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CONDITIONAL MULTIVARIATE CALIBRATION

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ABSTRACT

The problem of simple linear calibration is not new and dates back to the late 1930's. In 1982 Brown presented a number of important results for the multivariate case. In this paper we extend Brown's work to cover the situation where one is interested in calibrating for an unknown q-vector X on the basis of an observed p-vector Y given that $k \geq 1$ components of X are fixed in advance.

An outline of the theoretical development in the multivariate normal case will be given and the procedure illustrated with the application to previously published data.

1. Introduction

The task of calibrating an instrument or measuring device is something that most people have had some experience with. In its simplest form we take readings Y on some physical process X from which an empirical model of the relationship between Y and X is established. This model can then be used to 'predict' the value of X given some future observation y_0. If we assume a linear statistical model (although not necessarily linear in Y and X) we can write :

$$Y = \beta_0 + \beta_1 X + \xi \tag{1.1}$$

where β_0 and β_1 are unknown parameters and ξ is a random error component.

Using OLS we may estimate β_0 and β_1 in the usual manner to obtain a predicted Y (denoted by $\hat{Y}$) as :

$$\hat{Y} = \hat{\beta}_0 + \hat{\beta}_1 X \tag{1.2}$$

Note, however ,that whereas in regression we use equation (1.2) directly to predict a value of Y for some given X=x, the problem in a calibration setting is reversed. In this case we wish to predict X given a future observation y_0. Exactly how this is best achieved has been the subject of considerable discussion (for example see Lwin and Maritz (1980),(1982)). Berkson (1950) formally raised the issue when he asked are there two regressions in a calibration problem ? The so-called "classical" regression approach is to use the model in equation (1.1), estimate its parameters via OLS and simply rearrange the terms to provide :

$$\hat{x}_0 = \frac{y_o - \hat{\beta}_o}{\hat{\beta}_1} \tag{1.3}$$

Krutchkoff (1967) argued that since interest focuses on the determination of X and not of Y then one could perform the regression of X on Y directly. Thus the estimate obtained from this "inverse" regression is given by equation (1.4) :

$$\tilde{X}_0 = \hat{\beta}_0^* + \hat{\beta}_1^* Y_0 \tag{1.4}$$

where β_0^* and β_1^* are used to denote the regression estimates for the regression of X on Y.

The dilemma over the utility of equations (1.3) and (1.4) arises from a lack of agreement on the most suitable criterion for assessing alternative approaches. An obvious criticism of the inverse regression approach is that if Y is random and X fixed then the model :

$$X = \beta_0^* + \beta_1^* Y + \zeta \tag{1.5}$$

where ζ is a random error, makes no sense. However, if the calibration experiment is strictly data analytic and not inferential then one is not so much concerned with identifying a meaningful statistical model , and criticisms of the type just alluded to may be of no concern. Whilst it is not the intent of this paper to give a comprehensive review of the relative merits of the many approaches to statistical calibration, the interested reader may consult Fox (1989) in which these issues are discussed more fully.

2. The multivariate extension.

In this section we outline some of the theoretical development for the multivariate extension of the linear statistical calibration model. Our treatment of the multivariate case utilizes results previously given by Brown (1982).

Before proceeding with the theory, we first give an example to illustrate the type of problem encountered.

2.1 An example of multivariate calibration.

Oman and Wax (1984) discuss the problem of accurately determining the gestational age of an unborn child. Standard practice is to compare the rate of fetal development with published charts and tables. Such quantities as bone lengths (femur length, F and biparietal diameter, BPD) are usually used. However, the comparison of each measurement separately with its respective 'standard' value ignores the inter-dependencies among all three factors (age,F,and BPD). The authors demonstrated that a model which took cognizance of all three variables simultaneously resulted in an index of gestational age which was significantly more accurate than either alone. Observe, that in this example both F and BPD are dependent, although our future interest centers on determining age from measurements on F and BPD.

2.2 The theory of multivariate calibration.

We have as our assumed model :

$$Y = 1^{T}\alpha^{T} + X\beta + \xi \qquad (2.2.1)$$

where Y is $(n \times p)$; 1 is $(n \times 1)$ vector of ones ;

α is $(p \times 1)$; X is $(n \times q)$;

β is $(q \times p)$; ξ is $(n \times p)$.

Furthermore, assume $\xi \sim N_q(0,\Sigma)$. Without loss of generality , we will first center both the X and Y data by subtracting their respective means. Now using standard results, the OLS estimator of β is given as :

$$\hat{\beta} = (X^T X)^{-1} X^T Y \qquad (2.2.2)$$

It can be shown that the m.l.e. for a calibrated X_0 (corresponding to some future observation y_0) is :

$$\hat{X}_0^T = (\hat{\beta}\,\hat{\Sigma}^{-1}\,\hat{\beta}^T)^{-1}\,\hat{\beta}\,\hat{\Sigma}^{-1}\,y_0^T \qquad (2.2.3)$$

where $\hat{\Sigma} = \frac{1}{\nu}\,\hat{\xi}^T\hat{\xi}$; $\hat{\xi} = Y - \hat{Y}$

and $\nu = n-q-1$.

It can also be established that $\hat{X}_o$ is unbiased.

2.3 Conditional calibration.

The idea now is that when calibrating for X_0 it may be that some of the components of X_0 are fixed in advance and we thus wish to modify the procedure so that not only will $\hat{X}_0$ have the required fixed or known values, but also that the remaining (free) components of $\hat{X}_0$ be such that $\hat{X}_0$ as a whole has the correct covariance structure. Before addressing this problem we first present some standard results for the conditional multivariate normal distribution.

2.3.1 The conditional normal p.d.f.

Let X and Y be two random vectors such that $\begin{bmatrix} X \\ Y \end{bmatrix} \sim N(\mu, C)$ where

$$\mu = E\begin{bmatrix} X \\ Y \end{bmatrix} = \begin{bmatrix} \mu_x \\ \mu_y \end{bmatrix} \quad \text{and} \quad C = \mathrm{Cov}\begin{bmatrix} X \\ Y \end{bmatrix} = \begin{bmatrix} C_{11} & C_{12} \\ C_{12}^T & C_{22} \end{bmatrix} .$$

Let $\tilde{Y}$ be the random vector $Y|X=x$ where x is a vector of deterministic scalars.

It can be shown that :

$$E[\tilde{Y}] = C_{12}^T C_{11}(x - \mu_x) + \mu_y \qquad (2.3.1.1)$$

and

$$\mathrm{Cov}[\tilde{Y}] = C_{22} - C_{12}^T C_{11}^{-1} C_{12} \qquad (2.3.1.2)$$

We now utilize these results to calibrate conditionally in the case where the data is multivariate normal.

Let $\hat{X}_0^T$ be partitioned as :

$$\hat{X}_0^T = \begin{bmatrix} \hat{S} \\ - \\ \hat{T} \end{bmatrix}$$

where $\hat{S}$ has ν_1 components and $\hat{T}$ has ν_2 components and $\nu_1+\nu_2=q$.

Furthermore, let $E[\hat{X}_0^T] = \begin{bmatrix} \mu_s \\ \mu_t \end{bmatrix}$ and $Cov[\hat{X}_0^T] = \begin{bmatrix} C_{11} & C_{12} \\ C_{12}^T & C_{22} \end{bmatrix}$ and let $\tilde{T}$ be the vector $T|S{=}s$.

Thus, using equations (2.3.1.1) and (2.3.1.2) we have that

$$E[\tilde{T}] = C_{12}^T C_{11}^{-1}(s - \mu_s) + \mu_t \qquad (2.3.1.3)$$

and

$$Cov[\tilde{T}] = C_{22} - C_{12}^T C_{11}^{-1} C_{12} \qquad (2.3.1.4)$$

We are now in a position to identify the steps involved in calibrating conditionally.

2.4 The conditional calibration procedure.

Step 1:

Conduct the *unconditional* calibration to obtain $\hat{X}_0^T$ using equation(2.2.3), that is :

$$\hat{X}_0^T = (\hat{\beta}\,\hat{\Sigma}_y^{-1}\,\hat{\beta}^T)^{-1}\hat{\beta}\,\,\hat{\Sigma}_y^{-1}\,Y_0^T \qquad (2.4.1)$$

(where $\hat{\Sigma}_y$ denotes the estimated covariance matrix of the y's).

Partition $\hat{X}_0^T$ as : $\hat{X}_0^T = \begin{bmatrix} \hat{S} \\ \hat{T} \end{bmatrix}$.

Step 2:

For given $S{=}s$ compute :

$$\tilde{T} = C_{12}^T C_{11}(s - \hat{S}) + \hat{T} \qquad (2.4.2)$$

where $\hat{S}$ and $\hat{T}$ are obtained from the *unconditional* calibration.

Observe that our ability to calibrate conditionally is dependent upon us having knowledge of Cov$[\hat{X}_0]$ .In order that we may develop an expression for Cov$[\hat{X}_0]$ it will be necessary for us to digress momentarily to consider the regression of X on Y.

3. The regression of X on Y

As noted by Brown (1982) and others, when both X and Y are multivariate normally distributed an alternative approach to the use of equation (2.2.3) is to perform the regression of X on Y and thus obtain the calibrated vector $\hat{X}_0^*$ directly from the estimated regression model. Furthermore, after suitably transforming both $\hat{X}_0^*$ and $\hat{X}_0$, the resulting quantities are in fact equivalent up to a constant of proportionality and that the constants are the cannonical correlations between X and Y. We now develop these ideas further.

In what follows we assume that X and Y have been centered on their respective means.

In the regression of X on Y let :

$$\hat{X} = Y\hat{\beta} + \zeta \tag{3.1}$$

where the dimensions of $\hat{X}$,Y, and $\hat{\beta}$ are respectively (n x q), (n x p), and (p x q) and $\hat{\beta}$ is the usual least-squares estimate :

$$\hat{\beta} = (Y^T Y)^{-1} Y^T X \tag{3.2}$$

Thus, given a new (1 x p) vector y_0, we obtain $\hat{X}_0^*$ as :

$$\hat{X}_0^{*T} = X^T Y (Y^T Y)^{-1} y_0^T \tag{3.3}$$

After some algebraic manipulation it can be shown that :

$$\hat{X}_0^{*T} = [(X^T X)^{-1} + \hat{\beta}\, \hat{\Sigma}^{-1}\ \hat{\beta}^T]^{-1} (\hat{\beta}\, \hat{\Sigma}_y^{-1}\ \hat{\beta}^T) \hat{X}_0^T \tag{3.4}$$

where $\hat{\beta}$ is obtained from the regression of Y on X i.e.

$$\hat{\beta} = (X^T X)^{-1} X^T Y \tag{3.5}$$

and

$$\hat{\Sigma}_y = Y^T Y - \hat{\beta}^T X^T X \hat{\beta} \tag{3.6}$$

Next, let $W = (X^T X)^{\frac{1}{2}}\, \hat{\beta}\, \hat{\Sigma}_y^{-\frac{1}{2}}$

$$\Rightarrow W\, W^T = (X^T X)^{\frac{1}{2}}\, \hat{\beta}\, \hat{\Sigma}_y\, \hat{\beta}^T (X^T X)^{\frac{1}{2}} \tag{3.7}$$

Using the Binomial Inverse Theorem [Press (1972),p.23] it can also be shown that

$$(X^T X)^{-\frac{1}{2}} \hat{X}_0^{*T} = [I_q + W\, W^T]^{-1} W\, W^T (X^T X)^{-\frac{1}{2}} \hat{X}_0^T \tag{3.8}$$

Let $\Omega = [I_q + W\, W^T]^{-1}$

$\Rightarrow \Omega\, [I_q + W\, W^T] = I$

and $\Omega + \Omega(W\, W^T) = I$

hence $\Omega(W\,W^T)^{-1} + \Omega = (W\,W^T)^{-1} \Rightarrow \Omega\,[(W\,W^T)^{-1} + I_q] = (W\,W^T)^{-1}$

$$\Rightarrow \quad \Omega = (W\,W^T)^{-1}\,[(W\,W^T)^{-1} + I_q]^{-1} \qquad (3.9)$$

Since $(W\,W^T)$ and I_q comute, equation (3.9) may be written as

$$\Omega = [I_q + (W\,W^T)^{-1}](W\,W^T)^{-1} \qquad (3.10)$$

Now from equation (3.8) we have

$$(X^TX)^{-\frac{1}{2}}\hat{X}_0^{*T} = [I_q + W\,W^T]^{-1}W\,W^T(X^TX)^{-\frac{1}{2}}\hat{X}_0^T$$
$$= [I_q + (W\,W^T)^{-1}]^{-1}(W\,W^T)^{-1}W\,W^T(X^TX)^{-\frac{1}{2}}\hat{X}_0^T$$
$$= [I_q + (W\,W^T)^{-1}]^{-1}(X^TX)^{-\frac{1}{2}}\hat{X}_0^T \qquad (3.11)$$

Next let $U = (X^TX)^{-\frac{1}{2}}X^TY(Y^TY)^{-\frac{1}{2}}$

$$= \Sigma_x^{-\frac{1}{2}}\Sigma_{xy}\,\Sigma_y^{-\frac{1}{2}} \qquad (3.12)$$

Thus the positive eigenvalues of U are the cannonical correlations between X and Y.

Now, $\hat{\Sigma}_y = Y^TY - Y^TX(X^TX)^{-1}X^TY \qquad (3.13)$

Letting $V = (Y^TY)^{-\frac{1}{2}}\hat{\Sigma}_y\,(Y^TY)^{-\frac{1}{2}}$ we have

$$V^{-1} = (Y^TY)^{\frac{1}{2}}\hat{\Sigma}_y^{-1}(Y^TY)^{\frac{1}{2}} \qquad (3.14)$$

Furthermore, it is relatively easy to show that

$$V = I - U^T U \tag{3.15}$$

Next consider $(I + W W^T)^{-1} W W^T$. In the most general case where X is (n x q) and Y is (n x p), U will be a (q x p) matrix and V is a (p x p) matrix.

Now

$$(I + W W^T)^{-1} W W^T = (I + UV^{-1}U^T)^{-1} UV^{-1}U^T$$

Again, using the Binomial Inverse theorem we have

$$(I + UV^{-1}U^T)^{-1} = [I - UV^{-1}(V^{-1} + V^{-1}U^T UV^{-1})^{-1} V^{-1}U^T]$$

and hence

$$\begin{aligned}
(I + UV^{-1}U^T)^{-1} UV^{-1}U^T &= [I - UV^{-1}(V^{-1} + V^{-1}U^T UV^{-1})^{-1} V^{-1}U^T] UV^{-1}U^T \\
&= UV^{-1}U^T - UV^{-1}(V^{-1} + V^{-1}U^T UV^{-1})^{-1} V^{-1}U^T UV^{-1}U^T \\
&= UV^{-1}(V^{-1} + V^{-1}U^T UV^{-1})^{-1}(V^{-1} + V^{-1}U^T UV^{-1})U^T \\
&\quad - UV^{-1}(V^{-1} + V^{-1}U^T UV^{-1})^{-1} V^{-1}U^T UV^{-1}U^T \\
&= UV^{-1}(V^{-1} + V^{-1}U^T UV^{-1})^{-1}[(V^{-1} + V^{-1}U^T UV^{-1})U^T - V^{-1}U^T UV^{-1}U^T] \\
&= UV^{-1}(V^{-1} + V^{-1}U^T UV^{-1})^{-1} V^{-1}U^T \\
&= UV^{-1}[V^{-1}(I + U^T UV^{-1})]^{-1} V^{-1}U^T \\
&= UV^{-1}(I + U^T UV^{-1})^{-1} U^T \\
&= U(V + U^T U)^{-1} U^T
\end{aligned}$$

but by equation (3.15), $V + U^T U = I$. Thus substituting into the last expression we finally have that

$$(I + W W^T)^{-1} W W^T = (I + UV^{-1}U^T)^{-1} UV^{-1}U^T = UI^{-1}U^T = UU^T \tag{3.16}$$

Thus the eigenvalues of $(I + W W^T)^{-1} W W^T$ are the same as those of UU^T. However, as previously noted, the eigenvalues of U are the cannonical correlations between X and Y and hence the eigenvalues of UU^T are the corresponding correlations squared.

From equation (3.8) we have :

$$(X^TX)^{-\frac{1}{2}}\hat{X}_0^{*T} = [I_q + (W W^T)^{-1}]^{-1}(X^TX)^{-\frac{1}{2}}\hat{X}_0^T$$

$$\Rightarrow \quad [I_q + (W W^T)^{-1}](X^TX)^{-\frac{1}{2}}\hat{X}_0^{*T} = (X^TX)^{-\frac{1}{2}}\hat{X}_0^T \qquad (3.17)$$

Let $[I_q + (W W^T)^{-1}]$ have the spectral decomposition QDQ^T where the columns of Q are the normalized eigenvectors of $[I_q + (W W^T)^{-1}]$ and $D = \text{diag}(\lambda_1, \lambda_2, \ldots, \lambda_q)$ be a diagonal matrix of eigenvectors. Thus equation (3.16) can be written as :

$$QDQ^T(X^TX)^{-\frac{1}{2}}\hat{X}_0^{*T} = (X^TX)^{-\frac{1}{2}}\hat{X}_0^T$$

$$\Rightarrow \quad DQ^T(X^TX)^{-\frac{1}{2}}\hat{X}_0^{*T} = Q^T(X^TX)^{-\frac{1}{2}}\hat{X}_0^T \qquad (3.18)$$

If we let $\Delta = Q^T(X^TX)^{-\frac{1}{2}}$ we obtain :

$$D\ \Delta\ \hat{X}_0^{*T} = \Delta\ X_0^T \qquad (3.19)$$

In otherwords, after applying the same transformation (namely Δ) to both $\hat{X}_0^*$ and $\hat{X}_0$, we find they only differ by constants $(\lambda_1, \lambda_2, \ldots, \lambda_q)$ which, as we have shown, are the squared cannonical correlations between X and Y. We now utilize this fact to derive the covariance information for $\hat{X}_0$.

4. The covariance of $\hat{X}_0$.

For a given y_0 vector we can use the previous results to obtain $\hat{X}_0 = [\hat{x}_1, \hat{x}_2, \ldots \hat{x}_q]$. Observe that $\hat{X}_0$ is a random vector having some mean vector μ_{X_0} and covariance matrix Σ_{X_0}. In general, it will not be possible to estimate Σ_{X_0} using a sample covariance matrix since there will only be one q-vector $\hat{X}_0$. As an alternative, we use the relationship between $\hat{X}_0$ and $\hat{X}_0^*$ established in the previous section.

Returning to the regression of X on Y :

$$X = Y\beta^* + \zeta^*$$

thus

$$\hat{X}_0^* = y_0\hat{\beta}^*$$

where

$$\hat{\beta}^* = (Y^T Y)^{-1} Y^T X$$

and

$$\mathrm{Cov}[\hat{X}_0^*] = y_0 (Y^T Y)^{-1} y_0^T \, \Sigma_X \tag{4.1}$$

where Σ_X is the error-covariance matrix for the regression of X on Y. Now from equation (3.19) we have :

$$D \, \Delta \, \hat{X}_0^{*T} = \Delta \, X_0^T$$

$$\Rightarrow \quad \hat{X}_0 = \hat{X}_0^* \, \Omega \qquad \text{where} \quad \Omega = \Delta \, D \, \Delta^{-1}.$$

and thus :

$$\mathrm{Cov}[\hat{X}_0] = \hat{\Sigma}_{X_0} = \Omega \, \hat{\Sigma}_{X_0} \, \Omega^T \tag{4.2}$$

Thus, by performing the regression of **X** on **Y** we can obtain an estimate of $\mathrm{Cov}[\hat{X}_0]$. Knowledge of $\mathrm{Cov}[\hat{X}_0]$ allows us to calibrate conditionally using the procedure outlined in section 2.4.

It should be pointed out that we are not necessarily advocating the use of equation (2.2.3) over the seemingly more direct method of regressing X on Y (which as we have seen, needs to be performed anyway if estimates of $\mathrm{Cov}[\hat{X}_0]$ are to be obtained). All we are attempting to do is to provide a reasonable mechanism for calibrating conditionally *given* that one wishes to use the maximum likelihood estimate given by equation (2.2.3). We now illustrate the procedure using previously published data. A comparison of the methods will also be provided.

5. An example.

Brown (1982,p299) considered the multivariate calibration in which 21 samples of hard wheat had their percentage water and percentage protein compositions measured. In addition four infrared reflectance measurements were taken for each sample. The data are given in table I on the following page.

Preliminary data analysis

A cannonical correlation analysis of the data (n=15) gave the following (standardized) cannonical variates :

Table I : 21 samples of hard wheat, four infrared reflectance measurements plus laboratory determinations of percentage water and protein.

Observation	Y_1	Y_2	Y_3	Y_4	X_1 %water	X_2 %protein
1	361	108	96	243	9.00	10.73
2	361	107	98	245	8.94	11.05
3	362	110	94	241	9.12	9.86
4	362	105	94	246	9.06	11.41
5	362	104	70	221	10.02	11.57
6	367	113	75	221	10.06	9.42
7	366	108	82	233	9.52	10.93
8	360	104	86	236	9.32	11.61
9	362	113	85	229	9.56	8.82
10	360	103	90	242	9.10	11.81
11	351	97	88	238	9.14	12.33
12	353	95	73	227	9.70	12.93
13	352	97	77	228	9.60	12.69
14	355	96	52	206	10.62	13.13
15	357	106	69	216	10.04	10.41
16	351	93	69	222	10.00	13.57
17	363	113	88	231	9.46	9.26
18	363	110	101	248	8.86	9.82
19	366	96	85	235	9.34	12.85
20	350	96	85	235	9.34	12.85
21	355	97	63	216	10.12	12.81

Note :

(i) only the first 15 observations in table 5.1 will be used for the purpose of model fitting. The remaining data will be used for calibration.

(ii) all data is centered prior to analysis.

Reflectivity : $\xi_1 = -0.3541Y_1 + 0.5195Y_2 + 0.0397Y_3 + 0.8691Y_4$

$\xi_2 = -0.6524Y_1 + 1.7849Y_2 - 1.2006Y_3 + 0.6315Y_4$

Composition : $\tau_1 = -0.9320X_1 - 0.2513X_2$

$\tau_2 = 0.3914X_1 - 0.9791X_2$

The cannonical correlations are : r_1=0.998067 and r_2=0.992321. The correlations squared (also the eigenvalues of equation 3.16). are λ_1=0.996138 and λ_2=0.984702.

For the regression of Y on X we obtain :

$\hat{\alpha}^T$= (359.40, 104.40, 81.933, 231.467)

$$\hat{\beta} = \begin{bmatrix} 0.0027 & -0.3747 & -11.4830 & -11.2304 \\ -3.3795 & -5.4193 & -2.6268 & -0.0576 \end{bmatrix}$$

$$\hat{\Sigma}_y = \begin{bmatrix} 154.323 & 68.159 & 30.857 & 71.739 \\ 68.159 & 34.082 & 16.089 & 28.259 \\ 30.857 & 16.089 & 19.606 & 19.853 \\ 71.739 & 28.259 & 19.853 & 45.024 \end{bmatrix}$$

$$W = \begin{bmatrix} 6.0425 & -2.2184 & -9.1563 & -10.6294 \\ 2.7771 & -8.5708 & -1.4343 & -0.8891 \end{bmatrix}$$

$$Q = \begin{bmatrix} -0.318778 & 0.947829 \\ 0.947829 & 0.318778 \end{bmatrix}$$

$$D = \begin{bmatrix} 0.9847 & 0.0000 \\ 0.0000 & 0.9961 \end{bmatrix} \qquad \Delta = \begin{bmatrix} -0.101054 & 0.252790 \\ 0.240629 & 0.064895 \end{bmatrix}$$

$$\Omega^T = \begin{bmatrix} 1.005046 & -0.004193 \\ -0.002829 & 1.014407 \end{bmatrix}$$

Regression of X on Y

$$\hat{\beta}^* = \begin{bmatrix} 0.038935 & 0.157483 \\ -0.010858 & -0.322290. \\ -0.027428 & 0.088771. \\ -0.060185 & -0.080345. \end{bmatrix}$$

$$\hat{\Sigma}_x = \begin{bmatrix} 0.068538 & -0.030882 \\ -0.030882 & 0.203757 \end{bmatrix}$$

Calibration of observation #16.

For this observation we have :

y_0 = [351, 93, 69, 222]

From the regression of X on Y we obtain :

$\hat{\bar{X}}_0^*$ = [0.72123, 1.96381] (NB: these are centered values)

The calibration data yield : $\bar{X}_1 = 9.520$ and $\bar{X}_2 = 11.247$. Adding these to the respective components of $\hat{\bar{X}}_0^*$ we obtain $\hat{X}_0^*$ = [10.241, 13.211]. Applying equation (3.19) gives $\hat{\bar{X}}_0$ = [0.73991, 1.198538] from which we obtain $\hat{X}_0$ = [10.260, 13.232] (NB: these are the unconditional estimates).

Now, $$\hat{\Sigma}_{x_0^*} = \begin{bmatrix} 0.0308109 & -0.0138828 \\ -0.0138828 & 0.0915984 \end{bmatrix}$$

from which we compute :

$$\hat{\Sigma}_{x_0} = \begin{bmatrix} 0.0312553 & -0.0138411 \\ -0.0138411 & 0.0937138 \end{bmatrix}$$

Table II : Calibration of %Protein|%water.

Observation.	Unconditional equation 2.2.3	Conditional equation 2.4.2	Unconditional equation 3.3	Actual
16	13.2320	13.3498	13.2105	13.57
17	9.6031	9.5842	9.6180	9.26
18	10.3569	9.9951	10.3730	9.82
19	9.5205	9.7108	9.5316	9.46
20	12.4693	12.2924	12.4620	12.85
21	12.5197	12.8733	12.5007	12.81

Table III : Comparison of various calibration methods for the calibrated values of Table II.

	Average error	mean square error
equation 2.2.3	-0.0114	0.1255
equation 2.4.2	0.0059	0.0937
equation 3.3	-0.0124	0.1358

Finally, *given* that % water for this observation is 10.00 we obtain the conditionally calibrated value of % protein as 13.3498. This represents a 40% reduction in error when compared with the actual value of 13.57 and the value of 13.2105 obtained from the regression of X on Y.

The procedure has been applied to all six observations *not* used as part of the model fitting exercise. These results are summarized in tables II and III.

Overall, the conditional calibration of %protein using the procedure outlined in this paper has resulted in an approximate 30% reduction of mean square error when compared with the unconditional results.

6. Conclusion.

In this paper we have developed a procedure for calibrating conditionally in the multivariate normal case. As a by-product of this approach an expression for the variance of a calibrated vector $\hat{X}_0$ has been derived which hitherto has been unavailable. This variance is necessary if one is to make any type of inference about the components of $\hat{X}_0$. Finally, the procedure has been applied to sample data and shown to substantially improve the quality of calibration when at least some of the components of $\hat{X}_0$ are known in advance. Intuitively, the magnitude of this improvement will depend largely on the covariance structure of the X,Y sample data. Preliminary investigations into this aspect of the method have confirmed this belief.

REFERENCES

Berkson, J. (1950) "Are there two regressions?" *Am. Statist. Assoc.* 164-180.

Brown, J.P. (1982) "Multivariate calibration," *J.R.Statist. Soc.* (*B*) 44, (3) 87-321.

Fox, D.R. (1989) "Statistical Calibration : Theory and Applications. *Unpublished Ph.D. manuscript.* Dept. of Statistics, University of Wyoming.

Krutchkoff, R.G. (1967) "Classical and Inverse regression methods of calibration," *Technometrics*, 9, (3) 229-234.

Lwin,T. and Maritz, J.S. (1980) "A note on the problem of statistical calibration," *Appl. Statist.* 29, (2) 135-141.

__________ (1982) "An analysis of the linear calibration controversy from the perspective of compound estimation," *Technometrics*, 24, (3) 235-242.

Oman, S.D. and Wax, Y. (1984) "Estimating fetal age by ultrasound measurements : an example of multivariate calibration," *Biometrics*, 40, 947-960.

Press,S.J. (1972) *Applied Multivariate Analysis*. New York : Holt,Rinehart and Winston.

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