidence Interval Lengths and Their Ratios

y_0'	L_1	L_2	$R=L_2/L_1$
(108, 363)	1.83552	1.97487	1.07592
(104, 360)	1.81083	1.95363	1.07886
(114, 366)	1.78252	2.08069	1.16728
(96, 350)	1.76446	2.03375	1.15262

Appendix

If $a>0$ and if $D=b^2-ac>0$, then $g(x_0)\leqq 0$ leads to a finite closed interval. Note that

$$\begin{aligned} b^2 &= [(\bar{y}_0-\bar{y})' S^{-1} \hat{\beta}]^2 \\ &= [(\bar{y}_0-\bar{y})' S^{-1} \hat{\beta}][(\bar{y}_0-\bar{y})' S^{-1} \hat{\beta}]' \\ &= (\bar{y}_0-\bar{y})' S^{-1} \hat{\beta}\hat{\beta}' S^{-1} (\bar{y}_0-\bar{y}) \\ &= \mathrm{tr}[(\bar{y}_0-\bar{y})' S^{-1} \hat{\beta}\hat{\beta}' S^{-1} (\bar{y}_0-\bar{y})] \\ &= (\bar{y}_0-\bar{y})' S^{-1} (\bar{y}_0-\bar{y}) \mathrm{tr}(\hat{\beta}\hat{\beta}' S^{-1}) \\ &= [(\bar{y}_0-\bar{y})' S^{-1} (\bar{y}_0-\bar{y})](\hat{\beta}' S^{-1} \hat{\beta}), \end{aligned}$$

where $\mathrm{tr}(A)$ denotes the trace of a square matrix A. Hence

$$\begin{aligned} D &= [(\bar{y}_0-\bar{y})' S^{-1} (\bar{y}_0-\bar{y})]\hat{\beta}' S^{-1} \hat{\beta} - a[(\bar{y}_0-\bar{y})' S^{-1} (\bar{y}_0-\bar{y}) - (n^{-1}+k^{-1})\, T^2_{0,r}] \\ &= \left(T^2_{0,r} \Big/ \sum_{i=1}^{n} x_i^2\right)[(\bar{y}_0-\bar{y})' S^{-1} (\bar{y}_0-\bar{y})] + a(n^{-1}+k^{-1})\, T^2_{0,r}. \end{aligned}$$

Since S^{-1} is positive semidefinite, $D>0$ if $a>0$. Therefore (2.7) leads to (2.8) if $a>0$.

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References

(1) Brown, G.H. (1979). An optimization criterion for linear inverse estimation. *Technometrics*, Vol. *21*, 575~579.

(2) Brown, P.J. (1982). Multivariate calibration. *J.R. Statist. Soc. B.*, Vol. *44*, 287~321.

(3) Cook, R.D. and Weisberg, S. (1982). *Residuals and Influence in Regression.* Chapman and Hall, New York.

(4) Draper, N. and Smith, H. (1981). *Applied Regression Analysis, 2nd edn.*, Wiley, New York.

(5) Graybill, F.A. (1976). *Theory and Application of the Linear Model.* Duxbury Press, North Scituate.

(6) Hoadley, B. (1970). A Bayesian look at inverse linear regression. *J. Amer. Statist. Assoc.*, Vol. *65*, 356~369.

(7) Hunter, W.G. and Lamboy, W.F. (1981). A Bayesian analysis of the linear calibration problem. *Technometrics*, Vol. *23*, 323~350.

(8) Lwin, T. and Maritz, J.S. (1982). An analysis of the linear calibration controversy from the perspective of compound estimation. *Technometrics*, Vol. *24*, 235~242.

(9) Naes, T. (1985). Multivariate calibration when the error covariance matrix is structured. *Technometrics*, Vol. *27*, 301~311.

(10) Oman, S.D. and Wax, Y. (1984). Estimating fetal age by ultrasound measurements; an example of multivariate calibration. *Biometrics*, Vol. *40*, 947~960.