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BAYESIAN INVERSE REGRESSION AND DISCRIMINATION:  
AN APPLICATION OF CREDIBILITY THEORY

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Bayesian Inverse Regression and Discrimination:

An Application of Credibility Theory

R. Avenhaus and W.S. Jewell

Abstract

Many measurement problems can be formulated as follows: a certain linear relationship between two variables is to be estimated by using pairs of input and output data; the value of an unknown input variable is then estimated, given an observation of the corresponding output variable. This problem is often referred to as inverse regression or discrimination.

In this paper, we formulate a general Bayesian calibration and measurement model for this problem, in which prior information is assumed to be available on the relationship parameters, the possible values of the unknown input, and the output observation error. Simplified and easily interpreted formulae for estimating the posterior mean and variance of the input are then developed using the methods of credibility theory, a linearized Bayesian analysis developed originally for insurance estimation problems. A numerical example of the calibration of a calorimeter to measure nuclear material is given.

1. Problem Formulation

In this paper, we consider problems of the following kind: we wish to estimate the value of a certain state variable  $x$  which cannot be measured directly, or only with very large error or effort. We know, however, of another state variable  $y$ , which is statistically dependent on  $x$ , and which can be measured more easily or accurately. Thus, in principle, we can estimate the relationship between  $x$  and  $y$ , and then, with small effort, obtain  $x$  by measuring  $y$  and using the inverse relationship.

However, difficulty arises because we must use other pairs,

$(x_i, y_i)$  ( $i = 1, 2, \dots, n$ ), to estimate the relationship. Often these will have been determined for other objectives and under different experimental conditions. Thus, the true values of independent and dependent variables may not be precisely known, or the relationship itself may be slightly different than it appears from the data.

Finally, as in most physical problems, we assume that a great deal of collateral information is available which gives us some prior idea of relationship between  $x$  and  $y$ , and even of the unknown value  $x$  we are trying to estimate. In other words, we wish to make a Bayesian formulation of the problem.

Three examples of this class of problem are given below.

A. Calibration and Indirect Measurement of Nuclear Materials

Nuclear materials, e.g. plutonium, are extremely difficult to measure directly by chemical means. Therefore, one uses indirect methods, based upon the heat production or the number of neutrons emitted, in order to estimate the amount of material present. From well-known physical laws, we have a general relationship between these variables, but any measurement instrument based on these principles needs first to be calibrated. Usually, this calibration can be done with the aid of standard inputs, containing known amounts of nuclear materials. However, these inputs ( $x_i$ ) are not generally under our control, and in some cases, may have residual

imprecisions in their values.

Measurement instruments often have longer-term drifts, during which they tend to lose their original calibration. For this reason, measurement of a given production run often consists of two distinct phases: (re)calibration of the instrument, and actual indirect measurement. With a fixed amount of time available, it is of interest to determine how much time should be spent on the two phases, assuming that additional time spent on each observation reduces observational error.

B. Estimation of Family Incomes by Polling

We wish to estimate, through a public opinion poll, the distribution of family incomes in a certain city district. As the major part of the population will not be willing to divulge their incomes, or will give only a very imprecise figure, we look for a dependent variable which can be more easily determined. According to the literature (see, e.g. [10]), housing expenses are strongly related to family income, and, furthermore, it may be assumed that the population is less reluctant to divulge this figure, even though they may not be able to do so precisely. Clearly, to determine this relationship exactly, we must have some families in this district who are willing to give both their total income and their household expenses. On the other hand, we have strong prior information on this relationship from similar surveys, and may have general information

on income distribution from census and other sources.

### C. Missing Variables in Bayesian Regression

In a paper with this title [11], Press and Scott consider a simple linear regression problem in which certain of the independent variables,  $x_i$ , are assumed to be missing in a nonsystematic way from the data pairs  $(x_i, y_i)$ . Then, under special assumptions about the error and prior distributions, they show that an optimal procedure for estimating the linear parameters is to first estimate the missing  $x_i$  from an inverse regression based only on the complete data pairs.

Problems of this kind are described in textbooks on the theory of measurements, and are sometimes called *discrimination problems* (Brownlee [1], Miller [9]).

In the following, we shall formulate these problems as *Bayesian calibration and measurement problems*, in the sense of Dunsmore [3] [4], Hoadley [5], and Lindley [8]. This formulation is quite general, and although the language corresponds to that of example A, the translation to other examples is easily made.

Because of the strong distributional specification requirements of the full Bayesian analysis, we shall then use the approach of *credibility theory* to find best linear approximations to moments of interest. The resulting formulae enable us to easily display the relative value of prior information, on the one hand, and information obtained in the calibration, on the other. We will develop further the optimization problem



described in Example A above, and will consider a numerical example of calibration and indirect measurement of nuclear material.

## 2. Bayesian Calibration and Measurement Model

To develop the Bayesian model, we suppose that:

(1) *Calibration* consists of  $n$  independent pairs of input and output observations  $(\underline{x}, \underline{y}) = ((x_i, y_i), i = 1, 2, \dots, n)$ . ( $x_i$  is a relatively precise or *standard input*, and  $y_i$  is the *observed output* on a *measurement instrument*, which specifies a statistical relationship between these pairs through a *conditional measurement density*,  $p(y_i | x_i, \theta)$ ; the measurement density depends upon a fixed but unknown *measurement parameter*  $\theta$ , for which we have a prior density,  $p(\theta)$ );\*

(2) *Measurement* consists of using the same instrument on a sample of *unknown input*,  $\tilde{x} = x$ , to obtain an output  $\tilde{y} = y$ , say; the problem is then to *infer* the value of  $x$ . Since this cannot be accomplished, we must, in general, settle for an estimate,  $\hat{x}$ , which, in the remainder of the paper, we will assume to be  $\mathcal{E}\{\tilde{x} | y; \underline{x}, \underline{y}\}$ . Other Bayes estimators may be important in other physical situations.

Following [8], we see that we must compute the posterior conditional density,

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\* We use the convention that the arguments of any  $p(\cdot)$  indicate the particular density in question, which may be with respect to Lebesgue or discrete measure. Where necessary, we indicate a random variable with a tilde; i.e.,  $\tilde{x}$  is the random variable corresponding to  $x$ , etc..

$$\begin{aligned}
 p(x|y;\underline{x},\underline{y}) &= \frac{p(x,y;\underline{y}|\underline{x})}{p(y;\underline{y}|\underline{x})} \\
 &= \frac{\int p(y,\underline{y}|\underline{x},\underline{x},\theta) p(\theta|\underline{x},\underline{x}) p(x|\underline{x},\theta) d\theta}{\int p(x',y,\underline{y}|\underline{x}) dx'} \quad (2.1)
 \end{aligned}$$

from which the mean,  $\mathcal{E}\{\tilde{x}|y;\underline{x},\underline{y}\}$ , will be our estimate of the unknown input, and the variance,  $\mathcal{V}\{\tilde{x}|y;\underline{x},\underline{y}\}$ , will be the norm for our optimization problem, since we wish to make the estimate as precise as possible in the least-squares sense.

To proceed further, we must make additional statistical assumptions appropriate to our problem:

(1) Given  $\theta$ , we assume that the measurements are independent:

$$p(y,\underline{y}|\underline{x},\underline{x},\theta) = p(y|\underline{x},\theta) \prod_{i=1}^n p(y_i|x_i,\theta) \quad ;$$

(2) We assume that the prior on the measurement parameter is unrelated to any of the inputs:

$$p(\theta|\underline{x},\underline{x}) = p(\theta) \quad ;$$

(3) Any unknown input in the measurement process,  $x$ , is selected independently from the standard inputs,  $\underline{x} = [x_1, x_2, \dots, x_n]'$ , and the parameter  $\theta$ :

$$p(x|\underline{x},\theta) = p(x) \quad .$$

The third assumption is the strongest, and may not hold, for example, when the calibration inputs and the test input come from the same production process. However, in our case, we assume that the calibration inputs are independent standards.

By elementary manipulations, we obtain:

$$p(x|y; \underline{x}, \underline{y}) = \frac{p(x) \int p(y|x, \theta) p(\theta | \underline{x}, \underline{y}) d\theta}{\int p(y|\theta') p(\theta' | \underline{x}, \underline{y}) d\theta'} , \quad (2.2)$$

where

$$p(\theta | \underline{x}, \underline{y}) = \frac{\prod_{i=1}^n p(y_i | x_i, \theta) p(\theta)}{\int \prod_{j=1}^n p(y_j | x_j, \theta') p(\theta') d\theta'} . \quad (2.3)$$

Notice that the denominators of (2.2) and (2.3) are just normalizations, which may be computed directly at any time.

In the above form, it is clear that the problem breaks apart mathematically into two problems:

- (1) The updating of  $p(\theta)$  to  $p(\theta | \underline{x}, \underline{y})$  (calibration);
- (2) The calculation of moments of interest for  $p(x|y, \theta)$ , averaged over the appropriate density of  $\theta$  measurement.

We tackle these problems in reverse order, since the only effect of calibration is to modify the prior information about the regression parameters and to improve the precision of this estimate.

### 3. Estimation of Input Using Credibility Theory

To find the moments of  $p(x|y, \theta) = p(y|x, \theta) p(x) / \int p(y|x', \theta) p(x') dx'$ , we must in the general case make distributional assumptions about  $p(x)$  and  $p(y|x, \theta)$ . However, since only the moments of this density are of interest, it is desirable to

have a simpler, distribution-free approach, such as that provided by *credibility theory* [6] [7]. In this approach, Bayesian means conditional on given data  $w$ , say, are approximated by linear combinations of certain functions of  $w$ , chosen from physical considerations; the coefficients are then chosen to minimize the mean-square approximation error prior to  $w$ . In certain cases, these approximation formulae are also the exact Bayesian conditional means [6].

The usual assumption about a measurement process is that, given the measurement parameter  $\theta$ , there is a linear relation between the true input and the true output, but that the observed process may contain an additional uncorrelated measurement observation error, with zero mean and known variance.

This may be conveniently expressed as:

$$\mathcal{E}\{\tilde{y}|x, \theta\} = \beta_1(\theta) + \beta_2(\theta) x \quad ; \quad (3.1)$$

$$\mathcal{V}\{\tilde{y}|x, \theta\} = \sigma_M^2 \quad . \quad (3.2)$$

(In other applications, the observation error may also depend upon  $\theta$  or the level of  $x$ .) We call  $\beta_1(\theta)$ ,  $\beta_2(\theta)$  the *instrument parameters*.

We know that, for general  $p(x,y|\theta)$ , the fact that the regression of  $y$  upon  $x$  (3.1) is linear does not necessarily mean that the regression of  $x$  upon  $y$  is linear in  $y$ . However, it is true in the case of the normal and some other bivariate distributions, and seems a desirable characteristic of any measurement process. Therefore, we shall assume that our prior estimate of the true input  $x$ , given an observed output  $y$ , may

be approximated by the linear function:

$$\mathcal{E}\{\tilde{x}|y\} = \mathcal{E}\mathcal{E}\{\tilde{x}|y, \tilde{\theta}\} \approx f(y) = z_0 + z_1 y \quad , \quad (3.3)$$

where the "credibility coefficients"  $z_0, z_1$  are chosen so as to minimize the approximation error variance:

$$H_A = \mathcal{E}[\mathcal{E}\{\tilde{x}|\tilde{y}\} - f(\tilde{y})]^2 \quad . \quad (3.4)$$

For the remainder of this section, we shall treat the averaging over  $\theta$  as if it were with respect to the prior  $p(\theta)$ , realizing that in the next section we shall change to  $p(\theta|\underline{x}, \underline{y})$ , to add the information provided by the calibration.

One can easily show [6,7] [2, Appendix 3] that the optimal credibility coefficients are given by:

$$z_0 = \mathcal{E}\{\tilde{x}\} - z_1 \mathcal{E}\{\tilde{y}\} \quad ; \quad (3.5)$$

$$z_1 = \frac{\mathcal{C}\{\tilde{y}; \tilde{x}\}}{\mathcal{V}\{\tilde{y}\}} \quad ; \quad (3.6)$$

so that the optimal estimator is unbiased.

$\mathcal{E}\{\tilde{x}\}$  represents our prior estimate of the value of the input to be measured; the remaining moments must be calculated from our measurement assumptions (3.1) (3.2). From (3.1):

$$\mathcal{E}\{\tilde{y}\} = b_1 + b_2 \mathcal{E}\{\tilde{x}\} \quad , \quad (3.7)$$

where

$$b_i = \mathcal{E}\{\beta_i(\tilde{\theta})\} \quad (i = 1, 2) \quad (3.8)$$

are the mean prior estimates of the instrument parameters.

By unconditioning (3.2) on  $x$  and  $\theta$ , we find:

$$\mathcal{V}\{\tilde{y}\} = \sigma_M^2 + \mathcal{V}\{\tilde{x}\} (b_2^2 + \Delta_{22}) + \Delta_{11} + 2\Delta_{12}\mathcal{E}\{\tilde{x}\} + \Delta_{22}[\mathcal{E}\{\tilde{x}\}]^2 ,$$

where

$$\Delta_{ij} = \mathcal{C}\{\beta_i(\tilde{\theta}) ; \beta_j(\tilde{\theta})\} \quad (i, j = 1, 2) \quad (3.10)$$

are the prior estimates of the (co)variances in the instrument parameters. We see that the total prior-to-measurement variance in the observation is composed of three groups of terms:

- (1) The observation error variance;
- (2) The prior variation in input;
- (3) (Co)variances in instrument parameters.

An increase in any one of these will reduce the weight,  $z_1$ , attached to the observed output,  $y$ , in (3.3).

There is only one prior source of covariance between input and output:

$$\mathcal{C}\{\tilde{y}; \tilde{x}\} = b_2 \mathcal{V}\{\tilde{x}\} , \quad (3.11)$$

which means that, as the uncertainty in the input increases, one must attach more importance to the observed output in (3.3).

For convenience, we reproduce the final formula for the estimate of the true input:

$$f(y) = \mathcal{E}\{\tilde{x}\} + z_1 (y - \mathcal{E}\{\tilde{y}\}) = (1 - b_2 z_1) \mathcal{E}\{\tilde{x}\} + z_1 (y - b_1) ;$$

$$z_1 = \frac{b_2 \mathcal{V}\{\tilde{x}\}}{\sigma_M^2 + \mathcal{V}\{\tilde{x}\} (b_2^2 + \Delta_{22}) + \Delta_{11} + 2\Delta_{12}\mathcal{E}\{\tilde{x}\} + \Delta_{22}[\mathcal{E}\{\tilde{x}\}]^2} . \quad (3.13)$$

Thus, in the credibility approach, only seven prior moments must

be specified: the mean and variance of the potential input, and the two means and three (co)variances of the instrument coefficients.

It is of interest to examine several limiting cases of the estimator (3.12) (3.13) in more detail. First, as already mentioned, if either the observation error variance  $\sigma_M^2$  or any of the instrument variances is very large (sometimes called a "diffuse" calibration prior), then, since  $z_1$  vanishes, the best estimate of  $\tilde{x}$  is its prior mean,  $\mathcal{E}\{\tilde{x}\}$ ; the measurement process gives little additional information. Similarly, the vanishing of  $\mathcal{V}\{\tilde{x}\}$  makes  $\mathcal{E}\{\tilde{x}\}$  very reliable.

On the other hand, suppose that we have a "diffuse" prior on the level of input, that is, although  $\mathcal{E}\{\tilde{x}\}$  is given,  $\mathcal{V}\{\tilde{x}\} \rightarrow \infty$ . In this case the forecast can be rewritten:

$$f(y) = \left[ 1 + (\Delta_{22}/b_2^2) \right]^{-1} \left[ (\Delta_{22}/b_2^2) \mathcal{E}\{\tilde{x}\} - (b_1/b_2) - (y/b_2) \right] \quad . \quad (3.14)$$

If  $\Delta_{22}/b_2^2$  is small compared with unity, we obtain exactly the deterministic result corresponding to (3.11),  $y = b_1 + b_2 x$ .

In the optimization model of Section 6, we shall need the mean-square value of the error between the true value  $x$  and the predictor  $f(y)$ , that is, the *variance of forecast error*:

$$H = \mathcal{E}\{(\tilde{x} - f(\tilde{y}))^2\} \quad . \quad (3.15)$$

But, by elementary manipulations,

$$H = H_O + H_A \quad , \quad (3.16)$$

where  $H_0$  is the irreducible forecast variance using the Bayesian conditional mean:

$$H_0 = \mathcal{E}\mathcal{E}\{(\tilde{x} - \mathcal{E}\{\tilde{x}|\tilde{y}\})^2|\tilde{y}\} = \mathcal{E}\mathcal{V}\{\tilde{x}|\tilde{y}\} \quad , \quad (3.17)$$

and  $H_A$  is given by (3.4).

With the optimal choice of credibility coefficients, we obtain:

$$H = \mathcal{V}\{\tilde{x}\} - z_1 \mathcal{C}\{\tilde{y};\tilde{x}\} = \mathcal{V}\{\tilde{x}\}(1 - z_1 b_2) \quad . \quad (3.18)$$

$H$  in (3.15) and (3.18) is the variance of forecast error for one inverse measurement. If  $r$  such measurements are performed, with independent, identically distributed inputs, then one can easily show that the variance of the total error will be:

$$\begin{aligned} H^{(r)} &= r\mathcal{V}\{\tilde{x}\}(1 - z_1 b_2) \\ &\quad + (r^2 - r) z_1^2 (\Delta_{11} + 2\Delta_{12}\mathcal{E}\{\tilde{x}\} + \Delta_{22}[\mathcal{E}\{\tilde{x}\}]^2) \quad . \end{aligned} \quad (3.19)$$

We see that, in addition to the expected first term which is  $r$  times (3.18), there is a component which is proportional to  $r^2$ . This represents a possible persistence of error due to instrument parameter covariances, which may cause the individual forecast errors to be positively correlated.



#### 4. Updating of Instrument Parameters Using Credibility Theory

We turn now to the problem of incorporating the results of the calibration experiments into our prior-to-measurement density on  $\theta$ . Remember that the number,  $n$ , of such experiments, and the previously calibrated levels of the inputs,  $x_i$  ( $i=1,2,\dots,n$ ), are assumed to be fixed by external considerations. See also Section 6 below.

Assuming that (3.1) and (3.2) apply also to calibration (i.e. the same instrument is used), we may write:

$$\mathcal{E}\{\tilde{y}|\underline{x},\theta\} = \underline{x} \underline{\beta}(\theta) \quad , \quad (4.1)$$

$$\mathcal{C}\{\tilde{\underline{y}};\tilde{\underline{y}}|\underline{x},\theta\} = \sigma_C^2 \underline{I}_n \quad (*) \quad , \quad (4.2)$$

where

$$\tilde{\underline{y}} = [\tilde{y}_1, \tilde{y}_2, \dots, \tilde{y}_n]' \quad , \quad \underline{x} = [x_1, x_2, \dots, x_n]' \quad ,$$

$$\underline{\beta}(\theta) = [\beta_1(\theta), \beta_2(\theta)]' \quad , \quad \underline{x} = [\underline{1}_n, \underline{x}] \quad ,$$

$\underline{1}_n$  is a vector of  $n$  ones,  $\underline{I}_n$  is the unit matrix of order  $n$ , and  $\sigma_C^2$  is the observation variance for each output  $y_i$  ( $i=1,2,\dots,n$ ). We thus have a formulation as a Bayesian regression problem, in which we want to estimate various moments of  $p(\underline{\beta}(\theta)|\underline{x},\underline{y})$ . In particular, from (3.8) (3.10) (3.13) (3.18), we see that the first and second moments:

$$\mathcal{E}\{\underline{\beta}(\tilde{\theta})|\underline{x},\underline{y}\} \quad ; \quad \mathcal{C}\{\underline{\beta}(\tilde{\theta});\underline{\beta}(\tilde{\theta})|\underline{x},\underline{y}\}$$

will be needed.

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(\*) Vector covariance is defined as

$$\mathcal{C}\{\tilde{\underline{w}};\tilde{\underline{z}}\} = \mathcal{E}\{\tilde{\underline{w}} \tilde{\underline{z}}'\} - \mathcal{E}\{\tilde{\underline{w}}\} [\mathcal{E}\{\tilde{\underline{z}}\}]'$$

for any two random vectors  $\tilde{\underline{w}}$  and  $\tilde{\underline{z}}$ .

Rather than make distributional assumptions, such as those followed in [13], we shall again make a credibility approximation, this time to  $\mathcal{E}\{\tilde{\beta}(\theta) \mid \underline{x}, \underline{y}\}$ . The appropriate theory has been developed in [7], and we shall give only the necessary results here.

First, we approximate the desired mean instrument parameter vector by a linear function of the data vector  $\underline{y}$ :

$$\mathcal{E}\{\tilde{\beta}(\theta) \mid \underline{x}, \underline{y}\} \approx \underline{g}(\underline{y}) = \underline{z}_0 + Z\underline{y} \quad , \quad (4.3)$$

where  $\underline{g}$ ,  $\underline{z}_0$  are two-vectors,  $Z$  is a  $2 \cdot n$  matrix, and the credibility coefficients are chosen so as to minimize the mean-square approximation of both components to those of the Bayesian conditional mean vector. After some algebra it is shown in [7] that the optimal credibility forecast can be written as:

$$\underline{g}(\underline{y}) = (\mathbb{I}_2 - \underline{z})\underline{b} + \underline{z} \hat{\underline{\beta}}(\underline{y}) \quad , \quad (4.4)$$

where  $\underline{b} = [b_1, b_2]'$  is the vector of prior-to-calibration means,  $\underline{z}$  is a new  $2 \cdot 2$  *credibility matrix*:

$$\underline{z} = [\Delta(X'E^{-1}X)] [\mathbb{I}_2 + \Delta(X'E^{-1}X)]^{-1} \quad (4.5)$$

(the terms in square brackets commute), and  $\hat{\underline{\beta}}(\underline{y})$  is the classical *regression estimator* of  $\tilde{\beta}$  :

$$\hat{\underline{\beta}}(\underline{y}) = (X'E^{-1}X)^{-1} X'E^{-1}\underline{y} \quad . \quad (4.6)$$

$\Delta$  is the  $2 \cdot 2$  matrix of prior-to calibration covariances defined in (3.10), and

$$E = \mathcal{E}\{\tilde{Y}; \tilde{Y} | \underline{x}, \tilde{\theta}\} = \sigma_C^2 I_n . \quad (4.7)$$

Thus, in our model, the "regression errors" are "homoscedastic", and we get the further simplifications:

$$\underline{z} = [\Delta X' X] [\sigma_C^2 I_2 + \Delta X' X]^{-1} , \quad (4.8)$$

and

$$\hat{\beta}(\underline{y}) = (X' X)^{-1} X' \underline{y} , \quad (4.9)$$

where

$$XX' = nM = n \begin{bmatrix} 1 & \sum_{i=1}^n x_i/n \\ \sum_{i=1}^n x_i/n & \sum_{i=1}^n x_i^2/n \end{bmatrix} = n \begin{bmatrix} 1 & m_1 \\ m_1 & m_2 \end{bmatrix} , \quad (4.10)$$

i.e.  $n$  times a matrix of deterministic moments  $m_1, m_2$  describing the predetermined calibration inputs. One may easily verify that:

$$M^{-1} = \frac{1}{(m_2 - m_1^2)} \begin{bmatrix} m_2 & -m_1 \\ -m_1 & 1 \end{bmatrix} .$$

The results (4.4) (4.8) (4.9) are intuitively very satisfying, for they show that our estimate of the instrument coefficients prior to calibration should be taken as a linear mixture of our prior hypothesis,  $\underline{b}$ , and of the well-known classical estimator,  $\hat{\beta}(\underline{y})$ . The credibility attached to the latter depends upon the so-called *design matrix*,  $X$ , the observation error variance,  $\sigma_C^2$ , and the instrument covariances,  $\Delta$ . (See Jewell [7]).

Several limiting cases are of interest. First, as our observation error variance gets very large,  $\underline{z}$  vanishes, and no credibility is attached to the calibration experiment -- it is better to stick with the prior estimates.

Conversely, if all the prior instrument covariances,  $\Delta_{ij}$ , get very large, then  $\underline{z} \rightarrow I_2$ , and "full credibility" is attached to the calibration data; the same result occurs as  $\sigma_C^2 \rightarrow 0$ . Note also that full credibility occurs as the length of the calibration run,  $n$ , increases, as long as the successive inputs are chosen in such a way as to keep  $m_1$  and  $m_2$  about the same; in other words, the more calibration, the more weight is attached to the results.

The above model may be easily generalized to the case where the standard inputs themselves are subject to errors. In this case, we suppose that the selection of a "target input"  $i$  specifies  $\mathcal{E}\{\tilde{x}_i\}$ , rather than  $x_i$ ; the actual input differs from the mean by a known variance,  $\mathcal{V}\{\tilde{x}_i\}$ . The reader may easily verify that the above formulae again apply, with  $X = [\underline{1}_n, \mathcal{E}\{\tilde{x}\}]$  and with (4.7) replaced by a new diagonal matrix, with terms:

$$E_{ii} = \sigma_C^2 + (b_2^2 + \Delta_{22}) \mathcal{V}\{\tilde{x}_i\} \quad (i=1,2,\dots,n) \quad , \quad (4.11)$$

In the general case, the formulae (4.5) (4.6) must now be used; however, if the precision of the standards is the same, the regression is again homoscedastic, and (4.8) (4.9) may be used, but with  $\sigma_C^2$  replaced by (4.11).

As far as the mean-square error in fitting  $\underline{\beta}(\tilde{\theta})$  by (4.4) is concerned, we can also show that the prior covariance matrix,

with optimal choice of credibility coefficients, is:

$$\begin{aligned}\phi(X) &= \mathcal{E}\{(\underline{\beta}(\tilde{\theta}) - \underline{g}(\tilde{y}))(\underline{\beta}(\tilde{\theta}) - \underline{g}(\tilde{y}))' | X\} \\ &= (I_2 - \underline{z})\Delta = \underline{z}(X'E^{-1}X)^{-1} .\end{aligned}\tag{4.12}$$

If this fit is good, then  $\phi_{ij}$  will be a good approximation to  $\mathcal{E}\{\beta_i(\tilde{\theta}) ; \beta_j(\tilde{\theta})\}$  after the calibration, at least as we perceive it to be before we actually obtain the outputs  $\underline{y}$ . In other words,  $\phi(X)$  is our *preposterior estimate* of the covariance between instrument parameters.

It should be remembered that only the diagonal terms of (4.12) were individually optimized in the choice of credibility coefficients; one can easily show that the diagonal elements of  $\phi(X)$  are less than those of  $\Delta$ .

## 5. Integration of the Calibration and Measurement Stages

We may now complete our arguments about the relationship between Sections 3 and 4, in light of the knowledge available at each stage of the physical problem.

First, with only a prior hypothesis about our instrument available, and no calibration contemplated, our best estimate of  $\underline{\beta}(\tilde{\theta})$  is  $\underline{b}$ , with covariance  $\Delta$ . If an inverse measurement were to be performed at this point, (3.12) (3.13) is the formula we would use to estimate the true input, and  $H$  in (3.18) is the estimate now of the variance in this estimate.

Now, suppose we contemplate performing a calibration experiment  $(X,n)$ , with a fixed number of standards and fixed input design, but the results of the calibration are not yet available.

We still have no basis for revising  $\mathcal{E}\{\underline{\beta}(\tilde{\theta})\}$ , since the formula (4.4) is, prior-to-calibration, unbiased. However, the knowledge that there will be a calibration will reduce our instrument covariance terms from  $\Delta$  to  $\phi(X)$ . Therefore, prior to calibration, our estimate of the forecast error variance after measurement changes from (3.18) to:

$$H(X) = \mathcal{V}\{\tilde{x}\} - \frac{b_2^2 [\mathcal{V}\{\tilde{x}\}]^2}{\sigma_M^2 + \mathcal{V}\{\tilde{x}\} (b_2^2 + \phi_{22}) + \phi_{11} + 2\phi_{12}\mathcal{E}\{\tilde{x}\} + \phi_{22} [\mathcal{E}\{\tilde{x}\}]^2} \quad (5.1)$$

(This is the point at which optimization of the next section will be carried out). Similar modification applies to (3.19).

We now perform the calibration experiment, obtaining  $\underline{y}$  and the revised estimates,  $\underline{g}(\underline{y})$ , of  $\mathcal{E}\{\underline{\beta}(\tilde{\theta}) | \underline{y}, X\}$  from (4.4). These revised estimates of the instrument coefficients are then used in (3.12) and (3.13), which become:

$$f(\underline{y} | \underline{y}, X) = [1 - g_2(\underline{y}) z_1(\underline{y}, X)] \mathcal{E}\{\tilde{x}\} + z_1(\underline{y}, X) [\underline{y} - g_1(\underline{y})] \quad ; \quad (5.2)$$

$$z_1(\underline{y}, X) = \frac{g_2(\underline{y}) \mathcal{V}\{\tilde{x}\}}{\sigma_M^2 + \mathcal{V}\{\tilde{x}\} \{ [g_2(\underline{y})]^2 + \phi_{22} \} + \phi_{11} + 2\phi_{12}\mathcal{E}\{\tilde{x}\} + \phi_{22} [\mathcal{E}\{\tilde{x}\}]^2} \quad (5.3)$$

This is the final estimator for any unknown input, after the calibration has been performed.

We admit that it should, in principle, be possible to revise our estimate of the covariance of the instrument coefficients,  $\phi$ , after the actual calibration outputs,  $\underline{y}$ , are

obtained; however, these terms are probably already small for any reasonable calibration run, and to construct an additional credibility approximation for the posterior-to-calibration variance would require additional moments and complex formulae. Similarly, it should be possible in principle to revise our estimate of  $H(X)$  after the measurement  $y$  is made, but this leads to the same additional complexity. If one wishes, posterior to the calibration, one can replace  $b_2$  in (5.1) by  $g_2(\underline{y})$ .

We mention again some of the limiting cases of (5.2) (5.3), assuming that the revised instrument covariances are small. First, if the observation error variance  $\sigma_M^2$  is very large, or the variance in input is small, then the credibility in (5.3) will be very small, and the best estimate of the input is the prior mean. Conversely, a diffuse input,  $\mathcal{V}\{\bar{x}\} \rightarrow \infty$ , will lead to  $z_1(\underline{y}, X) \approx (g_2(\underline{y}))^{-1}$ , and a forecast:

$$f(\underline{y}|\underline{y}, X) \approx [\underline{y} - g_1(\underline{y})]/g_2(\underline{y}) \quad . \quad (5.4)$$

## 6. Optimization

For the optimization, we assume that there is a total of  $T$  hours to be split among  $n$  calibration measurements, say a total of  $T_C$  hours, and the remainder,  $T_M = T - T_C$  hours, to be spent upon  $r$  inverse inference measurements. We assume that one hour spent on a single measurement or calibration gives an observation error variance of  $\sigma^2$ ; therefore the individual observation variances used previously are then:

$$\sigma_C^2 = \frac{n\sigma^2}{T_C} \quad ; \quad \sigma_M^2 = \frac{r\sigma^2}{T_M} \quad . \quad (6.1)$$

To minimize the prior-to-calibration estimation of the forecast variance of a typical measurement, we must minimize the denominator of the second term of  $H(X)$  in (5.1):

$$D(T_C, T_M) = \frac{r\sigma^2}{T_M} + \mathcal{V}\{\tilde{x}\}(b_2^2 + \phi_{22}) + \phi_{11} + 2\phi_{22}\mathcal{E}\{\tilde{x}\} + \phi_{22}[\mathcal{E}\{\tilde{x}\}]^2 \quad (6.2)$$

where  $\phi$  is given by (4.12), with  $\sigma_C^2$  replaced by  $n\sigma^2/T_C$  in (4.8), subject to  $T_C + T_M = T$ . In general, this optimization must be carried out numerically. However, if  $n\sigma^2/T_C$  is much smaller than the diagonal terms of  $\Delta M$ , then the calibration will have practically full credibility, and

$$\phi = (I_2 - \underline{z})\Delta \approx \left[ I_2 - (I_2 - \frac{n\sigma^2}{T_C}(X'X)^{-1}) \right] = \frac{\sigma^2}{T_C} M^{-1} \quad (6.3)$$

This shows the expected result, namely, that a good calibration run gives vanishing  $\phi$  as  $T_C$  increases. The effect of the number of runs,  $n$ , is essentially cancelled out, as long as  $M$  is stable over different designs.

With this approximation, (6.2) can be written:

$$D(T_C, T_M) = \frac{r\sigma^2}{T_M} + \frac{\mu\sigma^2}{T_C} + \mathcal{V}\{\tilde{x}\} b_2^2 \quad (6.4)$$

where

$$\mu = \frac{m_2 - 2m_1\mathcal{E}\{\tilde{x}\} + \mathcal{E}\{\tilde{x}^2\}}{m_2 - m_1^2} \quad (6.5)$$

In this form, the optimization is obvious--the total time  $T$  should be split:

$$T_C^* / T_M^* = \sqrt{\mu/r} \quad (6.6)$$



giving a minimal value for D of:

$$D^* = \frac{\sigma^2}{T} (1 + \sqrt{\mu/r})^2 + \mathcal{V}\{\tilde{x}\} b_2^2 \quad (6.7)$$

An increase in the number of production runs,  $r$ , decreases the time used for calibration in an interesting way (6.6).

It is also interesting to note, in this approximation, that the ratio of effort depends, in addition to  $r$ , only on the first and second moments of the calibration design inputs, and on the measurement input. If the design  $X$  is considered to be variable, we see that we can further minimize (6.4) by decreasing  $\mu$ , i.e. we choose inputs  $\tilde{x}$  so that:

$$m_1 \approx \mathcal{E}\{\tilde{x}\} \quad ; \quad (m_2 - m_1^2) \text{ is as large as possible; } \quad (6.8)$$

which is very intuitive from a physical point of view.

This design choice would make  $\mu$  close to unity, and then  $T_C^*/T_M^* = r^{-1/2}$ . Of course, there may be many other physical reasons why the calibration input must be chosen in a different manner.

Even if the approximation (6.3) does not hold, (6.6) is suggested as an initial trial solution.

## 7. Numerical Example: Calorimetric Measurement of Nuclear Material

In order to illustrate the models developed in previous sections we use three kinds of information:

- (1) a-priori information on the relationship between dependent and independent variable;
- (2) results of calibration;
- (3) results of measurement of the dependent variable.

The following realistic example will illustrate circumstances under which certain information is more important, and the improvement is achieved by using credibility procedures.

Let us consider the quantitative measurement of plutonium with the help of a *calorimeter*. The problem is to measure a voltage induced by the heat produced by the plutonium. For this purpose, one has to know the isotopic composition of the plutonium to be measured as well as the specific heat production of the different isotopes. Typical data are given in Table 1.

Let the amount of plutonium of one batch to be measured, and let  $w$  be the specific heat production of the plutonium under consideration. Then the heat  $x$  produced by the amount  $P$  of plutonium is given by

$$x = w \cdot P \quad . \quad (7.1)$$

The voltage  $E_M$  induced in the measurement chamber of the calorimeter is proportional to this heat:

$$E_M = a \cdot x = a \cdot (wP) \quad . \quad (7.2)$$

In a second, identical chamber, a reference heat  $x_0$  is generated which induces a voltage  $E_0$ . Because of the assumed symmetry of the chambers, we have

$$E_0 = a \cdot x_0 \quad . \quad (7.3)$$

The value of  $x_0$  is kept constant throughout the operation of the instrument. The quantity actually measured is the differential voltage  $y$ ,

$$y = E_0 - E_M = a \cdot x_0 - a \cdot (wP) \quad ; \quad (7.4)$$

or, in other words,

$$y = \beta_1 + \beta_2 \cdot (wP) \quad , \quad (7.5a)$$

where

$$\beta_1 = a \cdot x_0 \quad , \quad \beta_2 = -a \quad , \quad a > 0 \quad . \quad (7.5b)$$

The value of  $x_0$  may be assumed to be known precisely. In addition, we assume there exists experience from past measurements, expressed as expectation and variance of  $\tilde{a}$ , now considered as a random variable. This means we know

$$b_1 = \mathcal{E}\{a\}x_0 \quad ; \quad b_2 = -\mathcal{E}\{a\} \quad ; \quad (7.6a)$$

$$\Delta = \begin{pmatrix} \mathcal{V}\{\tilde{\beta}_1\} & \mathcal{C}\{\tilde{\beta}_1:\tilde{\beta}_2\} \\ \mathcal{C}\{\tilde{\beta}_1:\tilde{\beta}_2\} & \mathcal{V}\{\tilde{\beta}_2\} \end{pmatrix} = \mathcal{V}\{\tilde{a}\} \begin{pmatrix} x_0^2 & -x_0 \\ -x_0 & 1 \end{pmatrix} \quad . \quad (7.6b)$$

The calibration is performed by putting an electric heater into

the measurement chamber and generating different values  $x_{i2}$  of heat which generates corresponding differential voltages  $y_i$ :

$$\Delta E_i = \beta_1 + \beta_2 \cdot x_{i2} \quad , \quad i = 1, \dots, n \quad . \quad (7.7)$$

Typical data for such a measurement problem are given in Table 2. According to this table, we have

$$b_1 = 600 \text{ [mV]} \quad , \quad (7.8a)$$

$$b_2 = -240 \text{ [mV/Watt]} \quad ; \quad (7.8b)$$

and furthermore,

$$\mathcal{V}\{\tilde{a}\} = (.02)^2 \cdot [\mathcal{E}\{\tilde{a}\}]^2 = 23.04 \cdot [\text{mV}^2/\text{Watt}^2] . \quad (7.8c)$$

In addition, we have

$$\mathcal{E}\{\tilde{x}\} = 2.668, \quad \mathcal{V}\{\tilde{x}\} = .07118, \quad \mathcal{E}\{\tilde{x}^2\} = 7.189 \quad . \quad (7.9)$$

Therefore, we get for  $\Delta_{ij}$ , as defined by (3.10) and given by (7.6),

$$\Delta = 23.04 \begin{pmatrix} 6.25 & -2.5 \\ -2.5 & 1 \end{pmatrix} = \begin{pmatrix} 144 & -57.6 \\ -57.6 & 23.04 \end{pmatrix} . \quad (7.10)$$

Let us consider first the case that we do not perform any calibration, but use only the prior information given by equations (7.8) and (7.9). According to (3.12) the estimate of the heat production is given by

$$\begin{aligned}
 f(y) &= \mathcal{E}\{\tilde{x}\} + z_1(y - \mathcal{E}\{\tilde{y}\}) \\
 &= 2.48 \cdot 10^{-3} + \frac{y - 600}{b_2 + 0.2234} \quad , \quad (7.11)
 \end{aligned}$$

which is to a good approximation

$$f(y) \sim \frac{1}{b_2} (y - 600) \quad .$$

We can easily determine the preposterior improvement in precision if we use (7.11) instead of simply using  $\mathcal{E}\{\tilde{x}\}$ ; if we take  $\mathcal{E}\{\tilde{x}\}$ , then the variance of this estimate is

$$H_0 = \mathcal{V}\{\tilde{x}\} = .07118 \quad .$$

Now, according to (3.18) we get for the variance of the forecast error of a single measurement

$$\begin{aligned}
 H &= \mathcal{V}\{\tilde{x}\} \cdot (1 - z_1 \cdot b_2) \\
 &= \mathcal{V}\{\tilde{x}\} \cdot 9.31 \cdot 10^{-4} \\
 &\approx 10^{-3} \cdot \mathcal{V}\{\tilde{x}\} \quad ,
 \end{aligned}$$

and according to (3.19), for the variance of the forecast error of the sum of  $r$  measurements

$$\begin{aligned}
 H^{(r)} &= r \cdot \mathcal{V}\{\tilde{x}\} (1 - z_1 \cdot b_2) + (r^2 - r) \cdot z_1^2 \cdot (\Delta_{11} + 2\Delta_{12} \cdot \mathcal{E}\{\tilde{x}\} \\
 &\quad + \Delta_{22} [\mathcal{E}\{\tilde{x}\}]^2) \\
 &= 4.3 \cdot 10^{-3} + 4 \cdot 10^{-2} \\
 &\approx 4.4 \cdot 10^{-2} \quad ,
 \end{aligned}$$

which shows that this variance is mainly determined by the uncertainty of the instrument parameters, which is common to

all measurements.

Let us now use the calibration given in Table 2. With

$$X = \begin{pmatrix} 1 & .8 \\ 1 & 1.1 \\ \vdots & \vdots \\ 1 & 2.9 \end{pmatrix} \quad (7.12)$$

we have

$$X'X = 8 \begin{pmatrix} 1 & 1.85 \\ 1.85 & 3.845 \end{pmatrix} = 8 \cdot M \quad (7.13)$$

We can use the approximate formula (6.6) for the optimal distribution of calibration and measurement effort, if  $n \cdot \sigma^2 / T_C$  is much smaller than the diagonal terms of  $\Delta \cdot M$ . We check this assumption by first using equation (6.6) and then seeing whether or not the result fulfills the assumption.

According to equation (6.6) and Table 2 the optimal distribution of the time T available is given by

$$\frac{T_C^*}{T_M^*} = .214 \quad , \quad T_C^* + T_M^* = 720 \quad ,$$

or, in other words,

$$T_C^* = 127 \quad , \quad T_M^* = 593 \quad . \quad (7.14)$$

Therefore, we have

$$\sigma_C^2 = \frac{n \cdot \sigma^2}{T_C^*} = 1.154 \ll \begin{pmatrix} |(\Delta M)_{11}| \\ |(\Delta M)_{22}| \end{pmatrix} = \begin{pmatrix} 300 \\ 142 \end{pmatrix} \quad , \quad (7.15)$$

which means that our assumptions are fulfilled.

Finally, we want to determine the improvement in precision by using the calibration. According to equation (4.12) we have

$$\phi(X) = (I_2 - \underline{z}) \cdot \Delta \quad ,$$

where  $\underline{z}$  is given by (4.8). With (7.10), (7.13), and (7.15) we obtain

$$\underline{z} = \begin{pmatrix} 5.96 & 12.54 \\ -2.36 & -4.94 \end{pmatrix} \quad ,$$

which gives for (4.12)

$$\phi = \begin{pmatrix} 8.06 & -3.22 \\ -2.34 & 0.96 \end{pmatrix} \quad . \quad (7.16)$$

Even though the forecast error variance after calibration and measurement according to (5.1) can be determined only if the calibration data  $(x_i, y_i)$ ,  $i = 1, \dots, n$ . are available, a comparison of (7.16) and (7.10) shows that the use of the calibration represents a considerable improvement in precision.

Table 1: Typical Plutonium Mixture

(Source: Schneider et al. [12])

	Pu238	Pu239	Pu240	Pu241	Pu242	Am241
Mean concentration [%]	0.041	90.51	8.265	1.113	0.064	0.05
Specific heat flux [mW/g]	569.0	1.923	7.03	4.62	0.12	108.4
Contribution to w [mW/g]	0.2333	1.7405	0.581	0.052	$7.69 \cdot 10^{-5}$	0.0612

Mean specific heat flux w: 2.668 [mW/g Pu]



Table 2: Typical Measurement Problem  
(Source: Schneider et al. [12])

No. of batches $r$	60
Mean Pu content $P$ [hg] of one batch	1
Mean heat production $x = w \cdot P$ [W] of one batch	2.668
Batch-to-batch variation	10%
Variance of a single measurement $\sigma^2(t)$ [(mV) <sup>2</sup> ] as a function of time $t$ [h] for $t > 6$	$\frac{18.324}{t}$
Total time $T$ [h] available	720
No. of calibrations $n$	8
Range $R$ of calibrations [Watt]	$0.8 \leq R \leq 3.0$
Values $x_{i2}$ of calibration procedure	0.8, 1.1, ..., 2.9
A priori information $\mathcal{E}\beta_1$ [mV] on intercept $\beta_1$	600
A priori information $\mathcal{E}\beta_2$ [mV/Watt] on the slope of the calibration line	-240
A priori information on the variance of $\beta$ (parametrically)	2%, 5%

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