



## Classical and Inverse Regression Methods of Calibration

R. G. Krutchkoff

*Technometrics*, Vol. 9, No. 3. (Aug., 1967), pp. 425-439.

Stable URL:

<http://links.jstor.org/sici?sici=0040-1706%28196708%299%3A3%3C425%3ACAIRMO%3E2.0.CO%3B2-5>

*Technometrics* is currently published by American Statistical Association.

---

Your use of the JSTOR archive indicates your acceptance of JSTOR's Terms and Conditions of Use, available at <http://www.jstor.org/about/terms.html>. JSTOR's Terms and Conditions of Use provides, in part, that unless you have obtained prior permission, you may not download an entire issue of a journal or multiple copies of articles, and you may use content in the JSTOR archive only for your personal, non-commercial use.

Please contact the publisher regarding any further use of this work. Publisher contact information may be obtained at <http://www.jstor.org/journals/astata.html>.

Each copy of any part of a JSTOR transmission must contain the same copyright notice that appears on the screen or printed page of such transmission.

---

The JSTOR Archive is a trusted digital repository providing for long-term preservation and access to leading academic journals and scholarly literature from around the world. The Archive is supported by libraries, scholarly societies, publishers, and foundations. It is an initiative of JSTOR, a not-for-profit organization with a mission to help the scholarly community take advantage of advances in technology. For more information regarding JSTOR, please contact [support@jstor.org](mailto:support@jstor.org).

# Classical and Inverse Regression Methods of Calibration

R. G. KRUTCHKOFF

*Virginia Polytechnic Institute*

The Classical and Inverse least squares methods of linear calibration are compared by Monte Carlo methods. The Inverse approach is found to be superior to the Classical approach from a mean squared error point of view.

## INTRODUCTION

Consider the problem of calibrating an instrument, say a pressure gauge. Let us assume that it has already been determined that the gauge response is a linear function, that is, the increase in gauge marking is proportional to the increase in pressure. In order to calibrate the gauge, one subjects it to two or more controlled pressures and notes the gauge markings. Using these data, the calibration parameters are calculated, and the gauge is calibrated. The gauge then is used to determine unknown pressures simply by reading the calibrated markings.

The problem of calibration is quite general, and could have been given in terms of measuring temperature, acidity, salinity, etc. The pressure gauge example will, however, be used throughout the introduction as an illustration.

If one uses  $x$  to represent the controlled variable (the pressure) and  $y$  the measured variable (the gauge marking) the relation between  $x$  and  $y$  can be given by

$$y = \alpha + \beta x + \epsilon \quad (1)$$

where  $\alpha$  and  $\beta$  are the parameters in the linear relationship (i.e. the intercept and slope), and where  $\epsilon$  represents the reading error. Two methods of calibration will be considered and compared in the following sections.

### *Method A: The Classical Approach.*

Using the model given by (1) with  $N$  values of  $x$  (not necessarily different values), and independent identically distributed errors with zero mean, one can write the model as

$$y_i = \alpha + \beta x_i + \epsilon_i \quad i = 1, 2, \dots, N. \quad (2)$$

If we let

$$\bar{x} = \sum_{i=1}^N x_i / N$$

$$\bar{y} = \sum_{i=1}^N y_i / N$$

$$u_i = x_i - \bar{x}$$

and

$$v_i = y_i - \bar{y}$$

then the least squares estimators  $b$  of  $\beta$  and  $a$  of  $\alpha$  are

$$b = \frac{\sum_{i=1}^N u_i v_i}{\sum_{i=1}^N u_i^2} \quad (3)$$

and

$$a = \bar{y} - b\bar{x}. \quad (4)$$

The least squares line is

$$y = a + bx \quad (5)$$

and the corresponding calibration equation becomes

$$x = \frac{y - a}{b}. \quad (6)$$

If one now uses the gauge to measure an unknown pressure (say  $X$ ) from a gauge reading  $Y$  the estimate for the pressure is

$$\hat{X} = \frac{Y - a}{b}. \quad (7)$$

*Method B: The Inverse Approach.*

The model (1) can be rewritten so that it becomes

$$x = \gamma + \delta y + \epsilon' \quad (8)$$

where

$$\gamma = -\frac{\alpha}{\beta}, \quad \delta = \frac{1}{\beta}, \quad \text{and} \quad \epsilon' = -\frac{\epsilon}{\beta}.$$

Considering the same data as in *Method A* the model may be written

$$x_i = \gamma + \delta y_i + \epsilon'_i \quad i = 1, 2, \dots, N. \quad (9)$$

The least squares estimators  $d$  of  $\delta$  and  $c$  of  $\gamma$  are

$$d = \frac{\sum_{i=1}^N u_i v_i}{\sum_{i=1}^N v_i^2} \quad (10)$$

and

$$c = \bar{x} - d\bar{y}. \quad (11)$$

The calibration equation then is

$$x = c + dy. \quad (12)$$

If one now reads  $Y$  on the gauge, the estimate of the unknown pressure is

$$\hat{X} = c + dY. \quad (13)$$

The estimates given by equations (7) and (13) in general will not be the same. One has, therefore, to choose between the two.

In an invited paper presented to the American Statistical Association in Detroit on December 29, 1938, Dr. C. Eisenhart discussed the problem of choosing between these methods. In the subsequent paper (Eisenhart (1939)) he says,

*It does not seem to be generally realized that the fitting should be done in terms of the deviations which actually represent 'error.' Thus when the research worker selects the  $X$  values in advance, and holds  $x$  to these values without error, and then observes the corresponding  $y$  values, the errors are in the  $y$  values, so that even if he is interested in using observed values of  $Y$  to estimate  $X$ , he should nevertheless fit  $\hat{Y} = a + bX$  and then use the inverse of this relation to estimate  $X$ , i.e.  $X = (\hat{Y} - a)/b$ , with the best available estimate of  $Y$  substituted for  $\hat{Y}$ .*

Eisenhart then presents two analysis of variance tables. The table he places on the left is the usual analysis of variance table, while the one he places on the right is a corresponding analysis which assumes that  $y$  is controlled and  $x$  is measured with error. He then states,

*"In short, remembering that we are dealing with the case in which the values of  $X$  are chosen by the research worker and only the values of  $Y$  are subject to error, the relation between  $X$  and  $Y$  being as in (1) [ $\alpha_0 + \alpha_1 X + \alpha_2 Y = 0$ ] or its equivalent form (2) [ $Y = \alpha + \beta X$ ], we see that the analysis of variance table on the left separates  $\sum (y - \bar{y})^2$  into portions whose meanings are clear."*

He then says "The analysis of variance table on the right, on the other hand, can be misleading if it is interpreted hastily." Without any further comparisons he concludes;

*"Briefly stated, when the values of  $x$  have been selected by the research worker and the corresponding  $y$  values observed, the line obtained by minimizing  $\sum (X - \hat{Y})^2$  [he means  $\sum (X - \hat{X})^2$ ] is meaningless, and (4) [ $\hat{Y} = a + bX$ ] is accordingly the only correct estimate of the postulated linear relationship between  $X$  and  $Y$ , wherefore, if it is desired to reason from  $Y$  to  $X$  this must be done by means of  $X = (\hat{Y} - a)/b$ , namely (4) solved for  $X$ ."*

After the appearance of this article *Method B*, unfortunately, seems to have been put aside. Subsequent texts and journal articles which deal with the calibration problem use *Method A* exclusively. See, for example, Bennett and Franklin (1954), Mandel and Linning (1957), Mandel (1958), Williams (1959), Brownlee (1960), Linning and Mandel (1964), and Ott (1966). Since no numer-

ical comparison of these two methods was made by Eisenhart it is now proposed that the problem of deciding between them be reopened.

As a basis for the criterion for choosing the better method of calibration, we will use the standard criterion of mean squared error

$$E(\hat{X} - X)^2. \quad (14)$$

Since  $\hat{x}$  is a function of the observations  $y_1, \dots, y_k$  and  $Y$ , the expectation must be with respect to these random variables. The mean squared error is then a function of the unknown pressure  $X$ . One could now require, for the criterion, that the mean squared error be smallest with respect to some weighting function (say  $f(x)$ ) giving the criterion as

$$\int E(\hat{X} - X)^2 f(X) dX. \quad (15)$$

Another possible criterion, still using the mean squared error, is to choose the method with the smallest maximum mean squared error, that is, choose the method which minimizes the

$$\max_x E(\hat{X} - X)^2. \quad (16)$$

Other criteria could also be used. This discussion, however, will turn out to be quite academic since the results will indicate that *Method B* has a smaller mean squared error than *Method A* for all  $X$ . This being the case, any criterion based on the mean squared error will favor the Inverse approach, *Method B*, over the Classical approach, *Method A*. In the following sections, the mean squared errors for *Method A* and for *Method B* will be compared using Monte Carlo methods.

#### THE MONTE CARLO PROCEDURE

As a starting point, let us consider the model of equation (1) i.e.  $y = \alpha + \beta x + \epsilon$  with  $\alpha = 0$  and  $\beta = .5$  (a line through the origin with a slope of  $30^\circ$ ). Since the range will enter into the problem merely as a scale factor, let us assume that the range of  $x$  is  $[0, 1]$  and that the standard deviation of the error is 10% of the range (i.e.  $\sigma = .1$ ).

Imagine designing the calibration experiment so that there are three observations at each of the end points ( $x = 0, x = 1$ ). After obtaining six values for  $y$  one can use equations (3) and (4) to obtain  $b$  and  $a$  and equations (10) and (11) to obtain  $d$  and  $c$ . One can now use *Method A* and *Method B* and obtain two (different) calibration equations, namely those given by equations (7) and (13). Using these, squared errors can be found for  $x = 0, .2, .4, .6, .8, 1$ .

Using the IBM 7040 at the Virginia Polytechnic Institute, and a program generating pseudo-normal random numbers, Monte Carlo experiments of 10,000 sets each were conducted. The values  $X = 1.2, 2, 5, 10$  were added to allow for the case where the maximum of the controlled variable in the laboratory is well below the maximum value for which the gauge is to be calibrated. The values should be considered separately. The results and conclusions, however,

will be seen to hold even for these values. Table I contains the average squared errors for the Classical approach, *Method A*, their standard errors, the average squared errors for the Inverse approach, *Method B*, their standard errors and the ratios of the two averages for the given  $X$  values.

TABLE I:  
*Comparison between classical and inverse methods of calibration*

| $\alpha = 0 \quad \beta = .5 \quad \sigma = .1 \quad \text{Design: } 3(x = 0), \quad 3(x = 1)$ |     |         |          |          |          |          |         |           |         |         |          |
|------------------------------------------------------------------------------------------------|-----|---------|----------|----------|----------|----------|---------|-----------|---------|---------|----------|
|                                                                                                |     | $X = 0$ | $X = .2$ | $X = .4$ | $X = .6$ | $X = .8$ | $X = 1$ | $X = 1.2$ | $X = 2$ | $X = 5$ | $X = 10$ |
| AV. $(\hat{X} - X)^2$                                                                          | CL. | .062    | .054     | .052     | .051     | .054     | .060    | .070      | .132    | .135    | .133     |
| STD. ERR.                                                                                      |     | .001    | .001     | .001     | .001     | .001     | .001    | .001      | .003    | .003    | .003     |
| AV. $(\hat{X} - X)^2$                                                                          | IN. | .049    | .043     | .041     | .041     | .043     | .048    | .055      | .103    | .104    | .104     |
| STD. ERR.                                                                                      |     | .001    | .001     | .001     | .001     | .001     | .001    | .001      | .002    | .002    | .002     |
| RATIO                                                                                          |     | 1.28    | 1.26     | 1.25     | 1.25     | 1.25     | 1.25    | 1.28      | 1.27    | 1.30    | 1.28     |

AV.  $(\hat{X} - X)^2$  CL. is the average squared error using the Classical Approach, *Method A*.

AV.  $(\hat{X} - X)^2$  IN. is the average squared error using the Inverse Approach, *Method B*.

One can conclude from the table that the average squared error of the Classical approach, *Method A*, is uniformly larger than the average squared error of the Inverse approach, *Method B*, (even for  $X$  values outside the range).

In order to establish that this result does not depend on the choice of parameters or design, these factors will now be investigated.

## COMPARISONS

### *The Effect of Intercept*

Is the choice  $\alpha = 0$  necessary for the above conclusion? Since the squared error involves a difference in  $X$  values, the value of  $\alpha$  should cancel out. In order to check to see whether this was actually the case several  $\alpha$  values were chosen and the procedure repeated leaving the other parameters and design unchanged. The results are given in Table II. As in Table I and in all subsequent tables the averages are for 10,000 repetitions.

The values in Table II differ by no more than two standard deviations from the corresponding values in Table I (repeated in Table II where  $\alpha = 0$ ). It can, therefore, be concluded that the results and conclusion indicated by Table I are in no way effected by the choice of a value for  $\alpha$  (the intercept of the line).

### *The Effects of Slope*

Since the choice of intercept has no effect on the results, it was decided to hold this constant (at  $\alpha = 0$ ) and vary the slope of the line (i.e. the  $\beta$  value). This was done, and the results are reported in Table III.

The effect of slope can be seen to be quite significant. Note that both methods have average squared errors which are essentially zero when  $\beta > 10$ . The average squared error for *Method B* remains below .4 for all  $\beta$  (for  $0 \leq X \leq 1$ ), whereas the average squared error for *Method A* becomes excessively large for  $\beta < .5$ . It can be seen that the Classical approach, *Method A*, has a 1%

TABLE II;  
*Comparison between classical and inverse methods of calibration: the effect of intercept*

| $\beta = .5 \quad \sigma = .1 \quad \text{Design: } 3(x = 0), \quad 3(x = 1)$ |       |        |        |        |        |       |         |       |       |        |
|-------------------------------------------------------------------------------|-------|--------|--------|--------|--------|-------|---------|-------|-------|--------|
|                                                                               | $X=0$ | $X=.2$ | $X=.4$ | $X=.6$ | $X=.8$ | $X=1$ | $X=1.2$ | $X=2$ | $X=5$ | $X=10$ |
| $\alpha = -10$                                                                |       |        |        |        |        |       |         |       |       |        |
| AV. $(\hat{X} - X)^2$ CL.                                                     | .061  | .054   | .052   | .051   | .056   | .059  | .068    | .131  | .130  | .135   |
| STD. ERR.                                                                     | .001  | .001   | .001   | .001   | .001   | .001  | .001    | .003  | .003  | .003   |
| AV. $(\hat{X} - X)^2$ IN.                                                     | .048  | .044   | .042   | .041   | .045   | .048  | .055    | .105  | .103  | .106   |
| STD. ERR.                                                                     | .001  | .001   | .001   | .001   | .001   | .001  | .001    | .002  | .001  | .002   |
| RATIO                                                                         | 1.27  | 1.24   | 1.25   | 1.25   | 1.24   | 1.23  | 1.23    | 1.25  | 1.25  | 1.27   |
| $\alpha = -2$                                                                 |       |        |        |        |        |       |         |       |       |        |
| AV. $(\hat{X} - X)^2$ CL.                                                     | .062  | .054   | .052   | .051   | .054   | .060  | .070    | .132  | .135  | .133   |
| STD. ERR.                                                                     | .001  | .001   | .001   | .001   | .001   | .001  | .001    | .003  | .003  | .003   |
| AV. $(\hat{X} - X)^2$ IN.                                                     | .049  | .043   | .041   | .041   | .043   | .048  | .055    | .103  | .104  | .104   |
| STD. ERR.                                                                     | .001  | .001   | .001   | .001   | .001   | .001  | .001    | .002  | .002  | .002   |
| RATIO                                                                         | 1.28  | 1.26   | 1.25   | 1.25   | 1.25   | 1.25  | 1.28    | 1.27  | 1.30  | 1.28   |
| $\alpha = 0$                                                                  |       |        |        |        |        |       |         |       |       |        |
| AV. $(\hat{X} - X)^2$ CL.                                                     | .062  | .054   | .052   | .051   | .054   | .060  | .070    | .132  | .135  | .133   |
| STD. ERR.                                                                     | .001  | .001   | .001   | .001   | .001   | .001  | .001    | .003  | .003  | .003   |
| AV. $(\hat{X} - X)^2$ IN.                                                     | .049  | .043   | .041   | .041   | .043   | .048  | .055    | .103  | .104  | .104   |
| STD. ERR.                                                                     | .001  | .001   | .001   | .001   | .001   | .001  | .001    | .002  | .002  | .002   |
| RATIO                                                                         | 1.28  | 1.26   | 1.25   | 1.25   | 1.25   | 1.25  | 1.28    | 1.27  | 1.30  | 1.28   |
| $\alpha = 1$                                                                  |       |        |        |        |        |       |         |       |       |        |
| AV. $(\hat{X} - X)^2$ CL.                                                     | .061  | .054   | .052   | .051   | .056   | .059  | .068    | .131  | .130  | .135   |
| STD. ERR.                                                                     | .001  | .001   | .001   | .001   | .001   | .001  | .001    | .003  | .003  | .003   |
| AV. $(\hat{X} - X)^2$ IN.                                                     | .048  | .044   | .042   | .041   | .045   | .048  | .055    | .105  | .103  | .106   |
| STD. ERR.                                                                     | .001  | .001   | .001   | .001   | .001   | .001  | .001    | .002  | .001  | .002   |
| RATIO                                                                         | 1.27  | 1.24   | 1.25   | 1.25   | 1.24   | 1.23  | 1.23    | 1.25  | 1.25  | 1.27   |
| $\alpha = 5$                                                                  |       |        |        |        |        |       |         |       |       |        |
| AV. $(\hat{X} - X)^2$ CL.                                                     | .062  | .054   | .052   | .051   | .054   | .060  | .070    | .132  | .135  | .133   |
| STD. ERR.                                                                     | .001  | .001   | .001   | .001   | .001   | .001  | .001    | .003  | .003  | .003   |
| AV. $(\hat{X} - X)^2$ IN.                                                     | .049  | .043   | .041   | .041   | .043   | .048  | .055    | .103  | .104  | .104   |
| STD. ERR.                                                                     | .001  | .001   | .001   | .001   | .001   | .001  | .001    | .002  | .002  | .002   |
| RATIO                                                                         | 1.28  | 1.26   | 1.25   | 1.25   | 1.25   | 1.25  | 1.28    | 1.27  | 1.30  | 1.28   |
| $\alpha = 10$                                                                 |       |        |        |        |        |       |         |       |       |        |
| AV. $(\hat{X} - X)^2$ CL.                                                     | .061  | .053   | .052   | .053   | .054   | .060  | .068    | .128  | .131  | .132   |
| STD. ERR.                                                                     | .001  | .001   | .001   | .001   | .001   | .001  | .001    | .003  | .003  | .003   |
| AV. $(\hat{X} - X)^2$ IN.                                                     | .048  | .043   | .041   | .042   | .043   | .048  | .054    | .101  | .100  | .102   |
| STD. ERR.                                                                     | .001  | .001   | .001   | .001   | .001   | .001  | .001    | .001  | .001  | .001   |
| RATIO                                                                         | 1.27  | 1.25   | 1.25   | 1.26   | 1.25   | 1.27  | 1.26    | 1.27  | 1.31  | 1.30   |

larger average squared error at a slope of 60% ( $\beta = 2$ ). The difference increases to 6% at a slope of 45% ( $\beta = 1$ ) going through 25% at 30° ( $\beta = .5$ ) and becoming excessive (above 7500%) when the slope is below 11° ( $\beta = .2$ ).

*Remark:* For  $\beta = .2$  four values of  $b$  in 10,000 were below .001 in absolute value, while for  $\beta = .1$  there were forty-one, and for  $\beta = .05$  there were seventy-nine such values. To prevent an excessively high squared error using *Method A* these values were replaced with  $b = .001$ . The values for the average squared error of *Method A* presented in Table III for these situations are, therefore, lower than they should actually be. This, of course, only helps strengthen the conclusions obtained. It should also be pointed out that in no other instance in any table presented in this paper did this truncation have to be performed.

The conclusion, for any slope, remains unchanged. *Method B* has a uniform

|                           | $\alpha = 0 \quad \sigma = .1 \quad \text{Design: } 3(x = 0), \quad 3(x = 1)$ |          |          |          |          |         |           |         |         |          |
|---------------------------|-------------------------------------------------------------------------------|----------|----------|----------|----------|---------|-----------|---------|---------|----------|
|                           | $X = 0$                                                                       | $X = .2$ | $X = .4$ | $X = .6$ | $X = .8$ | $X = 1$ | $X = 1.2$ | $X = 2$ | $X = 5$ | $X = 10$ |
| $\beta = .05$             |                                                                               |          |          |          |          |         |           |         |         |          |
| AV. $(\hat{X} - X)^2$ CL. | 174.4                                                                         | 193.2    | 151.3    | 197.5    | 183.0    | 188.7   | 199.8     | 274.8   | 245.2   | 225.1    |
| STD. ERR.                 | 18.1                                                                          | 21.1     | 14.8     | 24.0     | 23.8     | 22.9    | 25.8      | 33.0    | 24.0    | 23.1     |
| AV. $(\hat{X} - X)^2$ IN. | .347                                                                          | .212     | .144     | .134     | .215     | .355    | .550      | 2.11    | 2.10    | 2.13     |
| STD. ERR.                 | .005                                                                          | .005     | .007     | .005     | .006     | .006    | .006      | .01     | .01     | .02      |
| RATIO                     | 502.6                                                                         | 911.8    | 1052.3   | 1473.3   | 850.6    | 531.7   | 363.2     | 130.2   | 116.6   | 105.7    |
| $\beta = .1$              |                                                                               |          |          |          |          |         |           |         |         |          |
| AV. $(\hat{X} - X)^2$ CL. | 128.4                                                                         | 93.4     | 99.1     | 111.9    | 138.5    | 142.7   | 135.1     | 267.7   | 293.5   | 315.3    |
| STD. ERR.                 | 19.1                                                                          | 12.1     | 14.3     | 17.5     | 18.5     | 20.4    | 20.6      | 34.4    | 36.9    | 42.0     |
| AV. $(\hat{X} - X)^2$ IN. | .294                                                                          | .197     | .148     | .138     | .199     | .291    | .440      | 1.53    | 1.53    | 1.54     |
| STD. ERR.                 | .005                                                                          | .004     | .004     | .003     | .005     | .005    | .005      | .01     | .01     | .01      |
| RATIO                     | 436.9                                                                         | 474.9    | 667.5    | 810.3    | 697.3    | 491.4   | 307.3     | 175.0   | 192.3   | 205.2    |
| $\beta = .2$              |                                                                               |          |          |          |          |         |           |         |         |          |
| AV. $(\hat{X} - X)^2$ CL. | 16.7                                                                          | 10.8     | 15.6     | 16.8     | 22.4     | 24.3    | 45.3      | 108.5   | 93.0    | 128.2    |
| STD. ERR.                 | 6.7                                                                           | 3.3      | 4.8      | 6.2      | 8.7      | 7.0     | 15.0      | 28.4    | 22.4    | 39.1     |
| AV. $(\hat{X} - X)^2$ IN. | .181                                                                          | .141     | .128     | .127     | .140     | .177    | .224      | .597    | .598    | .589     |
| STD. ERR.                 | .006                                                                          | .002     | .003     | .003     | .003     | .003    | .003      | .007    | .009    | .007     |
| RATIO                     | 92.1                                                                          | 76.7     | 122.3    | 131.8    | 160.1    | 137.3   | 202.2     | 181.7   | 155.5   | 217.4    |
| $\beta = .5$              |                                                                               |          |          |          |          |         |           |         |         |          |
| AV. $(\hat{X} - X)^2$ CL. | .062                                                                          | .054     | .052     | .051     | .054     | .060    | .070      | .132    | .135    | .133     |
| STD. ERR.                 | .001                                                                          | .001     | .001     | .001     | .001     | .001    | .001      | .003    | .003    | .003     |
| AV. $(\hat{X} - X)^2$ IN. | .049                                                                          | .043     | .041     | .041     | .043     | .045    | .055      | .103    | .104    | .104     |
| STD. ERR.                 | .001                                                                          | .001     | .001     | .001     | .001     | .001    | .001      | .002    | .002    | .002     |
| RATIO                     | 1.28                                                                          | 1.26     | 1.25     | 1.25     | 1.25     | 1.25    | 1.28      | 1.27    | 1.30    | 1.28     |
| $\beta = .75$             |                                                                               |          |          |          |          |         |           |         |         |          |
| AV. $(\hat{X} - X)^2$ CL. | .0252                                                                         | .0230    | .0221    | .0222    | .0229    | .0256   | .0285     | .0527   | .0528   | .0540    |
| STD. ERR.                 | .0004                                                                         | .0003    | .0003    | .0003    | .0003    | .0004   | .0005     | .0010   | .0010   | .0010    |
| AV. $(\hat{X} - X)^2$ IN. | .0228                                                                         | .0208    | .0200    | .0202    | .0207    | .0231   | .0258     | .0473   | .0471   | .0480    |
| STD. ERR.                 | .0003                                                                         | .0003    | .0003    | .0003    | .0003    | .0003   | .0004     | .0007   | .0007   | .0007    |
| RATIO                     | 1.11                                                                          | 1.10     | 1.10     | 1.10     | 1.10     | 1.11    | 1.11      | 1.11    | 1.12    | 1.13     |
| $\beta = 1$               |                                                                               |          |          |          |          |         |           |         |         |          |
| AV. $(\hat{X} - X)^2$ CL. | .0139                                                                         | .0124    | .0120    | .0122    | .0125    | .0138   | .0154     | .0275   | .0279   | .0284    |
| STD. ERR.                 | .0002                                                                         | .0002    | .0002    | .0002    | .0002    | .0002   | .0002     | .0004   | .0005   | .0004    |
| AV. $(\hat{X} - X)^2$ IN. | .0132                                                                         | .0118    | .0114    | .0116    | .0018    | .0130   | .0146     | .0260   | .0261   | .0266    |
| STD. ERR.                 | .0002                                                                         | .0002    | .0002    | .0002    | .0002    | .0002   | .0002     | .0004   | .0004   | .0004    |
| RATIO                     | 1.06                                                                          | 1.06     | 1.06     | 1.06     | 1.05     | 1.06    | 1.06      | 1.06    | 1.07    | 1.06     |
| $\beta = 2$               |                                                                               |          |          |          |          |         |           |         |         |          |
| AV. $(\hat{X} - X)^2$ CL. | .00342                                                                        | .00308   | .00299   | .00292   | .00317   | .00335  | .00376    | .00681  | .00678  | .00697   |
| STD. ERR.                 | .00005                                                                        | .00004   | .00004   | .00004   | .00004   | .00005  | .00005    | .00010  | .00010  | .00010   |
| AV. $(\hat{X} - X)^2$ IN. | .00337                                                                        | .00304   | .00295   | .00288   | .00313   | .00332  | .00373    | .00676  | .00672  | .00689   |
| STD. ERR.                 | .00005                                                                        | .00004   | .00004   | .00004   | .00004   | .00005  | .00005    | .00010  | .00009  | .00010   |
| RATIO                     | 1.01                                                                          | 1.01     | 1.01     | 1.01     | 1.01     | 1.01    | 1.01      | 1.01    | 1.01    | 1.01     |
| $\beta = 5$               |                                                                               |          |          |          |          |         |           |         |         |          |
| AV. $(\hat{X} - X)^2$ CL. | .00054                                                                        | .00050   | .00048   | .00048   | .00050   | .00055  | .00060    | .00108  | .00109  | .00111   |
| STD. ERR.                 | .00001                                                                        | .00001   | .00001   | .00001   | .00001   | .00001  | .00001    | .00002  | .00002  | .00002   |
| AV. $(\hat{X} - X)^2$ IN. | .00054                                                                        | .00050   | .00048   | .00048   | .00049   | .00055  | .00060    | .00108  | .00108  | .00110   |
| STD. ERR.                 | .00001                                                                        | .00001   | .00001   | .00001   | .00001   | .00001  | .00001    | .00002  | .00002  | .00002   |
| RATIO                     | 1.00                                                                          | 1.00     | 1.00     | 1.00     | 1.00     | 1.00    | 1.00      | 1.00    | .100    | 1.00     |



TABLE III- Continued

|                         | X=0    | X=.2   | X=.4   | X=.6   | X=.8   | X=1    | X=1.2  | X=2    | X=5    | X=10   |
|-------------------------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|
| $\beta = 10$            |        |        |        |        |        |        |        |        |        |        |
| AV. $(\hat{X}-X)^2$ CL. | .00013 | .00013 | .00012 | .00012 | .00012 | .00014 | .00015 | .00027 | .00027 | .00028 |
| STD. ERR.               | .00000 | .00000 | .00000 | .00000 | .00000 | .00000 | .00000 | .00000 | .00000 | .00000 |
| AV. $(\hat{X}-X)^2$ IN. | .00013 | .00013 | .00012 | .00012 | .00012 | .00014 | .00015 | .00027 | .00027 | .00028 |
| STD. ERR.               | .00000 | .00000 | .00000 | .00000 | .00000 | .00000 | .00000 | .00000 | .00000 | .00000 |
| RATIO                   | 1.00   | 1.00   | 1.00   | 1.00   | 1.00   | 1.00   | 1.00   | 1.00   | 1.00   | 1.00   |
| $\beta = 100$           |        |        |        |        |        |        |        |        |        |        |
| AV. $(\hat{X}-X)^2$ CL. | .00000 | .00000 | .00000 | .00000 | .00000 | .00000 | .00000 | .00000 | .00000 | .00000 |
| STD. ERR.               | .00000 | .00000 | .00000 | .00000 | .00000 | .00000 | .00000 | .00000 | .00000 | .00000 |
| AV. $(\hat{X}-X)^2$ IN. | .00000 | .00000 | .00000 | .00000 | .00000 | .00000 | .00000 | .00000 | .00000 | .00000 |
| STD. ERR.               | .00000 | .00000 | .00000 | .00000 | .00000 | .00000 | .00000 | .00000 | .00000 | .00000 |
| RATIO                   | 1.00   | 1.00   | 1.00   | 1.00   | 1.00   | 1.00   | 1.00   | 1.00   | 1.00   | 1.00   |

smaller (or at least no larger) average squared error (even outside the range of  $x$ ).

*The Effect of Error Variance*

Keeping the other parameters and the design the same as in the situation

TABLE IV:

*Comparison between classical and inverse methods of calibration: the effect of error variance*

|                         | $\alpha = 0 \quad \beta = .5 \quad \text{Design: } 3(x = 0), \quad 3(x = 1)$ |        |        |        |        |        |        |        |        |        |
|-------------------------|------------------------------------------------------------------------------|--------|--------|--------|--------|--------|--------|--------|--------|--------|
|                         | X=0                                                                          | X=.2   | X=.4   | X=.6   | X=.8   | X=1    | X=1.2  | X=2    | X=5    | X=10   |
| $\sigma = 0$            |                                                                              |        |        |        |        |        |        |        |        |        |
| AV. $(\hat{X}-X)^2$ CL. | 0.0                                                                          | 0.0    | 0.0    | 0.0    | 0.0    | 0.0    | 0.0    | 0.0    | 0.0    | 0.0    |
| STD. ERR.               | 0.0                                                                          | 0.0    | 0.0    | 0.0    | 0.0    | 0.0    | 0.0    | 0.0    | 0.0    | 0.0    |
| AV. $(\hat{X}-X)^2$ IN. | 0.0                                                                          | 0.0    | 0.0    | 0.0    | 0.0    | 0.0    | 0.0    | 0.0    | 0.0    | 0.0    |
| STD. ERR.               | 0.0                                                                          | 0.0    | 0.0    | 0.0    | 0.0    | 0.0    | 0.0    | 0.0    | 0.0    | 0.0    |
| RATIO                   | 1.00                                                                         | 1.00   | 1.00   | 1.00   | 1.00   | 1.00   | 1.00   | 1.00   | 1.00   | 1.00   |
| $\sigma = .05$          |                                                                              |        |        |        |        |        |        |        |        |        |
| AV. $(\hat{X}-X)^2$ CL. | .0140                                                                        | .0125  | .0121  | .0119  | .0129  | .0136  | .0154  | .0281  | .0280  | .0288  |
| STD. ERR.               | .0002                                                                        | .0002  | .0002  | .0002  | .0002  | .0002  | .0002  | .0004  | .00004 | .0005  |
| AV. $(\hat{X}-X)^2$ IN. | .0132                                                                        | .0119  | .0115  | .0113  | .0123  | .0130  | .0147  | .0269  | .0267  | .0274  |
| STD. ERR.               | .0002                                                                        | .0002  | .0002  | .0002  | .0002  | .0002  | .0002  | .0004  | .0004  | .0004  |
| RATIO                   | 1.06                                                                         | 1.05   | 1.05   | 1.05   | 1.05   | 1.05   | 1.04   | 1.04   | 1.05   | 1.05   |
| $\sigma = .1$           |                                                                              |        |        |        |        |        |        |        |        |        |
| AV. $(\hat{X}-X)^2$ CL. | .062                                                                         | .054   | .052   | .051   | .054   | .060   | .070   | .132   | .135   | .133   |
| STD. ERR.               | .001                                                                         | .001   | .001   | .001   | .001   | .001   | .001   | .003   | .003   | .003   |
| AV. $(\hat{X}-X)^2$ IN. | .049                                                                         | .043   | .041   | .041   | .043   | .048   | .103   | .104   | .104   | .104   |
| STD. ERR.               | .001                                                                         | .001   | .001   | .001   | .001   | .001   | .001   | .002   | .002   | .002   |
| RATIO                   | 1.28                                                                         | 1.26   | 1.25   | 1.25   | 1.25   | 1.25   | 1.28   | 1.30   | 1.30   | 1.28   |
| $\sigma = .2$           |                                                                              |        |        |        |        |        |        |        |        |        |
| AV. $(\hat{X}-X)^2$ CL. | 7.6                                                                          | .85    | .81    | 2.3    | 1.41   | 1.31   | 1.60   | 10.28  | 7.29   | 10.78  |
| STD. ERR.               | 6.4                                                                          | .18    | .17    | 1.5    | .65    | .27    | .33    | 4.37   | 2.13   | 5.24   |
| AV. $(\hat{X}-X)^2$ IN. | .141                                                                         | .116   | .109   | .109   | .115   | .138   | .166   | .386   | .385   | .382   |
| STD. ERR.               | .005                                                                         | .002   | .002   | .002   | .002   | .002   | .002   | .005   | .006   | .005   |
| RATIO                   | 53.7                                                                         | 7.35   | 7.39   | 20.6   | 12.28  | 9.48   | 9.67   | 26.61  | 18.91  | 28.17  |
| $\sigma = .5$           |                                                                              |        |        |        |        |        |        |        |        |        |
| AV. $(\hat{X}-X)^2$ CL. | 355.2                                                                        | 570.7  | 539.4  | 458.5  | 341.4  | 1212.6 | 898.7  | 1494.9 | 2015.0 | 2083.6 |
| STD. ERR.               | 76.7                                                                         | 152.0  | 210.2  | 107.9  | 109.7  | 397.3  | 248.6  | 402.5  | 587.2  | 608.5  |
| AV. $(\hat{X}-X)^2$ IN. | .289                                                                         | .190   | .132   | .139   | .189   | .289   | .438   | 1.533  | 1.520  | 1.530  |
| STD. ERR.               | .005                                                                         | .005   | .003   | .004   | .004   | .004   | .005   | .012   | .012   | .012   |
| RATIO                   | 1229.5                                                                       | 3006.1 | 4077.8 | 3290.7 | 1798.5 | 4189.3 | 2052.4 | 975.0  | 1326.4 | 1362.0 |

of Table I, the standard deviation of the error was varied. Table IV represents these results.

When there is a zero error variance, both methods fit the line exactly with no squared errors. As the error variance increases, the average squared errors of each method increase. However, the average squared error for *Method B* remains below .3 (for  $0 \leq X \leq 1$ ) while the average squared error for *Method A* becomes excessive (above 1,000).

The size of the error variance, therefore, does not effect the conclusion obtained previously.

It is interesting to note that the effects of slope and variance depend only on the ratio  $\beta/\sigma$ . This point can easily be derived and is born out in the entries in Tables III and IV where  $\beta/\sigma = 1, 5, 10$ , (for  $\beta/\sigma = 1$ , the discrepancy is due to the truncation carried out on the  $b$  values in the case  $\beta = \sigma = 0.1$ ).

### *The Effect of the Number of Observations at Each Design Point*

Keeping all the parameters and the design the same as in the situation of Table I, the number of observations taken at each design point was varied. The results are in Table V.

TABLE V:  
*Comparison between classical and inverse methods of calibration:  
effect of the number of observations at each design point*

|                           | $\alpha = 0 \quad \beta = .5 \quad \sigma = .1$ |        |        |        |        |       |         |       |       |        |
|---------------------------|-------------------------------------------------|--------|--------|--------|--------|-------|---------|-------|-------|--------|
|                           | $X=0$                                           | $X=.2$ | $X=.4$ | $X=.6$ | $X=.8$ | $X=1$ | $X=1.2$ | $X=2$ | $X=5$ | $X=10$ |
| <hr/>                     |                                                 |        |        |        |        |       |         |       |       |        |
| $2(x=0)$                  |                                                 |        |        |        |        |       |         |       |       |        |
| $2(x=1)$                  |                                                 |        |        |        |        |       |         |       |       |        |
| AV. $(\hat{X} - X)^2$ CL. | .075                                            | .061   | .058   | .059   | .063   | .073  | .089    | .202  | .200  | .195   |
| STD. ERR.                 | .002                                            | .001   | .001   | .001   | .001   | .002  | .003    | .007  | .007  | .006   |
| AV. $(\hat{X} - X)^2$ IN. | .060                                            | .050   | .048   | .049   | .052   | .059  | .070    | .144  | .144  | .142   |
| STD. ERR.                 | .001                                            | .001   | .001   | .001   | .001   | .001  | .002    | .004  | .004  | .004   |
| RATIO                     | 1.25                                            | 1.23   | 1.20   | 1.21   | 1.21   | 1.24  | 1.28    | 1.40  | 1.38  | 1.37   |
| $3(x=0)$                  |                                                 |        |        |        |        |       |         |       |       |        |
| $3(x=1)$                  |                                                 |        |        |        |        |       |         |       |       |        |
| AV. $(\hat{X} - X)^2$ CL. | .062                                            | .054   | .052   | .051   | .054   | .060  | .070    | .132  | .135  | .133   |
| STD. ERR.                 | .001                                            | .001   | .001   | .001   | .001   | .001  | .001    | .003  | .003  | .003   |
| AV. $(\hat{X} - X)^2$ IN. | .049                                            | .043   | .041   | .041   | .043   | .048  | .055    | .103  | .104  | .104   |
| STD. ERR.                 | .001                                            | .001   | .001   | .001   | .001   | .001  | .001    | .002  | .002  | .002   |
| RATIO                     | 1.28                                            | 1.26   | 1.25   | 1.25   | 1.25   | 1.25  | 1.28    | 1.27  | 1.30  | 1.28   |
| $5(x=0)$                  |                                                 |        |        |        |        |       |         |       |       |        |
| $5(x=1)$                  |                                                 |        |        |        |        |       |         |       |       |        |
| AV. $(\hat{X} - X)^2$ CL. | .051                                            | .048   | .048   | .047   | .049   | .051  | .055    | .086  | .088  | .086   |
| STD. ERR.                 | .001                                            | .001   | .001   | .001   | .001   | .001  | .001    | .001  | .001  | .001   |
| AV. $(\hat{X} - X)^2$ IN. | .041                                            | .038   | .037   | .036   | .038   | .042  | .046    | .083  | .084  | .083   |
| STD. ERR.                 | .001                                            | .001   | .001   | .001   | .001   | .001  | .001    | .001  | .001  | .001   |
| RATIO                     | 1.25                                            | 1.27   | 1.29   | 1.29   | 1.27   | 1.22  | 1.18    | 1.04  | 1.04  | 1.04   |
| $10(x=0)$                 |                                                 |        |        |        |        |       |         |       |       |        |
| $10(x=1)$                 |                                                 |        |        |        |        |       |         |       |       |        |
| AV. $(\hat{X} - X)^2$ CL. | .046                                            | .043   | .043   | .044   | .043   | .046  | .049    | .064  | .063  | .063   |
| STD. ERR.                 | .001                                            | .001   | .001   | .001   | .001   | .001  | .001    | .001  | .001  | .001   |
| AV. $(\hat{X} - X)^2$ IN. | .037                                            | .034   | .033   | .034   | .034   | .038  | .043    | .077  | .077  | .077   |
| STD. ERR.                 | .001                                            | .001   | .001   | .001   | .001   | .001  | .001    | .001  | .001  | .001   |
| RATIO                     | 1.22                                            | 1.27   | 1.32   | 1.32   | 1.27   | 1.20  | 1.14    | .83   | .81   | .83    |

From Table V it is clear that increasing the number of observations reduces the average squared errors of both methods proportionally. The number of observations will, therefore, not affect the conclusion already obtained.

### *The Effect of Design*

Using the same parameters as in the situation of Table I, and still using six observations for the calibration, the design was varied. The designs used and the results are given in Table VI.

TABLE VI:  
*Comparison between classical and inverse methods of calibration: the effect of design*

|                         | $\alpha = 0 \quad \beta = .5 \quad \sigma = .1$ |        |        |        |        |       |         |       |       |        |
|-------------------------|-------------------------------------------------|--------|--------|--------|--------|-------|---------|-------|-------|--------|
|                         | $X=0$                                           | $X=.2$ | $X=.4$ | $X=.6$ | $X=.8$ | $X=1$ | $X=1.2$ | $X=2$ | $X=5$ | $X=10$ |
| <hr/>                   |                                                 |        |        |        |        |       |         |       |       |        |
| 3( $x=0$ )              |                                                 |        |        |        |        |       |         |       |       |        |
| 3( $x=1$ )              |                                                 |        |        |        |        |       |         |       |       |        |
| AV. $(\hat{X}-X)^2$ CL. | .062                                            | .054   | .052   | .051   | .054   | .060  | .070    | .132  | .135  | .133   |
| STD. ERR.               | .001                                            | .001   | .001   | .001   | .001   | .001  | .001    | .003  | .003  | .003   |
| AV. $(\hat{X}-X)^2$ IN. | .049                                            | .043   | .041   | .041   | .043   | .048  | .103    | .104  | .104  | .104   |
| STD. ERR.               | .001                                            | .001   | .001   | .001   | .001   | .001  | .001    | .002  | .002  | .002   |
| RATIO                   | 1.28                                            | 1.26   | 1.25   | 1.25   | 1.25   | 1.25  | 1.28    | 1.30  | 1.30  | 1.28   |
| <hr/>                   |                                                 |        |        |        |        |       |         |       |       |        |
| 2( $x=0$ )              |                                                 |        |        |        |        |       |         |       |       |        |
| 2( $x=.5$ )             |                                                 |        |        |        |        |       |         |       |       |        |
| 2( $x=1$ )              |                                                 |        |        |        |        |       |         |       |       |        |
| AV. $(\hat{X}-X)^2$ CL. | .072                                            | .061   | .057   | .056   | .061   | .072  | .088    | .205  | .204  | .210   |
| STD. ERR.               | .002                                            | .001   | .001   | .001   | .001   | .002  | .002    | .006  | .006  | .007   |
| AV. $(\hat{X}-X)^2$ IN. | .049                                            | .042   | .039   | .039   | .042   | .049  | .059    | .132  | .132  | .134   |
| STD. ERR.               | .001                                            | .001   | .001   | .001   | .001   | .001  | .001    | .002  | .002  | .002   |
| RATIO                   | 1.48                                            | 1.46   | 1.44   | 1.43   | 1.45   | 1.48  | 1.49    | 1.55  | 1.54  | 1.57   |
| <hr/>                   |                                                 |        |        |        |        |       |         |       |       |        |
| 1( $x=0$ )              |                                                 |        |        |        |        |       |         |       |       |        |
| 1( $x=.2$ )             |                                                 |        |        |        |        |       |         |       |       |        |
| 1( $x=.4$ )             |                                                 |        |        |        |        |       |         |       |       |        |
| 1( $x=.6$ )             |                                                 |        |        |        |        |       |         |       |       |        |
| 1( $x=.8$ )             |                                                 |        |        |        |        |       |         |       |       |        |
| 1( $x=1$ )              |                                                 |        |        |        |        |       |         |       |       |        |
| AV. $(\hat{X}-X)^2$ CL. | .096                                            | .072   | .063   | .063   | .075   | .100  | .128    | .380  | .382  | .400   |
| STD. ERR.               | .005                                            | .002   | .002   | .001   | .004   | .008  | .007    | .036  | .039  | .047   |
| AV. $(\hat{X}-X)^2$ IN. | .050                                            | .040   | .036   | .036   | .040   | .050  | .065    | .172  | .170  | .172   |
| STD. ERR.               | .001                                            | .001   | .001   | .001   | .001   | .001  | .001    | .002  | .002  | .003   |
| RATIO                   | 1.92                                            | 1.81   | 1.75   | 1.74   | 1.89   | 1.99  | 1.98    | 2.21  | 2.25  | 2.33   |
| <hr/>                   |                                                 |        |        |        |        |       |         |       |       |        |
| 3( $x=.15$ )            |                                                 |        |        |        |        |       |         |       |       |        |
| 3( $x=.85$ )            |                                                 |        |        |        |        |       |         |       |       |        |
| AV. $(\hat{X}-X)^2$ CL. | .104                                            | .070   | .062   | .061   | .069   | .089  | .175    | .581  | .433  | .532   |
| STD. ERR.               | .017                                            | .003   | .002   | .002   | .002   | .008  | .068    | .290  | .144  | .233   |
| AV. $(\hat{X}-X)^2$ IN. | .050                                            | .041   | .037   | .036   | .042   | .051  | .065    | .170  | .167  | .169   |
| STD. ERR.               | .001                                            | .001   | .001   | .001   | .001   | .001  | .001    | .003  | .003  | .003   |
| RATIO                   | 2.07                                            | 1.71   | 1.70   | 1.69   | 1.64   | 1.75  | 2.69    | 3.43  | 2.59  | 3.14   |

The end point design, used exclusively for the previous tables, can be seen to be the most efficient design for *Method A*. That is, the average squared errors for *Method A* are uniformly smallest in using the end point design. *Method B*, on the other hand, seems to be fairly robust to design. The average squared errors for *Method B* are slightly larger at the points  $X = 0$  and  $X = 1$  for the other designs, but smaller at the points  $X = .2, .4, .6, .8$ .

The fact that the end point design is most efficient for *Method A* and not most efficient for *Method B* only helps to strengthen the conclusion already obtained. That is, the Inverse approach, *Method B*, has a uniformly smaller (never larger) average squared error than the Classical approach, *Method A*.

### ROBUSTNESS

In all the above situations the errors were assumed to be normally distributed. What would be the effect of non-normal errors on the results obtained? In order to answer this question the pseudo-normal random number generator was replaced by a remarkable computer program (see Krutchkoff and Thomas 1966) which, among other things, can generate pseudo-random numbers from any Pearson distribution. These distributions are characterized by the values of skewness

$$\beta_1 = \frac{(\text{Third Central Moment})^2}{(\text{Variance})^3} \quad (17)$$

and kurtosis

$$\beta_2 = \frac{(\text{Fourth Central Moment})}{(\text{Variance})^2}. \quad (18)$$

For the normal distribution, which is a Pearson distribution,  $\beta_1 = 0$  and  $\beta_2 = 3$ .

### The Effect of Skewness

In Table VII the errors were distributed as Pearson variables with skewness as indicated.

TABLE VII:

*Comparison between classical and inverse methods of calibration: effect of skewness in the error*

| $\alpha = 0 \quad \beta = .5 \quad \sigma = .1 \quad \text{Design: } 3(x = 0), \quad 3(x = 1) \quad \beta_2 = 3$ |       |        |        |        |        |       |         |       |       |        |
|------------------------------------------------------------------------------------------------------------------|-------|--------|--------|--------|--------|-------|---------|-------|-------|--------|
|                                                                                                                  | $X=0$ | $X=.2$ | $X=.4$ | $X=.6$ | $X=.8$ | $X=1$ | $X=1.2$ | $X=2$ | $X=5$ | $X=10$ |
| $\sqrt{\beta_1} = -1$                                                                                            |       |        |        |        |        |       |         |       |       |        |
| AV. $(\hat{X} - X)^2$ CL.                                                                                        | .057  | .053   | .050   | .051   | .057   | .063  | .071    | .134  | .138  | .138   |
| STD. ERR.                                                                                                        | .001  | .001   | .001   | .001   | .001   | .001  | .001    | .003  | .003  | .003   |
| AV. $(\hat{X} - X)^2$ IN.                                                                                        | .049  | .045   | .041   | .040   | .043   | .047  | .053    | .098  | .101  | .102   |
| STD. ERR.                                                                                                        | .001  | .001   | .001   | .001   | .001   | .001  | .001    | .002  | .002  | .002   |
| RATIO                                                                                                            | 1.16  | 1.19   | 1.23   | 1.27   | 1.32   | 1.33  | 1.35    | 1.37  | 1.37  | 1.34   |
| $\beta_1 = 0$                                                                                                    |       |        |        |        |        |       |         |       |       |        |
| AV. $(\hat{X} - X)^2$ CL.                                                                                        | .062  | .054   | .052   | .051   | .054   | .060  | .070    | .132  | .135  | .133   |
| STD. ERR.                                                                                                        | .001  | .001   | .001   | .001   | .001   | .001  | .001    | .003  | .003  | .003   |
| AV. $(\hat{X} - X)^2$ IN.                                                                                        | .049  | .043   | .041   | .041   | .043   | .048  | .055    | .103  | .104  | .104   |
| STD. ERR.                                                                                                        | .001  | .001   | .001   | .001   | .001   | .001  | .001    | .002  | .002  | .002   |
| RATIO                                                                                                            | 1.28  | 1.26   | 1.25   | 1.25   | 1.25   | 1.25  | 1.28    | 1.27  | 1.30  | 1.28   |
| $\sqrt{\beta_1} = 1$                                                                                             |       |        |        |        |        |       |         |       |       |        |
| AV. $(\hat{X} - X)^2$ CL.                                                                                        | .063  | .056   | .051   | .051   | .054   | .057  | .064    | 1.21  | .127  | .122   |
| STD. ERR.                                                                                                        | .001  | .001   | .001   | .001   | .001   | .001  | .001    | .002  | .003  | .003   |
| AV. $(\hat{X} - X)^2$ IN.                                                                                        | .048  | .043   | .040   | .042   | .045   | .049  | .056    | .106  | .111  | .107   |
| STD. ERR.                                                                                                        | .001  | .001   | .001   | .001   | .001   | .001  | .001    | .001  | .002  | .002   |
| RATIO                                                                                                            | 1.33  | 1.31   | 1.27   | 1.23   | 1.20   | 1.16  | 1.14    | 1.14  | 1.14  | 1.13   |

For the Inverse approach the variation is less than two standard errors from the normal. Although the Classical approach demonstrates a slightly higher variation than this the results do not indicate any change in the conclusions obtained for normal errors.

*The Effect of Kurtosis*

In Table VIII the errors were distributed as Pearson variables with kurtosis as indicated.

TABLE VIII:  
*Comparison Between Classical and Inverse Methods of Calibration: Effect of Kurtosis in the Error*

| $\alpha = 0 \quad \beta = .5 \quad \sigma = .1 \quad \text{Design: } 3(x = 0), 3(x = 1) \quad \beta_1 = 0$                 |                           |      |      |      |      |      |      |      |      |      |      |
|----------------------------------------------------------------------------------------------------------------------------|---------------------------|------|------|------|------|------|------|------|------|------|------|
| $X = 0 \quad X = .2 \quad X = .4 \quad X = .6 \quad X = .8 \quad X = 1 \quad X = 1.2 \quad X = 2 \quad X = 5 \quad X = 10$ |                           |      |      |      |      |      |      |      |      |      |      |
| <hr/>                                                                                                                      |                           |      |      |      |      |      |      |      |      |      |      |
| “U”                                                                                                                        | $\beta_2 = 1.7$           |      |      |      |      |      |      |      |      |      |      |
|                                                                                                                            | AV. $(\hat{X} - X)^2$ CL. | .059 | .054 | .051 | .051 | .055 | .060 | .066 | .126 | .130 | .126 |
|                                                                                                                            | STD. ERR.                 | .001 | .001 | .001 | .001 | .001 | .001 | .001 | .002 | .002 | .002 |
|                                                                                                                            | AV. $(\hat{X} - X)^2$ IN. | .049 | .044 | .041 | .042 | .044 | .049 | .055 | .106 | .109 | .108 |
|                                                                                                                            | STD. ERR.                 | .001 | .001 | .001 | .001 | .001 | .001 | .001 | .002 | .002 | .002 |
|                                                                                                                            | RATIO                     | 1.21 | 1.24 | 1.24 | 1.24 | 1.23 | 1.23 | 1.21 | 1.19 | 1.19 | 1.17 |
| $\beta_2 = 2$                                                                                                              |                           |      |      |      |      |      |      |      |      |      |      |
|                                                                                                                            | AV. $(\hat{X} - X)^2$ CL. | .060 | .054 | .051 | .051 | .055 | .060 | .067 | .125 | .131 | .127 |
|                                                                                                                            | STD. ERR.                 | .001 | .001 | .001 | .001 | .001 | .001 | .001 | .002 | .003 | .003 |
|                                                                                                                            | AV. $(\hat{X} - X)^2$ IN. | .049 | .044 | .041 | .041 | .044 | .048 | .055 | .104 | .108 | .109 |
|                                                                                                                            | STD. ERR.                 | .001 | .001 | .001 | .001 | .001 | .001 | .001 | .001 | .002 | .002 |
|                                                                                                                            | RATIO                     | 1.22 | 1.24 | 1.24 | 1.24 | 1.24 | 1.23 | 1.22 | 1.21 | 1.21 | 1.19 |
| $\beta_2 = 3$                                                                                                              |                           |      |      |      |      |      |      |      |      |      |      |
|                                                                                                                            | AV. $(\hat{X} - X)^2$ CL. | .062 | .054 | .052 | .051 | .054 | .060 | .070 | .132 | .135 | .133 |
|                                                                                                                            | STD. ERR.                 | .001 | .001 | .001 | .001 | .001 | .001 | .003 | .003 | .003 | .003 |
|                                                                                                                            | AV. $(\hat{X} - X)^2$ IN. | .049 | .043 | .041 | .041 | .043 | .048 | .055 | .103 | .104 | .104 |
|                                                                                                                            | STD. ERR.                 | .001 | .001 | .001 | .001 | .001 | .001 | .001 | .002 | .002 | .002 |
|                                                                                                                            | RATIO                     | 1.28 | 1.26 | 1.25 | 1.25 | 1.25 | 1.25 | 1.28 | 1.27 | 1.30 | 1.28 |
| $\beta_2 = 4$                                                                                                              |                           |      |      |      |      |      |      |      |      |      |      |
|                                                                                                                            | AV. $(\hat{X} - X)^2$ CL. | .062 | .055 | .051 | .051 | .056 | .061 | .067 | .128 | .135 | .132 |
|                                                                                                                            | STD. ERR.                 | .001 | .001 | .001 | .001 | .001 | .001 | .001 | .003 | .004 | .004 |
|                                                                                                                            | AV. $(\hat{X} - X)^2$ IN. | .048 | .043 | .040 | .040 | .044 | .048 | .054 | .099 | .104 | .103 |
|                                                                                                                            | STD. ERR.                 | .001 | .001 | .001 | .001 | .001 | .001 | .001 | .001 | .002 | .002 |
|                                                                                                                            | RATIO                     | 1.28 | 1.26 | 1.26 | 1.26 | 1.26 | 1.26 | 1.26 | 1.29 | 1.30 | 1.28 |

The effect of kurtosis on either method is not significant anywhere in this table. It is interesting to note the lack of significance even when the distribution is “U” shaped ( $\beta_2 = 1.7$ ).

*The Effect of a Quadratic Term*

Ott (1966), working with *Method A* only, shows that if one designs in from the end points, the linear calibration given by equation (7) is a fair representation for the calibration even when the true model is quadratic e.g.

$$y = \alpha + \beta X + \theta X^2 + \epsilon. \tag{19}$$

The values in Table IX were obtained by adding positive quadratic terms (values for  $\theta$ ) to the model, obtaining the corresponding observations and then using equations (7) and (13) to estimate  $X$  as if the model were linear.

TABLE IX:

*Comparison Between Classical and Inverse Methods of Calibration: The Effect of a Positive Quadratic Term*

|                           | $\alpha = 0 \quad \beta = .5 \quad \sigma = .1 \quad \text{Design: } 3(x = .15), \quad 3(x = .85)$ |          |          |          |          |         |           |         |         |          |
|---------------------------|----------------------------------------------------------------------------------------------------|----------|----------|----------|----------|---------|-----------|---------|---------|----------|
|                           | $X = 0$                                                                                            | $X = .2$ | $X = .4$ | $X = .6$ | $X = .8$ | $X = 1$ | $X = 1.2$ | $X = 2$ | $X = 5$ | $X = 10$ |
| $\theta = 0$              |                                                                                                    |          |          |          |          |         |           |         |         |          |
| AV. $(\hat{X} - X)^2$ CL. | .104                                                                                               | .070     | .062     | .061     | .069     | .089    | .175      | .581    | .433    | .532     |
| STD. ERR.                 | .017                                                                                               | .003     | .002     | .002     | .002     | .008    | .068      | .290    | .144    | .233     |
| AV. $(\hat{X} - X)^2$ IN. | .050                                                                                               | .041     | .037     | .036     | .042     | .051    | .065      | .170    | .167    | .189     |
| STD. ERR.                 | .001                                                                                               | .001     | .001     | .001     | .001     | .001    | .001      | .003    | .003    | .003     |
| RATIO                     | 2.07                                                                                               | 1.71     | 1.70     | 1.69     | 1.64     | 1.75    | 2.69      | 3.43    | 2.59    | 3.14     |
| $\theta = .2$             |                                                                                                    |          |          |          |          |         |           |         |         |          |
| AV. $(\hat{X} - X)^2$ CL. | .0356                                                                                              | .0302    | .0283    | .0269    | .0292    | .0397   | .0688     | .647    | .655    | .651     |
| STD. ERR.                 | .0007                                                                                              | .0005    | .0005    | .0004    | .0005    | .0008   | .0016     | .010    | .010    | .010     |
| AV. $(\hat{X} - X)^2$ IN. | .0310                                                                                              | .0231    | .0217    | .0220    | .0237    | .0276   | .0381     | .321    | .326    | .323     |
| STD. ERR.                 | .0005                                                                                              | .0004    | .0003    | .0003    | .0003    | .0005   | .0009     | .005    | .005    | .005     |
| RATIO                     | 1.15                                                                                               | 1.31     | 1.31     | 1.22     | 1.23     | 1.44    | 1.81      | 2.02    | 2.01    | 2.01     |
| $\theta = .5$             |                                                                                                    |          |          |          |          |         |           |         |         |          |
| AV. $(\hat{X} - X)^2$ CL. | .0187                                                                                              | .0141    | .0159    | .0149    | .0140    | .0218   | .0614     | 1.315   | 1.317   | 1.323    |
| STD. ERR.                 | .0003                                                                                              | .0002    | .0002    | .0002    | .0002    | .0004   | .0008     | .008    | .008    | .009     |
| AV. $(\hat{X} - X)^2$ IN. | .0200                                                                                              | .0121    | .0137    | .0139    | .0131    | .0165   | .0423     | 1.017   | 1.019   | 1.024    |
| STD. ERR.                 | .0003                                                                                              | .0002    | .0002    | .0002    | .0002    | .0003   | .0006     | .007    | .007    | .007     |
| RATIO                     | .94                                                                                                | 1.16     | 1.16     | 1.07     | 1.07     | 1.32    | 1.45      | 1.29    | 1.29    | 1.29     |
| $\theta = 1$              |                                                                                                    |          |          |          |          |         |           |         |         |          |
| AV. $(\hat{X} - X)^2$ CL. | .0133                                                                                              | .0064    | .0112    | .0106    | .0064    | .0151   | .0728     | 2.113   | 2.116   | 2.120    |
| STD. ERR.                 | .0002                                                                                              | .0001    | .0001    | .0001    | .0001    | .0002   | .0006     | .007    | .007    | .007     |
| AV. $(\hat{X} - X)^2$ IN. | .0146                                                                                              | .0058    | .0103    | .0104    | .0064    | .0125   | .0616     | 1.918   | 1.920   | 1.924    |
| STD. ERR.                 | .0002                                                                                              | .0001    | .0001    | .0001    | .0001    | .0002   | .0005     | .007    | .007    | .007     |
| RATIO                     | .91                                                                                                | 1.10     | 1.08     | 1.01     | 1.00     | 1.21    | 1.18      | 1.10    | 1.10    | 1.10     |
| $\theta = 5$              |                                                                                                    |          |          |          |          |         |           |         |         |          |
| AV. $(\hat{X} - X)^2$ CL. | .0139                                                                                              | .0129    | .0108    | .0107    | .0013    | .0140   | .1124     | 3.748   | 3.749   | 3.750    |
| STD. ERR.                 | .0001                                                                                              | .0000    | .0000    | .0000    | .0000    | .0001   | .0002     | .003    | .003    | .003     |
| AV. $(\hat{X} - X)^2$ IN. | .0140                                                                                              | .0126    | .0108    | .0107    | .0013    | .0137   | .1112     | 3.725   | 3.726   | 3.727    |
| STD. ERR.                 | .0001                                                                                              | .0000    | .0000    | .0000    | .0000    | .0001   | .0002     | .003    | .003    | .003     |
| RATIO                     | .99                                                                                                | 1.03     | 1.00     | 1.00     | 1.00     | 1.02    | 1.01      | 1.01    | 1.01    | 1.01     |
| $\theta = 10$             |                                                                                                    |          |          |          |          |         |           |         |         |          |
| AV. $(\hat{X} - X)^2$ CL. | .0149                                                                                              | .0107    | .0116    | .0115    | .0108    | .0149   | .1226     | 4.106   | 4.107   | 4.108    |
| STD. ERR.                 | .0000                                                                                              | .0000    | .0000    | .0000    | .0000    | .0000   | .0001     | .002    | .002    | .002     |
| AV. $(\hat{X} - X)^2$ IN. | .0149                                                                                              | .0106    | .0115    | .0115    | .0109    | .0148   | .1222     | 4.100   | 4.100   | 4.100    |
| STD. ERR.                 | .0000                                                                                              | .0000    | .0000    | .0000    | .0000    | .0000   | .0001     | .002    | .002    | .002     |
| RATIO                     | 1.00                                                                                               | 1.01     | 1.00     | 1.00     | 1.00     | 1.00    | 1.00      | 1.00    | 1.00    | 1.00     |

Both *Method A* and *B* tend to improve (smaller average squared errors) for larger positive quadratic terms. At one point ( $X = 0$ ) and for some positive quadratic terms ( $.5 \leq \theta \leq 5$ ) the values for the average squared error of *Method A* become slightly lower than that of *Method B*. Thus, one cannot say that *Method B* is uniformly more robust, unless one eliminates the point  $X = 0$ . However, *Method B* still has, in general, a smaller average squared error. It should also be pointed out that unless one suspected a positive quadratic term one would not, using *Method A*, design away from the end points. *Method B*, however, appears to be robust to design and, therefore, one could protect against a quadratic term without sacrificing mean squared error.

It seems intuitively unreasonable that the methods should have decreasing average squared errors when the ignored quadratic term increases. However,

the positive quadratic term is in effect increasing the slope of the approximating line. From Table III we see that the squared error decreases with increasing slope. Evidently the increase in squared error due to the quadratic term is more than offset by the decrease caused by the increase in effective slope. If this is the case, then both methods should have an increasing average squared error when the effective slope is decreased. This can be checked by introducing a negative quadratic term. Table X gives the results of ignoring a negative quadratic term.

As was anticipated, the average squared error of both methods increased as the magnitude of the negative quadratic term increased. The average squared errors for *Method B* remained relatively small (no larger than .4 for  $0 \leq X \leq 1$ ) while the average squared errors for *Method A* became excessive (over 15)

TABLE X:  
*Comparison Between Classical and Inverse Methods of Calibration: The Effect of a Negative Quadratic Term*

|                           | $\alpha = 0 \quad \beta = .5 \quad \sigma = .1 \quad \text{Design: } 3(x = .15), \quad 3(x = .85)$ |          |          |          |          |         |           |         |         |          |
|---------------------------|----------------------------------------------------------------------------------------------------|----------|----------|----------|----------|---------|-----------|---------|---------|----------|
|                           | $X = 0$                                                                                            | $X = .2$ | $X = .4$ | $X = .6$ | $X = .8$ | $X = 1$ | $X = 1.2$ | $X = 2$ | $X = 5$ | $X = 10$ |
| $\theta = 0$              |                                                                                                    |          |          |          |          |         |           |         |         |          |
| AV. $(\hat{X} - X)^2$ CL. | .104                                                                                               | .070     | .062     | .061     | .069     | .089    | .175      | .582    | .433    | .532     |
| STD. ERR.                 | .017                                                                                               | .003     | .002     | .002     | .002     | .008    | .068      | .291    | .144    | .233     |
| AV. $(\hat{X} - X)^2$ IN. | .055                                                                                               | .041     | .037     | .036     | .042     | .051    | .065      | .170    | .167    | .169     |
| STD. ERR.                 | .001                                                                                               | .001     | .001     | .001     | .001     | .001    | .001      | .003    | .003    | .003     |
| RATIO                     | 2.07                                                                                               | 1.71     | 1.70     | 1.69     | 1.64     | 1.75    | 2.69      | 3.43    | 2.59    | 3.14     |
| $\theta = -.01$           |                                                                                                    |          |          |          |          |         |           |         |         |          |
| AV. $(\hat{X} - X)^2$ CL. | .206                                                                                               | .086     | .076     | .075     | .075     | .137    | .561      | 2.148   | 1.187   | 1.774    |
| STD. ERR.                 | .112                                                                                               | .014     | .012     | .013     | .003     | .052    | .448      | 1.854   | .896    | 1.478    |
| AV. $(\hat{X} - X)^2$ IN. | .052                                                                                               | .042     | .038     | .037     | .043     | .053    | .068      | .190    | .188    | .190     |
| STD. ERR.                 | .001                                                                                               | .001     | .001     | .001     | .001     | .001    | .001      | .003    | .003    | .003     |
| RATIO                     | 3.99                                                                                               | 2.04     | 2.01     | 2.04     | 1.73     | 2.61    | 8.22      | 11.29   | 6.33    | 9.37     |
| $\theta = -.05$           |                                                                                                    |          |          |          |          |         |           |         |         |          |
| AV. $(\hat{X} - X)^2$ CL. | .136                                                                                               | .098     | .083     | .080     | .096     | .111    | .161      | .405    | .371    | .403     |
| STD. ERR.                 | .008                                                                                               | .007     | .003     | .002     | .003     | .004    | .017      | .055    | .028    | .046     |
| AV. $(\hat{X} - X)^2$ IN. | .058                                                                                               | .048     | .043     | .042     | .049     | .062    | .085      | .326    | .323    | .323     |
| STD. ERR.                 | .001                                                                                               | .001     | .001     | .001     | .001     | .001    | .001      | .003    | .003    | .003     |
| RATIO                     | 2.36                                                                                               | 2.04     | 1.95     | 1.93     | 1.96     | 1.79    | 1.89      | 1.24    | 1.15    | 1.25     |
| $\theta = -.1$            |                                                                                                    |          |          |          |          |         |           |         |         |          |
| AV. $(\hat{X} - X)^2$ CL. | 2.46                                                                                               | 15.07    | 4.22     | .174     | .302     | .742    | .757      | 5.33    | 9.65    | 14.82    |
| STD. ERR.                 | 1.96                                                                                               | 14.73    | 4.00     | .034     | .082     | .549    | .489      | 4.17    | 8.71    | 13.44    |
| AV. $(\hat{X} - X)^2$ IN. | .067                                                                                               | .057     | .050     | .048     | .057     | .077    | .117      | .656    | .651    | .650     |
| STD. ERR.                 | .001                                                                                               | .001     | .001     | .001     | .001     | .001    | .001      | .004    | .004    | .004     |
| RATIO                     | 36.70                                                                                              | 266.9    | 84.37    | 3.63     | 5.26     | 9.66    | 6.47      | 8.13    | 14.81   | 22.80    |
| $\theta = -.2$            |                                                                                                    |          |          |          |          |         |           |         |         |          |
| AV. $(\hat{X} - X)^2$ CL. | 17.25                                                                                              | 4.06     | 8.04     | 10.03    | 9.68     | 6.76    | 10.33     | 6.49    | 15.44   | 5.99     |
| STD. ERR.                 | 7.42                                                                                               | 1.16     | 4.39     | 6.26     | 4.58     | 3.05    | 4.30      | 2.46    | 8.20    | 2.16     |
| AV. $(\hat{X} - X)^2$ IN. | .093                                                                                               | .079     | .069     | .062     | .079     | .126    | .242      | 2.166   | 2.156   | 2.147    |
| STD. ERR.                 | .002                                                                                               | .001     | .001     | .001     | .002     | .002    | .002      | .007    | .007    | .007     |
| RATIO                     | 186.1                                                                                              | 51.3     | 117.5    | 162.7    | 123.2    | 53.6    | 42.6      | 3.00    | 7.16    | 2.79     |
| $\theta = -.5$            |                                                                                                    |          |          |          |          |         |           |         |         |          |
| AV. $(\hat{X} - X)^2$ CL. | 257.1                                                                                              | 161.3    | 222.4    | 235.5    | 177.1    | 241.6   | 653.2     | 16678   | 16719   | 16152    |
| STD. ERR.                 | 29.9                                                                                               | 17.5     | 23.2     | 26.0     | 20.1     | 27.6    | 57.1      | 1166    | 1175    | 1122     |
| AV. $(\hat{X} - X)^2$ IN. | .330                                                                                               | .155     | .095     | .093     | .154     | .341    | .732      | 8.300   | 8.264   | 8.286    |
| STD. ERR.                 | .004                                                                                               | .006     | .009     | .005     | .003     | .009    | .012      | .240    | .234    | .237     |
| RATIO                     | 778                                                                                                | 1040     | 2337     | 2534     | 1153     | 708     | 892       | 2010    | 2023    | 1949     |

for  $\theta \leq -1$ . Therefore, except for very few points, where *Method A* had a very slightly smaller average squared error than *Method B*, one can conclude, for the misclassification problem, that the Inverse approach, *Method B*, has a smaller average squared error than the Classical approach, *Method A*.

### CONCLUSION

The Classical approach to the linear calibration problem is compared with the Inverse approach by Monte Carlo methods. Although a mathematical proof is not given the Monte Carlo results are such that one can safely conclude that the Inverse approach to the calibration problem has a uniformly smaller mean squared error than the Classical approach.

It is evident that this conclusion opens more questions than it settles. For example, how do these methods compare using other criteria such as expected absolute deviation or expected bias? The answer to this is presently being assembled by the author.

Since the usual method, the Classical approach, is clearly not optimal for the calibration problem then what is? This question is being investigated by the author and his colleagues but at the time of this writing no solution is available.

### ACKNOWLEDGMENT

The author would like to thank Dr. John Mandel for deriving the fact that the expected squared errors for both methods are functions of  $\beta/\sigma$ .

### REFERENCES

- BENNETT, C. A., AND FRANKLIN, N. L., 1954. *Statistical Analysis in Chemistry and the Chemical Industry*. John Wiley and Sons, New York, p. 231.
- BROWNLIE, K. A., 1960. *Statistical Theory and Methodology in Science and Engineering*. Second Edition. John Wiley and Sons, New York, pg. 346.
- EISENHART, C., 1939. The interpretation of certain regression methods and their use in biological and industrial research. *Ann. Math. Statist.* 10, 162.
- KRUTCHKOFF, R. G. AND THOMAS, D., 1967. The PURGE 2 subroutine for generating Pearson type pseudo-random variates. *Virginia Polytechnic Institute Statistical Research Report No. 20*.
- LINNING, F. J., AND MANDEL, J., 1964. Which measure of precision? *Analytic Chemistry* 36, 25A.
- MANDEL, J., 1958. A note on confidence intervals in regression problems. *Ann. Math. Statist.* 29, 903.
- MANDEL, J., AND LINNING, F. J., 1957. Study of accuracy in chemical analysis using linear calibration curves. *Analytic Chemistry*, 29, 743.
- OTT, L., 1966. Optimal designs for inverse estimation in regression analysis. Ph.D. Dissertation V.P.I.
- WILLIAMS, E. J., 1959. *Regression Analysis*. John Wiley and Sons, New York., p. 10.