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An improved approach to multivariate linear calibration

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Abstract. The article presents an approach to multivariate linear calibration based on the best linear predictor. The bias and mean squared error for the suggested predictor are derived in order to examine its properties. It has been examined that Bias/σ^2 and MSE/σ^2 are functions of five invariant quantities. A simulation study is made for different values of response variables and sample sizes assuming different distributions for the explanatory variable. It is observed that the proposed estimator performs quite well. Some approximations to mean squared error have been suggested and the pivotal functions based on these approximations have been defined. Lower and upper tail probabilities have been calculated and it is examined that they are quite reasonable. These probabilities suggest that the relevant intervals have sensible confidence coefficient. Moreover, it is also shown that the multivariate classical and inverse estimators are special cases of the proposed estimator.

1. Introduction

Multivariate calibration is a two-step procedure and has many applications in science and industry. In the first step, we have data from a multivariate regression experiment (X_i, T_i), $i = 1, 2, \cdots, N$; X_i is $q \times 1$ and T_i is $p \times 1$ vector. Usually, the T values are precise and expansive and the X values are cheap and easily made on the same objects. In the second step, called current situation, a $q \times 1$ vector ε is observed and $p \times 1$ vector T is to be predicted using data of multivariate regression experiment ($p \leq q$) available from the first step.

Consider multivariate linear regression model as follows:

$$X = T\beta^{\#} + \varepsilon, \tag{1}$$

where X is an $N \times q$ matrix of q response variables for each of the N individuals. T is $N \times (p+1)$ matrix whose first column consists of 1's and the other vector columns list p explanatory variables measured on N individuals. $\beta^{\#}$ is a $(p+1) \times q$ matrix of regression parameters and ε is a matrix of $N \times q$ random errors whose rows ε_i^T are independent and normally distributed with $E(\varepsilon_i) = 0$ and $E(\varepsilon_i \varepsilon_i^T) = \Gamma$. The maximum likelihood estimators of $\beta^{\#}$ and Γ for the regression experiment are:

$$\hat{\beta}^{\#} = \left(T^T T\right)^{-1} T^T X,$$

$$\hat{\Gamma} = \left\{ X^T \left(I - T \left(T^T T\right)^{-1} T^T \right) X \right\} / N, \tag{2}$$

but the unbiased estimate of Γ is:

$$\hat{\Gamma} = \left\{ X^T \left(I - T \left(T^T T\right)^{-1} T^T \right) X \right\} / (N - p - 1). \tag{3}$$

If $\beta^{\#}$ in Eq. (1) is partitioned as $\begin{bmatrix} \alpha^T \\ \beta^T \end{bmatrix}$, β is $q \times p$.

Two commonly used estimators to predict T are the classical and the inverse estimators. The classical

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or maximum likelihood estimator for $p \times 1$ vector T is:

$$\breve{T} = \bar{T} + \left(\hat{\beta}^T \hat{\Gamma}^{-1} \hat{\beta}\right)^{-1} \hat{\beta}^T \hat{\Gamma}^{-1} \left(X - \bar{X}\right). \tag{4}$$

and the inverse estimator is:

$$\tilde{T} = \bar{T} + S_{TX} S_{XX}^{-1} \left(X - \bar{X}\right). \tag{5}$$

S_{TX} is $p \times q$ matrix of sums of products corrected for the mean and S_{XX} is $q \times q$ matrix of sums of corrected squares and products. These estimators have been studied by Brown [1], Brown [2] along with the extension to the Lwin and Maritz [3] approach, Fujikoshi and Nishii [4], Naes [5], Rinco and Chuiv [6], Spezzaferri [7], Osborne [8], Kubokawa and Robert [9], Sundberg [10,11], Mathew and Sharma [12], Olivieri [13], Jose and Isaac [14], and Gabrielsson and Trygg [15]. Some recent literature on the topic may be seen in Dinc et al. [16], Tan et al. [17], Ebadi and Amiri [18], Xuemei et al. [19], Forbes and Minh [20], Jensen and Ramirez [21], and John [22] and the references therein.

Sundberg [23] and Brown and Sundberg [24] discussed confidence and conflict of these estimators. Sundberg and Brown [25] suggested considering one explanatory variable at a time, forgetting the existence of the other $(p-1)$ variables. Very often, $(p = 1)$ is of interest in practical situations, as has been discussed by Wood [26] and Oman and Wax [27], where they estimated only one variable age using more response variables of different body measurements. Srivastava [28], Oman and Srivastava [29], and Takeuchi [30] also discuss general (q) and $(p = 1)$. In such situations, one may think of the current situation (X, T) with $p(x, t)$, where T is to be predicted based on the observed q-vector X in (X, T) and available data of multivariate regression experiment, i.e. (X_i, T_i); $i = 1, 2, \cdots, N$, from the first step. We believe that some of the conflicts may be avoided by separating the issue of regression parameter estimation in the first step from that of choosing the best linear function in the second step and proposing an estimator, i.e. the best linear predictor approach. We concentrate on $p = 1$ and general q, i.e. the most practical situation. Bias and mean squared error are derived. Also, interval estimates are suggested based on the approximated mean squared error.

2. Derivation of the best linear predictor

The multivariate normal linear regression model (Eq. (1)) with q-vector X and an explanatory variable T can be written as $X_i = \alpha_{q\times 1} + T_i \beta_{q\times 1} + \varepsilon_i$, $i = 1, 2, \cdots, N$; X_i and ε_i are $(q\times 1)$ vectors with $E(\varepsilon_i) = 0$ and $E(\varepsilon_i \varepsilon_i^T) = \Gamma$, but ε_i's are independent for $i = 1, 2, 3, \cdots N$.

In the current situation (X, T), the joint distribution $p(x, t)$ is such that $p(X|T = t)$ is $N(\alpha + T\beta, \Gamma)$. The best linear $\hat{T}$ is derived by minimizing:

$$E[T - (C + D^T X)]^2. \tag{6}$$

Eq. (6) is minimized by:

$$C = E(T) - D^T E(X) = \mu - D^T(\alpha + \mu\beta),$$

and:

$$D = \sigma^2[\Gamma + \sigma^2 \beta\beta T]^{-1}\beta,$$

so the best linear predictor will be:

$$\hat{T} = C + D^T X = E(T) - D^T[X - E(X)]$$

$$= \mu(1 - D^T\beta) + D^T(X - \alpha)$$

$$= \mu(1 - p^2) + (X - \alpha)^T \sigma^2 \left\{\Gamma + \sigma^2 \beta\beta^T\right\}^{-1} \beta, \tag{7}$$

where:

$$\rho^2 = D^T\beta = \sigma^2 \beta^T \{\Gamma + \sigma^2 \beta\beta^T\}^{-1}\beta. \tag{8}$$

The current situation with $p = 1$ and general q is $\alpha_{q\times 1}$, $\beta_{q\times 1}$, $\Gamma_{q\times q}$, all described by the parameters μ, σ^2. These parameters define all the first- and second-order moments of current $p(x, t)$. According to the proposed approach, the regression experiment provides estimates of α, β, and Γ, because the joint distribution $p(x, t)$ is such that $p(X|T = t)$ is the same in both regression and future situations, i.e. $N(\alpha + T\beta, \Gamma)$ and the first two moments $\mu = E(T)$ and $\sigma^2 = \text{VAR}(T)$ of $p(t)$ are assumed to be known. The parameters μ and σ^2 are not known exactly, but may be assessed as follows:

i. An assumption implicit in any calibration technique is $t_* \leq T \leq t*$, Otherwise the experimental regression has to be extrapolated. Bounds for μ and σ^2 can be deduced;

ii. Sometimes a random sample of T's (or more commonly of X's [31]) is available. Natural estimates $\hat{\mu}$ and $\hat{\sigma}^2$ result in:

$$E(X) = EE(X|T) = \alpha + \beta\mu,$$

$$\text{VAR}(X) = \text{VAR}(E(X|T)) + E(\text{VAR}(X|T))$$

$$= \beta^2\sigma^2 + \sigma^2_{x|t}.$$

iii. In the absence of (ii), μ and σ^2 may be the parameters of a subjective probability distribution.

It is interesting to note that the proposed best linear predictor in Eq. (7) gives classical estimator Eq. (4) for $\sigma^2 = \infty$., as:

$$\rho^2 = D^T\beta = \sigma^2\beta^T\{\Gamma + \sigma^2\beta\beta^T\}^{-1}\beta = 1.$$

The inverse estimator (Eq. (5)) is obtained when $\mu = \bar{t}$ and $\sigma^2 = S_{TT}/N-2$ is inserted in Eq. (7).

For $p = q = 1$, the model Eq. (1) becomes the simple linear regression model and the whole calibration situation becomes univariate [32]. Kubokawa and Robert [9] obtained inverse estimator using Bayesian approach by inserting the estimated mean and variance of T.

3. Bias and mean squared error

There are two situations: (i) α, β, and Γ known; it is just of theoretical nature; and (ii) α, β, and Γ known unknown; it is the most practical situation:

i. α, β, and Γ known:

$$\text{Bias} = E(T - (C + D^T X) = 0,$$

$$\begin{aligned}\text{MSE} &= E[T-(C+D^TX)]^2\sigma^2 - D^T\text{COV}(T,X)\\ &= \sigma^2[1-\sigma^2\beta^T(\Gamma+\sigma^2\beta\beta^T)^{-1}\beta]\\ &= \sigma^2(1-\rho^2),\end{aligned}$$

by definition of ρ^2 as in Eq. (8);

ii. α, β, and Γ unknown:

$$\text{Bias} = E\left[T-\left(\hat{C}+\hat{D}^TX\right)\right] = -\left[E\left(\hat{C}\right)-C\right] - \left[E\left(\hat{D}\right)-D\right]^T\{\alpha+\beta\mu\} \neq 0, \qquad (9)$$

so estimator biased.

$$\begin{aligned}\text{MSE} &= E\left(T-\hat{C}-\hat{D}^TX\right)^2\\ &= EE\left[\left(T-\hat{C}-\hat{D}^TX\right)^2 \middle| \hat{C},\hat{D}\right].\end{aligned}$$

The expression $E[(T-\hat{C}-\hat{D}^TX)^2|\hat{C},\hat{D}]$ is quadratic in $\hat{C}$ and $\hat{D}$, and is minimized by $\hat{C} = C$ and $\hat{D} = D$ and its minimum is $\sigma^2(1-\rho^2)$. Thus:

$$E\left[\left(T-\hat{C}-\hat{D}^TX\right)^2 \middle| \hat{C},\hat{D}\right] = \begin{pmatrix}\hat{\mathbf{C}}-\mathbf{C}\\ \hat{\mathbf{D}}-\mathbf{D}\end{pmatrix} M \begin{pmatrix}\hat{\mathbf{C}}-\mathbf{C}\\ \hat{\mathbf{D}}-\mathbf{D}\end{pmatrix} + \sigma^2(1-\rho^2).$$

Here, M is a $(q+1)\times(q+1)$ symmetric matrix, i.e.:

$$M = \begin{bmatrix} 1 & EX_1 & . & . & EX_q\\ & Ex_1^2 & . & . & EX_1X_q\\ & & . & . & .\\ & & & . & .\\ & & & & EX_q^2\end{bmatrix}.$$

Now, $\text{MSE} = \sigma^2(1-\rho^2) + E$ trace MN, here:

$$N = \begin{pmatrix}\hat{\mathbf{C}}-\mathbf{C}\\ \hat{\mathbf{D}}-\mathbf{D}\end{pmatrix}\left(\hat{\mathbf{C}}-\mathbf{C} \quad \hat{\mathbf{D}}^{\mathbf{T}}-\mathbf{D}^{\mathbf{T}}\right).$$

Finally:

$$\begin{aligned}\text{MSE} =& E\left(\hat{C}-C\right)^2 + 2(EX_1)E\left(\hat{C}-C\right)\left(\hat{D}_1-D_1\right)\\ &+\cdots+2(EX_q)E\left(\hat{C}-C\right)\left(\hat{D}_q-D_q\right)\\ &+E(X_1^2)E\left(\hat{D}_1-D_1\right)^2+\cdots\\ &+2(EX_1X_q)E\left(\hat{D}_1-D_1\right)\left(\hat{D}_q-D_q\right)\\ &+\cdots+\cdots+(EX_q^2)E\left(\hat{D}_q-Dq\right)^2\\ &+\sigma^2(1-\rho^2). \end{aligned} \qquad (10a)$$

For $q = p = 1$, it decreases to simple linear calibration [15] and $\text{MSE} = (1-\rho^2)\sigma^2(1+Q_s)$. Therefore:

$$\text{MSE}/\sigma^2 = (1-\rho^2)(1+Q_s). \qquad (10b)$$

Using Taylors series, Gabrielsson and Trygg [15] approximated the value of Q_s and denoted it by Q_A.

$$Q_A = \frac{\rho^2}{N} + \frac{1}{N-2}[2\rho^2(1-\rho^2)+(1-2\rho^2)C_N+\rho^2B_N]. \qquad (11)$$

Eq. (11) depends only on four invariants, i.e. N, B_N, C_N and ρ^2. Here, N is size of the experiment; $C_N = (N-2)\sigma^2/S_{TT}$ is the relative concentration of the experiment; $B_N = (N-2)(t-\mu)^2/S_{TT}$ is the relative bias of the experiment; and ρ^2 is squared correlation coefficient.

Eq. (10a) includes uncertainty due to estimation of parameters in addition to the intrinsic uncertainty due to multivariate situation. We show in Theorem 1 that MSE/σ^2 in Eq. (10a) depends only upon N, B_N, C_N, ρ, and q.

Theorem 1. MSE/σ^2 depends only upon N, B_N, C_N, ρ, and q. It would be proved in five steps:

- **Step 1:** MSE/σ^2 depends upon: (i) the unconditional moments μ, σ^2, EX, $\text{COV}(X)$ and $\beta\sigma^2$ and (ii) the parameters of the distribution of ($\hat{\mathbf{C}}$, $\hat{\mathbf{D}}$).

  Proof: Note that ρ^2 is merely a function of (i), so MSE/σ^2 depends only on: (i) μ, σ^2, α, β, and Γ, and (ii) the distribution of $\hat{\alpha}$, $\hat{\beta}$, and $\hat{\Gamma}$, ([33], Theorem 8.2.2), so MSE/σ^2 depends only on μ, σ^2, α, β, Γ; t, S_{TT}, and N;

- **Step 2:** MSE/σ^2 is not changed by:
  (i) Changes of origin/scale of T;
  (ii) Changes of origin of X;
  (iii) $X \to HX$, where H is non-singular.
  These will be proved in Step 2 of Theorem 2;
- **Step 3:** MSE/σ^2 depends only on q, N, ρ, $\sqrt{(\bar{t}-\mu)^2/(S_{TT}q/(N-2))}$, $(N-2)\sigma^2/S_{TT}$; $\bar{t}$, S_{TT}, α, β and Γ.

  Proof: This follows at once from Step 1. Note that q, N, ρ, $\sqrt{(\bar{t}-\mu)^2/(S_{TT}q/(N-2))}$ and $(N-2)\sigma^2/S_{TT}$ are invariants for transformations (i), (ii), and (iii) of Step 2;
- **Step 4:** Consider two calibration situations or systems A and B which have the same values of q, N, ρ, $\sqrt{B_N}$, and C_N. By transformation of T and X (of types mentioned in Step 2), system A becomes system A' with:

$$\bar{t}=0, \qquad S_{TT}=N-2, \qquad \alpha=0, \qquad \Gamma=1,$$

$$\beta=\left[\frac{\rho}{\sqrt{(N-2)\sigma^2/S_{TT}(1-\rho^2)}}0,0,\cdots,0\right]. \quad (12)$$

  Possibility of this transformation is shown in Step 5.

  By a transformation of similar type, system B becomes system B' with $\bar{t}=0$, $S_{TT}=N-2$, $\alpha=0$ and $\Gamma=1$, and β is same as the above in Eq. (12).

  By Step 3, A' and B' agree in all quantities on which MSE/σ^2 depends. By Step 2, $(\text{MSE}/\sigma^2)_A = (\text{MSE}/\sigma^2)_{A'}$ and $(\text{MSE}/\sigma^2)_B = (\text{MSE}/\sigma^2)_{B'}$, thus $(\text{MSE}/\sigma^2)_A = (\text{MSE}/\sigma^2)_B$. In other words, MSE/$\sigma^2$ depends only on q, N, ρ, B_N and C_N;
- **Step 5:** To show the possibility of $A \to A'$, by (i), (ii), and/or (iii) of Step 2, where A' has $\bar{t}=0$, $S_{TT}=N-2$, $\alpha=0$ and $\Gamma=1$ and β is as in Eq. (12) in Step 4, we have the following reasoning.

  First, $\bar{t}=0$ and $S_{TT}=N-2$ are ensured by choice of origin/scale of T. These values will not be disturbed by transformation of X, which are about to be described.

  After a linear transformation, $X \to HX$ has simultaneously achieved $\Gamma=1$ and the required β; a change of origin in X will ensure $\alpha=0$ without disturbing Γ or β.

  The transformation $X=HX$ can be done in the following stages:
  (a) Linearly independent combinations $Y_2, Y_3, \cdots, Y_q$ are chosen with zero regression on T, i.e. $Y_j = m_j^T X$, where $m_j^T\beta=0$ $(j=2,3,\cdots,q)$;
  (b) $Y_1 = m_1^T X$ is chosen to be uncorrelated (conditional on T) with $Y_2, Y_3, \cdots, Y_q$), thus $m_1^T\Gamma m_j = 0$ $(j=2,3,...,q)$;
  (c) Write $Y=(Y_2,Y_3,\cdots,Y_q)^T$ and $\text{COV}(Y|T) = GG^T$ where G is $(q-1)\times(q-1)$ and non-singular.
  Now, $\text{COV}(G^{-1}Y|T) = \text{COV}(G^{-1}GG^T(G^{-1})^T) = I$. The components of $Z=G^{-1}Y$ are uncorrelated (conditional on T) with Y_1, by (b). Change of scale of Y_1 is all that is needed to achieve $\Gamma=1$. Z has zero regression on T by (a);
  (d) Consider:

$$HX=\begin{bmatrix}\text{Scaled version of } Y_1\\ \cdots\cdots\cdots\cdots\\ Z\end{bmatrix}$$

  If its regression vector is $(\beta^*,0,0,\cdots,0)^T$ and its conditional covariance matrix is I, then the identity $\rho^2=\sigma^2\beta^T(\Gamma+\sigma^2\beta\beta^T)^{-1}\beta$ shows that:

$$\rho^2 = \sigma^2(\beta^*,0,0,\cdots,0)\left\{I+\begin{bmatrix}\sigma^2\beta^{*2} & 0\cdots & 0\\ 0 & 0 & 0\\ 0 & 0 & 0\end{bmatrix}\right\}^{-1}\begin{bmatrix}\beta^*\\0\\0\end{bmatrix}$$
$$=\frac{\sigma^2\beta^{*2}}{1+\sigma^2\beta^{*2}}, \quad (13)$$

  thus:

$$\beta^{*2}=\frac{\rho^2}{\sigma^2(1-\rho^2)}. \quad (14)$$

  Since system A' has $S_{TT}=N-2$, we replace σ^2 by $(N-2)\sigma^2/S_{TT}$. Thus:

$$\beta^{*^2}=\frac{\rho^2}{[(N-2)\sigma^2/S_{TT}](1-\rho^2)}$$
$$=\frac{\rho^2}{C_N(1-\rho^2)}. \quad (15)$$

These steps complete the proof that MSE/σ^2 depends only on q, N, ρ, B_N, and C_N.

Theorem 2: σ^{-1} Bias depends only on q, N, ρ, B_N, and C_N.

Proof: From Eq. (9)

$$\text{Bias}/\sigma = -\left[E\left(\hat{C}\right)-C\right] - \left[E\left(\hat{D}\right)-D\right]^T\{\alpha+\beta\mu\}/\sigma. \quad (16)$$

The steps in this proof are very similar to the proof for MSE/σ^2 in Theorem 1, except Step 2 which is slightly different:

- **Step 1:** Same as above in Theorem 1;
- **Step 2:** Bias/σ is not changed by:
  - (i) Changes of origin/scale in T;
  - (ii) Changes of origin in X;
  - (iii) $X \to HX$, where H is non-singular.

Proof: $D = \sigma^2\{\Gamma + \sigma^2\beta\beta^T\}^{-1}\beta$; $C = \mu - D^T(\alpha + \mu\beta)$

(i) Change of origin/scale in T.

Consider T', where $T = f + gT'$ and $\alpha + \beta T = \alpha' + \beta' T'$, so $\alpha + \beta f + \beta g T' = \alpha' + \beta' T'$, thus $\beta' = \beta g$ and $\alpha' = \alpha + \beta f$; also $\mu' = E(T') = E[(T-f)/g] = (\mu - f)/g$; $\sigma'^2 = \text{VAR}(T') = \text{VAR}[(T-f)/g] = \sigma^2/g$; so, Γ is unchanged, i.e. $\Gamma = \Gamma'$.

The results given above show that $\sigma\beta$ is unchanged, therefore $\{\Gamma + \sigma^2\beta\beta^T\}$ is unchanged and $D' = \sigma'^2\{\Gamma' + \sigma'^2\beta'\beta'^T\}^{-1} = \sigma' D/\sigma = D/g$. Similarly, $E(\hat{D}') = E(\hat{D}')/g$; therefore, $E(\hat{D}' - D') = E(\hat{D}' - D)/g$.

Now, $\alpha' + \beta'\mu' = \alpha + \beta f + \beta g[(\mu - f)/g] = \alpha + \mu\beta$. Therefore, the second term in Bias/σ, i.e. Bias/$\sigma = -[E(\hat{D}) - D]^T\{\alpha + \beta\mu\}/\sigma$, is invariant.

Now, $C' = \mu' - D'(\alpha' + \mu'\beta') = [(\mu - f)/g] - [D^T/g][\alpha + \mu\beta] = (C - f)/g$. Similarly, $\hat{C}' = (\hat{C} - f)/g$ and $E(\hat{C}') = [E(\hat{C}) - f]/g$; therefore, the first term in Bias/σ, i.e. $-[E(\hat{C}) - C]/\sigma$, is also invariant. Thus, Bias/σ is invariant for changes of origin or scale in T, as required for (i).

(ii) $X' = m + X$.

μ, σ, unchanged; $\alpha' + \beta' T = E(X'|T) = m + \alpha + \beta T$. Therefore, $\alpha' = m + \alpha$ and $\beta' = \beta$; $\Gamma' = \Gamma$; $D' = D$; $\hat{D}' = \hat{D}$; and $C' = \mu - D^T(\alpha' + \mu\beta') = C - D^T m$. Similarly, $\hat{C}' = \hat{C} - \hat{D}^T m$ and $E\hat{C}' = E\hat{C} - E(\hat{D}^T)m$. Thus:

$$\begin{aligned}\text{Bias} = &-\left[E\hat{C} - E\left(\hat{D}^T\right)m - (C - D^T m)\right] \\ &- E\left[E\hat{D} - D\right]^T\{m + \alpha + \beta\mu\}\left[E\hat{C} - C\right] \\ &- \left[E\hat{D} - D\right]^T\{\alpha + \beta\mu\},\end{aligned}$$

that is not changed. So Bias/σ is also invariant. Note that $E\hat{C} - C$ is not invariant.

(iii) $X' = HX$, where, H is $q \times q$ non-singular.

μ, σ, unchanged, $\alpha' + \beta' T = E[X'|T] = H(\alpha + \beta T)$, therefore, $\alpha' = H\alpha$ and $\beta' = H\beta$; and $\Gamma' = \text{COV}[X'|T] = \text{COV}[HX|T] = H\Gamma H^T$; thus:

$$\left\{\Gamma' + \sigma'^2\beta'^T\right\} = \left(H^T\right)^{-1}\left\{\Gamma + \sigma^2\beta\beta^T\right\}H^{-1},$$

and:

$$D' = \left(H^T\right)^{-1} D.$$

Similarly, $\hat{D}' = (H^T)^{-1}\hat{D}$, $E\hat{D}' = (H^T)^{-1}E\hat{D}$ and $E[\hat{D}' - D] = (H^T)^{-1}E[\hat{D} - D]$, therefore, the second term in Bias becomes $E[\hat{D}' - D]H^{-1}H\{\alpha + \beta\mu\}$, i.e. not changed.

$C = \mu - D^T\{\alpha + \mu\beta\}$ is also unchanged; therefore, C', EC', $(EC' - C)$ and the first term in Bias/σ are seen successively to be unchanged.

Thus, Bias/σ is invariant for non-singular transformations $H' = HX$, as required for (iii).

Steps 3, 4, and 5 are same as those in Theorem 1. These steps complete the proof.

4. Simulations

MSE/σ^2 in Eq (10b) depends only on the four invariants N, ρ^2, B_N, and C_N and on q for any value of q and also it is invariant under changes of origin/scale of T and X. Therefore, it is enough to simulate the canonical system with: $\bar{t} = 0$, $S_{TT} = N - 2$, $\alpha = 0$, $\Gamma = 1$, and:

$$\beta = (\beta^*, 0, 0, \cdots, 0)^T,$$

where $\beta^* = \rho/\sqrt{[C_N(1-\rho^2)]}$, $\mu = \sqrt{B_N}$, and $\sigma^2 = C_N$.

In the canonical form, we have:

$$EX_1 = \beta^*\mu; \quad EX_2 = EX_3 = \cdots = EX_q = 0.$$

$$EX_1^2 = \beta^{*2}\sigma^2 + (\beta^{*2}\mu)^2 + 1 = \beta^{*2}(\sigma^2 + \mu^2) + 1;$$

$$EX_2^2 = EX_3^2 = \cdots = EX_q^2 = 1;$$

$$EX_1X_2 = EX_1X_3 = \cdots = EX_{q-1}X_q = 0.$$

Substituting these values in Eq. (10a), we get:

$$\begin{aligned}\text{MSE} =& \sigma^2(1-\rho^2) + E\left(\hat{C} - C\right)^2 \\ &+ 2\beta^*\mu E\left(\hat{C} - C\right)\left(\hat{D}_1 - D_1\right) \\ &+ [\beta^{*2}(\sigma^2 + \mu^2) + 1\}E\left(\hat{D}_1 - D_1\right)^2 \\ &+ (q-1)E\left(\hat{D}_2 - D_2\right)^2. \end{aligned} \tag{17}$$

The last term in Eq. (17) is in symmetry with $X_2, X_3, \cdots, X_q$.

$$D = \left[\frac{\sigma^2\beta^*}{1 + \sigma^2\beta^{*2}}, 0, \cdots, 0\right]^T,$$

i.e. $D_2, D_3, \cdots, D_q = 0$;

$$C = \mu - D^T\{\alpha + \mu\beta\} = \frac{\mu}{1 + \sigma^2\beta^{*2}}.$$

Therefore, the best linear predictor is:

$$C + D^T X = C + D_1 X_1 = \{\alpha + \mu\beta\} = \frac{\mu + \sigma^2\beta^{*2}X_1}{1 + \sigma^2\beta^{*2}}. \quad (18)$$

To evaluate Eq. (17), we require simulating $\hat{C}$ and $\hat{D}$, and thus estimates of $\text{VAR}(\hat{C})$, $\text{VAR}(\hat{D}_1)$, $\text{VAR}(\hat{D}_2)$, $\text{COV}(\hat{C}, \hat{D}_1)$, $E(\hat{C}) - C$, $E(\hat{D}_1) - D_1$, $E(\hat{D}_2)$, $E(\hat{C} - C)^2 = \text{VAR}(\hat{C}) + (\text{Bias } C)^2$, etc.

These can be estimated by simulating $\hat{\alpha}, \hat{\beta}$, and $\hat{\Gamma}$ from their distributions. Anderson ([33], Theorem 8.2.2) states that if $X_{a(q\times 1)}$ is $N(\beta_{(q'\times P')}, t_{a(p'\times 1)}, \Gamma_{q\times q})$, $a = 1, 2, \cdots, N$, let $p' = p + 1$, where p is the number of explanatory variables, $t_a = (1, t_{1a}, \cdots, t_{pa})^T$. Then:

$$\hat{\beta}_q \times p' \quad \text{is} \quad N(\beta, \cdots),$$

and:

$$\text{COV } (i\text{th and } j\text{th rows of } \hat{\beta}) \quad \text{is} \quad \gamma_{ij} A^{-1}, \quad (19)$$

where $A_{p'\times p'} = \sum t_a t_a^T$ and $\Gamma = \{\gamma_{ij}\}$ and $N\hat{\Gamma}_{\text{MLE}}$ is $W(\Gamma, N - p')$, independent of $\hat{\beta}$.

In linear calibration, when $p = 1$, $X_{a(q\times 1)}$ is:

$$N\left[[\alpha_1\beta_1, \alpha_2\beta_2, \cdots, \alpha_q\beta_q]^T \begin{bmatrix} 1 \\ t_a \end{bmatrix}, \Gamma_{q\times q}\right],$$

$$a = 1, 2, \cdots, N,$$

and in the X_a canonical form, X_a is $N[(\beta^* t_a, 0, 0, \cdots, 0)^T, \mathbf{I}]$, $a = 1, 2, \cdots, N$; thus, $\Gamma = 1$ and:

$$A = \sum_a \begin{bmatrix} 1 & t_a \\ t_a & t_a^2 \end{bmatrix} = \begin{bmatrix} N & 0 \\ 0 & S_{TT} \end{bmatrix},$$

because $\bar{t} = 0$, $\hat{\alpha}_i, \hat{\beta}_i (i = 1, 2, \cdots, q)$ are independent by Eq. (19); also by Eq. (19), covariance matrix of $(\hat{\alpha}_i, \hat{\beta}_i)$ is:

$$A^{-1} = \begin{bmatrix} N^{-1} & 0 \\ 0 & S_{TT}^{-1} \end{bmatrix}.$$

$\hat{\alpha}_i$ is $N(0, 1/N)$, $i = 1, 2, \cdots, q$; $\hat{\beta}_1$ is $N(\beta^*, 1/(N - 2))$ and $\hat{\beta}_i$ is $N(0, 1/(N - 2))$, $i = 1, 2, \cdots, q$. Also, independent $N\hat{\Gamma}_{\text{MLE}}$ is $W(I, N - 2)$ and unbiased $\hat{\Gamma}$ is $(N - 2)^{-1}W(I, N - 2)$. Bartlett's decomposition of Wishart matrix ([33], Corollary 7.2.1) was used to simulate $\hat{\Gamma}$.

10000 values of $\hat{C}$ and $\hat{D}$ are obtained by the follows equation:

$$\hat{D} = \sigma^2 \left\{\hat{\Gamma} + \sigma^2\hat{\beta}\hat{\beta}^T\right\}^{-1} \hat{\beta},$$

$$\hat{C} = \mu - \hat{D}^T\left(\hat{\alpha} + \mu\hat{\beta}\right),$$

by simulating $\hat{\alpha}$, $\hat{\beta}$, $\hat{\Gamma}$ from their distributions mentioned above with $\mu = \sqrt{B_N}$ and $\sigma^2 = C_N$. Ultimately, natural estimates of $\text{VAR}(\hat{C})$, $\text{VAR}(\hat{D}_1)$, $\text{VAR}(\hat{D}_2)$, $\text{COV}(\hat{C}, \hat{D}_1)$, $E(\hat{C}) - C$, $E(\hat{D}_1) - D_1$, and $E(\hat{D}_2)$ are obtained from these simulations.

$$\text{MSE}/\sigma^2 = (1 - \rho^2)(1 + Q_s),$$

so:

$$Q_s = \text{MSE}/[\sigma^2(1 - \rho^2)] - 1. \quad (20)$$

MSE/σ^2 is invariant, so it would be Q_s.

Q_s is calculated by Eq. (20) for the $81 = (3 \times 3 \times 3 \times 3)$ combinations of 4 invariants by choosing their most plausible values, i.e. $N = 10, 30, 50$; $B_N = 0.0, 1.0, 4.0$; $C_N = 0.25, 1.0, 4.0$ and $\rho^2 = 0.7, 0.8, 0.9$, and for $q = 1, 2, 3, 4, 8$ by the procedure described above. The results are given in Table 1(a) and the following messages are obtained.

(i) Q_S is an increasing function of q when ρ^2, B_N, C_N, and N are fixed;

(ii) Q_S for small values of N is greater than that for large values of N, i.e. Q_S is greater for $N = 10$ than for $N = 30$ and 50 (ρ^2, B_N, C_N, and q are fixed).

For $q = 1$, these values quite agreed with the simulated values of Muhammad and McLaren [32]. It should be noted that inverse estimator corresponds to $B_N = 0$ and $C_N = 1$, as also discussed by Srivastava [28], Oman and Srivastava [29], and Takeuchi [30].

5. Approximations and interval estimates

Approximation to $Q_S(N-2)$ when $q > 1$ and $p = 1$ can be obtained using simulated values and this can be used to define an interval estimate for T. The procedure to obtain approximations to $Q_S(N - 2)$ is based on regressing simulated values and is described as follows.

For any particular value of q, Q_S is a function of N, ρ^2, B_N, C_N, i.e. $Q_S(N, \rho^2, B_N, C_N)$. Muhammad and McLaren [32] made an extensive study for simple linear calibration problem ($p = q = 1$) by considering simulated values Q_S and an approximated value Q_A was obtained with the help of Taylor's series. Using Taylor's series, they got a mathematical expression for Q_A when $q = 1$.

$$Q_A = \frac{\rho^2}{N} + \frac{1}{N-2}[2\rho^2(1-\rho^2) + (1-2\rho^2)C_N + \rho^2 B_N]. \quad (21)$$

Table 1(a). 81 values of $\hat{Q}_S$ for $q = 1, 2, 3$, and 4.

	$q=1$			$q=2$			$q=3$			$q=4$		
C_N	**0.25**	**1.0**	**4.0**	**0.25**	**1.0**	**4.0**	**0.25**	**1.0**	**4.0**	**0.25**	**1.0**	**4.0**
B_N						$\rho_2 = 0.7$, $N = 10$						
0	0.134	0.163	0.344	0.308	0.377	0.711	0.560	0.662	1.108	1.015	1.110	1.562
1	0.232	0.258	0.415	0.426	0.487	0.802	0.709	0.800	1.239	1.212	1.298	1.746
4	0.521	0.258	0.623	0.773	0.809	1.069	1.158	1.221	1.635	1.804	1.862	2.294
						$\rho_2 = 0.7$, $N = 30$						
0	0.040	0.045	0.061	0.072	0.086	0.142	0.110	0.131	0.224	0.152	0.181	0.304
1	0.066	0.071	0.085	0.099	0.112	0.165	0.138	0.159	0.250	0.183	0.212	0.335
4	0.142	0.147	0.156	0.179	0.190	0.235	0.222	0.242	0.327	0.276	0.304	0.426
						$\rho_2 = 0.7$, $N = 50$						
0	0.024	0.027	0.0366??	0.042	0.049	0.081	0.060	0.072	0.124	0.082	0.099	0.170
1	0.038	0.041	0.050	0.057	0.065	0.095	0.077	0.088	0.139	0.098	0.115	0.186
4	0.082	0.085	0.092	0.104	0.110	0.137	0.125	0.136	0.183	0.148	0.165	0.235
						$\rho_2 = 0.8$, $N = 10$						
0	0.136	0.186	0.376	0.313	0.397	0.714	0.567	0.683	1.140	1.012	1.131	1.652
1	0.245	0.306	0.483	0.443	0.525	0.826	0.725	0.836	1.277	1.216	1.328	1.841
4	0.568	0.644	0.803	0.824	0.902	1.150	1.203	1.304	1.694	1.829	1.918	2.401
						$\rho_2 = 0.8$, $N = 30$						
0	0.041	0.052	0.091	0.075	0.092	0.157	0.116	0.138	0.227	0.159	0.188	0.300
1	0.071	0.082	0.122	0.106	0.122	0.186	0.147	0.169	0.257	0.194	0.222	0.334
4	0.158	0.170	0.214	0.196	0.212	0.271	0.242	0.263	0.345	0.296	0.324	0.433
						$\rho_2 = 0.8$, $N = 50$						
0	0.025	0.031	0.053	0.044	0.054	0.091	0.064	0.077	0.127??	0.087	0.103	0.167
1	0.041	0.047	0.071	0.062	0.071	0.108	0.082	0.095	0.144	0.105	0.121	0.185
4	0.091	0.097	0.122	0.115	0.124	0.159	0.137	0.149	0.197	0.161	0.177	0.239
						$\rho_2 = 0.9$, $N = 10$						
0	0.135	0.209	0.554	0.317	0.416	0.805	0.572	0.698	1.195	1.006	1.153	1.712
1	0.255	0.335	0.711	0.458	0.559	0.951	0.739	0.864	1.355	1.219	1.359	1.909
4	0.069	0.712	1.178	0.869	0.978	1.383	1.243	1.370	1.848	1.854	1.978	2.502
						$\rho_2 = 0.9$, $N = 30$						
0	0.042	0.060	0.135	0.078	0.100	0.185	0.121	0.146	0.244	0.166	0.195	0.309
1	0.075	0.093	0.170	0.112	0.134	0.219	0.155	0.180	0.278	0.204	0.233	0.347
4	0.172	0.192	0.276	0.213	0.234	0.320	0.260	0.287	0.382	0.316	0.346	0.458
						$\rho_2 = 0.9$, $N = 50$						
0	0.025	0.035	0.077	0.046	0.059	0.109	0.067	0.081	0.137	0.092	0.108	0.172
1	0.044	0.054	0.097	0.066	0.078	0.128	0.088	0.102	0.158	0.112	0.128	0.192
4	0.099	0.110	0.155	0.125	0.138	0.188	0.149	0.162	0.218	0.174	0.190	0.253

This expression suggests the following linear model for $q \geq 1$:

$$Q_{A1} = \frac{1}{N-2}\big[b_o + b_1\rho^2 + b_2\rho^4 + (b_3 + b_4\rho^2 + b_5\rho^4)C_N + (b_6 + b_7\rho^2 + b_8\rho^4)B_N\big]. \quad (22)$$

Simulated values Q_S corresponding to any set of values of the invariants for any $q\times 1$ can be generated and Q_A1 in Eq. (22) can be replaced by those simulated values Q_S for maximum $q = 8$. Thus, the following quadratic multiple regression model can be fitted.

$$Q_s(N-2) = \big[b_o + b_1\rho^2 + b_2\rho^4 + (b_3 + b_4\rho^2 + b_5\rho^4)C_N + (b_6 + b_7\rho^2 + b_8\rho^4)B_N\big] + \text{error}, \quad (23)$$

coefficients b_i's $(i = 0, 1, \cdots, 8)$ may depend on N and q. Q_R will represent fitted values of Eq. (23).

Here, to increase the scope of study, sample space for the invariants ρ^2, B_N, and C_N with five values for each, i.e. $\rho^2 = 0.3, 0.5, 0.7, 0.8, 0.9$; $B_N = 0.0, 1.0, 2.0,$

Table 1(b). Partial regression estimates and S.E.'s for different values of q and N.

	N	$q=1$	$q=2$	$q=3$	$q=4$	$q=8$
	10	-0.5422(0.3915)	1.2306(0.2769)	3.8386(0.3229)	8.9605(0.4232)	—
b_o	30	-0.4081(0.1578)	-0.1111(0.1246)	0.3101(0.1894)	0.9699(0.3221)	6.9410(1.3190)
	50	-0.2441(0.0978)	0.1838(0.0952)	-0.0243(0.1244)	0.3425(0.2283)	3.2410(1.0360)
	10	5.4520(1.4400)	3.0150(1.0180)	0.9560(1.1870)	-2.3600(1.5560)	—
b_1	30	4.6982(0.5804)	4.9255(0.4581)	5.2021(0.6964)	5.4810(1.1840)	1.5610(4.8490)
	50	4.0942(0.3597)	4.9598(0.3501)	5.6386(0.4574)	6.1038(0.8395)	5.0630(3.8100)
	10	-4.5930(1.1950)	-2.0116(0.8452)	-0.4754(0.9856)	1.1730(1.2920)	—
b_2	30	-3.5677(0.4818)	-2.8512(0.3802)	-2.2225(0.5781)	-1.8138(0.9831)	2.7340(4.0250)
	50	-3.0357(0.2986)	2.8091(0.2906)	-2.4855(0.3797)	-2.0672(0.6968)	1.4990(3.1620)
	10	1.6681(0.1386)	0.9969(0.0980)	0.1286(0.1143)	-1.4228(0.1498)	—
b_3	30	1.6608(0.0559)	2.1445(0.0441)	2.6063(0.0670)	2.9120(0.1140)	2.0545(0.4667)
	50	1.4414(0.0346)	2.3670(0.0337)	3.0648(0.0440)	3.5284(0.0808)	4.4555(0.3667)
	10	-5.4357(0.5096)	-1.4705(0.3604)	1.6764(0.4202)	5.0521(0.5509)	—
b_4	30	-5.9741(0.2054)	-5.2029(0.1621)	-4.5158(0.2465)	-3.8032(0.4192)	3.4460(1.7160)
	50	-5.3675(0.1273)	-5.9353(0.1239)	-5.9277(0.1619)	-5.3840(0.2971)	-1.2680(1.3480)
	10	5.1623(0.4230)	1.6352(0.2992)	-0.4441(0.3488)	-2.0651(0.4573)	—
b_5	30	5.4846(0.1705)	4.0896(0.1346)	2.8833(0.2046)	1.8909(0.3480)	-4.3480(1.4250)
	50	5.0425(0.1057)	4.6463(0.1028)	3.8767(0.1344)	2.8491(0.2466)	-2.2510(1.1190)
	10	0.2302(0.1336)	0.6018(0.0945)	1.0525(0.1102)	1.6213(0.1445)	—
b_6	30	-0.0064(0.0539)	0.2276(0.0425)	0.4776(0.0646)	0.7367(0.1099)	2.1522(0.4501)
	50	-0.0337(0.0334)	0.1329(0.0325)	0.3067(0.0425)	0.5147(0.0779)	1.5559(0.3536)
	10	-0.1597(0.4915)	-0.5000(0.3476)	-0.6582(0.4053)	-0.7725(0.5313)	—
b_7	30	0.8041(0.1981)	0.3100(0.1563)	-0.1125(0.2377)	-0.4330(0.4043)	-1.4080(1.6550)
	50	0.9501(0.1228)	0.5582(0.1195)	-0.2529(0.1561)	-0.0652(0.2865)	-1.0510(1.3000)
	10	1.2038(0.4080)	1.2048(0.2885)	1.0786(0.3364)	0.8851(0.4410)	—
b_8	30	0.2833(0.1645)	0.5443(0.1298)	0.7398(0.1973)	0.8692(0.3356)	0.5670(1.3740)
	50	0.1124(0.1019)	0.3982(0.0992)	0.5442(0.1296)	0.6540(0.2379)	0.6640(1.0790)
		S and R^2 (in parenthesis) for different N				
	10	0.2320(98.0%)	0.1641(99.2%)	0.1913(99.2%)	0.2508(99.2%)	—
	30	0.0935(99.6%)	0.0738(99.8%)	0.1122 (99.7%)	0.1908 (99.4%)	0.7814 (96.3%)
	50	0.0580(99.8%)	0.0564 (99.9%)	0.0737(99.9%)	0.1353(99.7%)	0.6139(98.0%)

3.0, 4.0; and $C_N = 0.25, 0.50, 1.0, 2.0, 4.0$, is considered and the values of N are $N = 10, 30, 50$. $Q_S(N-2)$ corresponding to $125 = (5 \times 5 \times 5)$ combinations of ρ^2, B_N, C_N is calculated for each $N = 10, 30, 50$, making a total of 375.

Linear model Eq. (23) is fitted by ordinary least squares for $q = 1, 2, 3, 4$, and 8, using 125 values of Q_S for $N = 10, 30, 50$, respectively. Estimates of partial regression coefficients along with other relevant statistics are given in Table 1(b). R^2 is coefficient of determination and S is such that $(125-9)S^2 =$ residual sum of squares. Table 1(c) summarizes $Q_S(N-2)$, $Q_A(N-2)$, and $Q_R(N-2)$.

5.1. *Results* ($q = 1$)

Table 1(b) indicates that the values of R^2 are greater than 98% and S decreases with the increase in N. This, along with the summary in Table 1(c), shows that the model fits the situation very well. 95% of the interval estimates constructed for regression parameters b_i's

Table 1(c). Summary statistics of 125 values of $Q_S(N-2)$, $Q_R(N-2)$ and $Q_A(N-2)$ for N and q.

q		**Minimum**			**Median**			**Maximum**		
	N	**10**	**30**	**50**	**10**	**30**	**50**	**10**	**30**	**50**
1	$Q_S(N-2)$	0.865	0.745	0.795	2.819	2.514	2.449	9.427	7.717	7.749
	$Q_R(N-2)$	0.806	0.768	0.782	2.782	2.489	2.461	8.720	7.616	7.411
	$Q_A(N-2)$	0.700	0.740	0.748	2.400	2.467	2.480	7.060	7.180	7.204
2	$Q_S(N-2)$	2.104	1.415	1.361	4.972	4.029	3.971	11.064	8.953	9.040
	$Q_R(N-2)$	2.130	1.348	1.303	4.917	3.965	3.920	10.817	8.900	8.990
3	$Q_S(N-2)$	4.025	2.167	1.958	7.935	5.557	5.348	14.784	10.688	10.468
	$Q_R(N-2)$	4.231	2.048	1.852	7.907	5.576	5.361	14.760	10.604	12.882
4	$Q_S(N-2)$	7.845	3.070	2.677	12.496	7.173	6.626	20.015	13.204	13.158
	$Q_R(N-2)$	7.986	2.936	2.530	12.394	7.130	6.703	20.164	12.956	12.882
8	$Q_S(N-2)$	—	8.325	6.099	—	15.100	12.816	—	26.557	26.310
	$Q_R(N-2)$	—	8.330	5.863	—	15.743	12.719	—	25.579	25.587

$(i = 0, 1, \cdots, 8)$ of Eq. (23) overlapped for $N = 30$, 50, and also for $N = 10$, most of the time. The approximation Eq. (23) suggests that bi would depend slightly on N.

To compare the mathematical (Eq. (22)) and multiple linear regression model (Eq. (23)), define two quantities S_A and S_R as:

$$S_A = E[Q_S(N-2) - Q_{A1}(N-2)]^2$$
$$= \frac{1}{125} \sum_{i=1}^{125} 1[Q_S(N-2) - Q_{A1}(N-2)]^2,$$

and:

$$S_R = E[Q_S(N-2) - Q_R(N-2)]^2$$
$$= \frac{1}{125-9} \sum_{i=1}^{125} 1[Q_S(N-2) - Q_R(N-2)]^2 = \hat{\sigma}^2.$$

Q_A, as in Eq. (21), is obtained by Taylor's series and Q_R is from regression model, where coefficients of ρ^2, ρ^4, etc. in Q_R are functions of $Q_1, Q_2, \cdots, Q_{125}$. The values of S_A and S_R for each N are given in Table 2.

These results indicate that the approximations get better for high values of N. It looks reasonable to pool these three regressions for $N = 10$, 30, 50, because there is a reason to think that three functions are the same (mathematical approximation).

Table 2. S_R and S_A for different values of N.

N	**10**	**30**	**50**
S_R	0.054	0.009	0.0034
S_A	0.445	0.045	0.0150
S_A/S_R	8.2	5.0	4.0

5.2. Combination of estimates

Let the linear model (Eq. (23)) be represented by $E(X) = A\theta$, where $A_{125\times 9}$ is a matrix of ρ^2, B_N, C_N and $\theta_{9\times 1}$ is a parameter vector; also, $\text{COV}(X) = \sigma^2 I$; then, $\hat{\theta} = ((A^T A)^{-1} A^T X$ and $\text{COV}(\hat{\theta}) = \sigma^2 (A^T A)^{-1}$.

If we assume $X_M (M = 1, 2, \cdots, 125)$ is $N(A\theta, \sigma^2 I)$, then:

$$\text{Loglik} = \text{Const} - 25 \log \sigma - \frac{1}{2\sigma^2}[X - A\theta]^T [X - A\theta]$$
$$= \text{Const} - 125 \log \sigma$$
$$- \frac{1}{2\sigma^2}\left[\left(\theta - \hat{\theta}\right)^T A^T A \left(\theta - \hat{\theta}\right) + \text{RSS}\right].$$

For three independent sets of data with $N = 10$, 30, 50, and 125 observations in each, let $\hat{\theta}_{10}$, $\hat{\theta}_{30}$, $\hat{\theta}_{50}$ be the estimates for $N = 10$, 30, 50 with error variances σ^2_{10}, σ^2_{30} and σ^2_{50}, respectively; then:

$$\text{Combined Loglik} = \text{Const} - 125 \sum \log \sigma_i$$
$$- \frac{1}{2} \sum \frac{1}{\sigma^2}_N \left(\theta - t\hat{h}eta_N\right)^T A^T A \left(\theta - \hat{\theta}_N\right).$$

$A^T A$ is the same each time, because values of A are determined by ρ^2, B_N and C_N and it is not a diagonal matrix; RSS_N is absorbed in Constant. This arrangement is equal to:

$$\text{Const} - 125 \sum \log \sigma_i$$
$$- \frac{1}{2}\left(\theta - \hat{\theta}\right)^T \left(\frac{1}{\sigma^2_{10}} + \frac{1}{\sigma^2_{30}} + \frac{1}{\sigma^2_{50}}\right) (A^T A) \left(\theta - \hat{\theta}\right),$$

for an appropriate choice of $\hat{\theta}$ and constant. By comparing linear terms in θ:

$$-2\hat{\theta}^T K\theta = -2\left[\frac{1}{\sigma_{10}^2}\hat{\theta}_{10}^T(A^TA)\theta + \frac{1}{\sigma_{30}^2}\hat{\theta}_{30}^T(A^TA)\theta + \frac{1}{\sigma_{50}^2}\hat{\theta}_{50}^T(A^TA)\theta\right],$$

where:

$$K = \left(\frac{1}{\sigma_{10}^2} + \frac{1}{\sigma_{30}^2} + \frac{1}{\sigma_{50}^2}\right)(A^TA),$$

coefficient vector:

$$K\hat{\theta} = \sum \frac{1}{\sigma_N^2}(A^TA)\hat{\theta}_N, \quad \hat{\theta} = \sum W_N\hat{\theta}_N,$$

and $\text{COV}(\hat{\theta}) = \sum W_N^2 \text{COV}(\hat{\theta}_N)$, and $W_N = \frac{a}{b}$, with $a = \frac{1}{\sigma_N^2}$, $b = \frac{1}{\sigma_{10}^2} + \frac{1}{\sigma_{30}^2} + \frac{1}{\sigma_{50}^2}$ and $\sum_1^3 w_i = 1$. Using the above theory, we combined estimates for $N = 10$, 30, 50, which are represented in Table 3.

Table 3 shows that only some of b_i's corresponding to $Q_A(N-2)$, i.e. coefficients for Eq. (21), lie in the pooled interval from regression. Presumably, Q_R is a better approximation than Q_A.

5.3. Results ($q = 2, 3, 4, 8$)

Linear model (Eq. (23)) is fitted to 125 values, each of $Q_S(N-2)$, for $q = 2$, 3, 4, 8 and $N = 10$, 30, 50 and the results are shown in Tables 1(b) and 1(c). It is clear from tables that R^2 is always very high, i.e. for $q = 2$, it is 99.2% for $N = 10$, and 99.9% for $N = 50$. S is very small, i.e. for $q = 2$, it is 0.1641 for $N = 10$, and 0.0564 for $N = 50$. Similarly, for $q = 3$, 4. For $q = 8$, R^2 is still high but S has increased. Results for $q = 8$ and $N = 10$ are not reported because of high estimation error in multivariate regression experiments as $N \geq p + q + 1$ is required to avoid singularity of the error covariance matrix Γ [25]. Table 1(c) suggests that the linear model Eq. (23) fits very well.

Table 3. Combined b_i's for different values of N.

Coef.	W.S.D	Interval estimate		(b_i) in Q_A
-0.300	0.081	-0.46	-0.14	0
4.310	0.299	3.72	4.90	2.80*
-3.244	0.24	-3.73	-2.76	-2.00
1.509	0.029	1.45	1.57	1.00
-5.531	0.106	-5.74	-5.32	-4.00
5.165	0.088	4.99	5.34	4.00
-0.015	0.028	-0.07	0.04	0.00
0.863	0.102	0.66	1.06	1.00
0.205	0.085	0.04	0.37	0.00

*: This value is for $N = 10$ and the values for any other N can be calculated by the relation $2 + (N-2)/N$.

5.4. Interval estimates

An approximate interval estimate of the form is proposed: $\hat{T} \pm 1.96\sqrt{\hat{\text{MSE}}}$. The unknown parameters can be estimated; then, the unconditional interval for T would reflect uncertainty about α, β, and Γ. To study the error probabilities using simulation, we define pivotal function F_1 as follows:

$$F_1 = \frac{T - \left(\hat{C} + \hat{D}X\right)}{\sqrt{\hat{\text{MSE}}}} = \frac{\text{Bias of } T}{\sqrt{\hat{\text{MSE}}}} = \frac{\text{Bias of } T/\sigma}{\sqrt{\hat{\text{MSE}}/\sigma^2}}. \quad (24)$$

Here:

$$M\hat{S}E = (1-\rho^2)\sigma^2(1+Q_R),$$

$$E(F_1) \approx E\left(\frac{T - \left(\hat{C} + \hat{D}X\right)}{\sqrt{\hat{\text{MSE}}}}\right) = \frac{-[\left(E\hat{C} - C\right) - \left(E\hat{D} - D\right)^T\{\alpha + \beta\mu\}}{\sqrt{\hat{\text{MSE}}_{\text{reg}}}},$$

$$E(F_1) \approx E\left(\frac{T - \left(\hat{C} + \hat{D}X\right)}{\sqrt{\hat{\text{MSE}}_{\text{reg}}}}\right) = \frac{\text{MSE}/E}{\sqrt{\hat{\text{MSE}}_{\text{reg}}}} \approx 1.$$

It follows from Theorems (1) and (2) that at least approximately both $E(F_1)$ and $\text{VAR}(F_1)$ depend only on the invariants q, N, ρ, B_N and C_N, because both numerator and denominator in (Eq. (24)) depend on these invariants.

To simulate the upper tail probability $P(F_1 > 1.96)$ and lower tail probability $P(F_1 < -1.96)$ for F_1 with $q = 1$, 2, 3, 4, it is required to obtain pivotal function F_1. F_1 is simulated for $\rho^2 = 0.7$ and $27 = (3 \times 3 \times 3)$ combinations of the invariants ($N = 10$, 30, 50; $B_N = 0.0$, 1.0, 4.0; $C_N = 0.25$, 1.0, 4.0). Q_R is used instead of Q_A in the calculations of F_1; then, $\hat{\text{MSE}} = (1-\rho^2)\sigma^2(1+\hat{Q}_R)$. $\hat{Q}_R$ is from Eq. (22); substitute $\rho^2 = \hat{\rho}^2$, so $\hat{\rho}^2 = \hat{\beta}^T\hat{D}$. To this end, the followings are simulated as in Section 4:

(i) T_i's and X_i's are simulated using canonical form;

(ii) $\hat{\alpha}$, $\hat{\beta}$, and $\hat{\Gamma}$ are generated from the distribution theory to get the estimates $\hat{\mathbf{C}}$, $\hat{\mathbf{D}}$, and ρ^2.

Two cases are studied for T:

(a) T is generated from $N(\mu, \sigma^2)$;

(b) T is generated from exponential distribution with μ and σ^2 as location and scale parameters which are calculated from the values of B_N and C_N.

β^* is calculated by the relation:

$$\beta^* = \frac{\rho}{\sqrt{C_N(1-\rho^2)}},$$

and X's are generated from the standardized normal distribution.

$\hat{Q}_R$ comes from the linear model (Eq. (22)) with regression coefficients b_i's $(i = 0, 1, \cdots, 8)$ as are given in Table 1(b) for different values of N. The corresponding b_i's of Table 1(b) were used at first. Then, the cases $N = 30$, 50 were repeated with b_i's corresponding to $N = 10$, and slightly lower tail probabilities were usually found. So, these latter b_i's were finally chosen for $q = 2$, 3, and 4. The coefficients used for $q = 1$ are the weighted coefficients previously given under the "Combination of Estimates".

Some extreme cases are picked to see the distribution of F_1. The summary statistics are provided in Table 4(a) for 1000 values of F_1 with normal and exponential distribution of T for $q = 1$, 2, 3, 4 and combinations of the invariants with $N = 10$. It is clear that the mean is approximately zero. We have also verified the approximate normality (using normal probability plots). The upper tail probability $P(F_1 > 1.96)$ and lower tail probability $P(F_1 < -1.96)$ for $P(t)$ to be normal and exponential are given in Table 4(b), for $N = 10$, 30, 50 and $q = 1$, 2, 3, and 4. These indicate that for $N = 10$, the error probabilities are high and have increasing trend with the increasing q. For $q = 1$, the sum of lower and upper tail probabilities is around 0.085 for $P(t)$ to be normal and 0.080 for P(t) to be exponential. For $N = 30$ and 50, the sums of error probabilities are very close and are always between 0.05 and 0.06. It is also observed that the lower and upper tail probabilities are near each other for $B_N = 0.0$ and get apart for higher values of B_N. For $q = 1$, the approximated value Q_A obtained using Taylor's series, as in Eq. (21), was also used to obtain error probabilities instead of Q_R in expression Eq. (24). For $N = 10$, the point estimates of lower tail probability, $P(F_1 < -1.96) = \hat{P}_L$, and upper tail probability, $P(F_1 > 1.96) = \hat{P}_U$, range in 0.042-0.057 and 0.026-0.046, respectively for normal $p(t)$. For $N = 30$, 50 they are between 0.021-0.030 and 0.029-0.035, respectively. The sums of $\hat{P}_L + \hat{P}_U$ are nearly 0.08, 0.06, 0.055 $\geq$ 0.05 for $N = 10$, 30, 50, respectively.

For exponential $p(t)$, $\hat{P}_L$ and $\hat{P}_U$ range in 0.030-0.056 and 0.032-0.050, respectively, and the sum $\hat{P}_L + \hat{P}_U$ is between 0.079-0.086 for $N = 10$. For $N = 30$, 50, they have tendency toward near 0.018 and 0.032, respectively, and the sum $\hat{P}_L + \hat{P}_U$ is nearly 0.050 $\geq$ 0.05. It can be concluded here that Error probabilities depend on q, N, B_N, C_N and to some extent on ρ^2.

Using the procedure of canonical from, the upper and lower tail probabilities were the same for $B_N = 0$ or $\bar{t} = \mu$, but when $\bar{t} \neq \mu$, the values of the upper and lower tail probabilities exchanged. This happened because always $\mu \leq \bar{t}$; whereas here it is opposite, i.e. $\bar{t} \leq \mu$. The change of sign of T exchanges the numerical values of the lower and upper tail probabilities, i.e.:

Lower error prob. $= P(F_1 < -1.96)$,

Table 4(a). Summary statistics of 1000 values of F_1, $n=10$, different values of q, $p(t)$, and invariants.

$p(t)$	$q=1$			$q=2$			$q=3$			$q=4$		
	B_N=4 C_N=0.25	B_N=4 C_N=4	B_N=0 C_N=4	B_N=4.0 C_N=0.25	B_N=4 C_N=4	B_N=0 C_N=4	B_N=4 C_N=0.25	B_N=4 C_N=4	B_N=0 C_N=4	B_N=4 C_N=0.25	B_N=4 C_N=4	B_N=0 C_N=4
Mean												
Normal	0.070	0.133	0.049	-0.008	0.191	-0.097	0.217	0.501	0.044	1.710	0.622	-0.013
Exponential	0.006	0.085	0.008	0.053	0.284	-0.014	0.234	0.553	0.077	1.443	0.670	0.028
S.D												
Normal	1.170	1.138	1.137	1.185	1.227	1.328	1.298	1.412	1.483	0.710	1.763	1.765
Exponential	1.129	1.133	1.140	1.249	1.231	1.239	1.399	1.669	1.713	1.443	1.801	1.902
Median												
Normal	0.039	0.031	0.018	-0.057	0.059	-0.054	0.138	0.324	0.029	0.106	0.429	-0.063
Exponential	-0.014	-0.014	-0.093	0.032	0.130	-0.055	0.178	0.315	-0.046	0.162	0.463	-0.089
Minimum												
Normal	-5.323	-3.284	-5.995	-5.270	-5.822	-9.490	-4.324	-4.041	-8.282	-9.785	-7.056	-7.598
Exponential	-5.744	-6.060	-5.474	-5.136	-2.521	-3.655	-5.829	-3.920	-5.534	-10.456	-7.071	-10.231
Maximum												
Normal	4.480	5.921	4.894	5.091	6.299	5.145	6.145	6.504	6.171	9.862	10.692	7.809
Exponential	4.064	8.381	7.003	5.690	6.533	5.989	10.002	20.134	19.230	6.376	17.914	17.323

Table 4(b). Lower (L) and Upper(U), $10^3\times$ error probabilities of F_1 for different values of q, $p(t)$ and N.

C_N	B_N	$q=1$			$q=2$			$q=3$			$q=4$		
		0.0	**1.0**	**4.0**	**0.0**	**1.0**	**4.0**	**0.0**	**1.0**	**4.0**	**0.0**	**1.0**	**4.0**
(i): $p(t)$ normal													
$N=10$													
0.25	L	40	38	37	50	44	39	60	51	44	80	68	57
	U	42	47	49	46	54	57	62	70	76	76	91	103
1.00	L	39	36	32	53	40	31	63	46	34	84	61	41
	U	44	50	53	49	61	67	65	81	92	80	106	126
4.00	L	40	31	22	58	40	22	80	49	27	103	65	36
	U	46	52	56	55	71	83	78	104	124	100	141	170
$N=30$													
0.25	L	29	27	26	32	30	27	29	26	24	30	26	23
	U	29	29	32	30	32	33	29	32	31	29	32	33
1.00	L	30	27	24	34	29	24	28	25	20	31	24	19
	U	39	31	33	31	34	36	31	34	37	31	36	39
4.00	L	31	27	23	34	28	23	34	25	18	39	27	18
	U	30	34	36	33	38	42	34	42	48	38	47	55
$N=50$													
0.25	L	29	27	27	26	24	22	26	24	22	29	27	23
	U	29	29	29	27	28	29	28	28	29	22	24	24
1.00	L	29	27	25	24	23	21	27	24	20	31	26	21
	U	29	30	31	27	30	32	29	31	32	23	27	29
4.00	L	31	27	26	25	23	20	29	24	18	33	27	19
	U	29	32	34	28	33	36	32	36	39	28	33	38
(ii): $P(t)$ exponential													
$N=10$													
0.25	L	34	31	33	45	38	37	54	47	42	74	61	54
	U	44	47	47	49	52	56	60	69	76	76	87	98
1.0	L	35	28	27	45	33	27	31	39	28	76	53	39
	U	45	48	49	51	58	63	64	80	93	82	102	121
4.00	L	31	21	17	41	25	15	57	30	15	88	49	24
	U	47	50	51	56	69	78	76	97	114	97	126	152
$N=30$													
0.25	L	26	24	24	26	24	22	26	23	20	23	19	18
	U	37	36	35	38	38	38	38	37	37	32	33	34
1.00	L	25	23	22	24	23	19	25	22	17	22	17	14
	U	37	36	38	38	40	41	39	41	41	34	38	39
4.00	L	24	21	18	23	18	13	25	17	12	27	16	10
	U	36	39	42	40	43	47	43	51	54	43	52	57
$N=50$													
0.25	L	23	23	22	23	22	21	22	18	15	20	18	16
	U	37	37	38	36	37	37	36	37	36	33	34	31
1.0	L	23	21	21	21	21	19	22	18	15	19	17	14
	U	36	38	39	36	38	38	36	38	40	34	36	37
4.0	L	23	20	18	22	19	17	21	17	12	19	15	11
	U	38	39	41	38	41	42	39	43	46	39	44	47

and:

Upper error prob. $= P(F_1 > 1.96)$.

Let:

$$T' = -T, \qquad \bar{T}' = -\bar{T}, \qquad S_{T'T'} = S_{TT},$$

$$E(X|T) = \alpha + \beta T' = \alpha' + \beta' T,$$

so $\alpha' = \alpha$, $\beta' = -\beta$, $\sigma^2_{X|T'} = \sigma^2_{X|T}$, $\mu' = -\mu$, $\sigma'^2 = \sigma'^2$ and N, ρ^2, B_N, C_N are unchanged so MSE unchanged.

$$C' + D'X = \hat{T}' = -\hat{T} = C - DX,$$

$$C' = -C, \qquad D' = -D.$$

$$\text{Lower error prob}' = P(F_1' < -1.96)$$

$$= P\left(\frac{T - \left(\hat{C} + \hat{D}X\right)}{\sqrt{\hat{\text{MSE}}}} < -1.96\right)$$

$$= P\left(-\frac{T - \left(\hat{C} + \hat{D}X\right)}{\sqrt{\hat{\text{MSE}}}} > -1.96\right)$$

$$= P\left(\frac{T - \left(\hat{C} + \hat{D}X\right)}{\sqrt{\hat{\text{MSE}}}} > -1.96\right)$$

$$= P(F_1 > -1.96) = \text{Upper error prob.}$$

5.5. Example: Wheat quality data

In this section, we provide an application example using the wheat quality data analyzed by Brown [2]. The data set consists of 21 samples of response variables, the 4-vector X, and the 2-vector T of explanatory variables. X_1, X_2, X_3, and X_4 are the infrared reflectance measurements and T_1, and T_2 denote the percentages of water and protein contents, respectively. The set of the first 16 observations on X_1, X_2, X_3, X_4 and T are treated as regression experiment and the next set of 5 observations are used to test the predicted values. We have taken only one explanatory variable, namely the protein percentage.

To predict T, we confined ourselves to these subsets of response variables: (a) X_2 only; (b) X_1 and X_2; (c) X_1, X_2, and X_3; and (d) X_1, X_2, X_3, and X_4. The values of $\hat{\mathbf{C}}$ and $\hat{\mathbf{D}}$ are calculated for the above subsets by obtaining α, β and Γ from the first 16 observations. μ and σ^2 may be taken as $\mu = \bar{t}$ and $\sigma^2 = S_{TT}/15$ approximately B_N =0.0 and $C_N = 1.0$, because the mean and standard deviation of 21 values of the variable T are 11.26 and 1.45, respectively, whereas the mean and standard deviation of 16 observations are 11.39 and 1.35, respectively. The point and interval estimates for protein percentage values T_{17}, T_{18}, T_{19}, T_{20}, and T_{21} are calculated and reported in Table 4(c) along with the data. It is clear that the values to be predicted are always in the 95%

Table 4(c). Point and interval estimates of wheat quality data for subsets of response variables.

	Point estimate	Interval estimates		MSE
(i) X_2	9.4704	8.7515	10.1894	0.1345
	10.0894	9.3705	10.8083	
	9.2641	8.5452	9.9830	
	12.9780	12.2591	13.6969	
	12.7717	12.0527	13.4906	
(ii) X_1, X_2	9.1669	8.7369	9.5969	0.0481
	10.0420	9.6120	10.4720	
	9.2325	8.8025	9.6625	
	12.5773	12.1473	13.0073	
	12.8811	12.4511	13.3112	
(iii) X_1, X_2, X_3	9.1295	8.7509	9.5080	0.0373
	10.1736	9.7951	10.5522	
	9.1149	8.7364	9.4935	
	12.6602	12.2816	13.0387	
	12.7719	12.3934	13.1505	
(iv) X_1, X_2, X_3, X_4	9.2490	8.8729	9.6265	0.0368
	10.1817	9.8055	10.5579	
	9.1522	8.7760	9.5284	
	12.7134	12.3372	13.0895	
	12.7666	12.3904	13.1428	

interval for all the four subsets of response variables (cf. Table 4). The interval estimate gets shorter with the increase in q until $q = 3$ and it is almost the same for $q = 3$ and $q = 4$.

6. Conclusions and recommendations

This study has suggested the classical and inverse estimators as special cases of the proposed multivariate linear calibration approach based on the best linear predictor. The bias and mean squared error are derived for the proposed predictor. The study has revealed that the ratios Bias/σ^2 and MSE/σ^2 are functions of five invariant quantities. The probabilities for the interval estimates have shown that they have reasonable confidence coefficient; thereby, we conclude that this estimator can be safely used. The scope of the study may be extended to be carried out in an extensive investigation on the same lines by including more explanatory variables, T's, instead of one variable T.

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