Notes

Classical and Inverse Regression Methods of Calibration in Extrapolation

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In an earlier paper (Krutchkoff, 1967) the Inverse Method of calibration is compared to the Classical Method by a Monte Carlo technique and found to have a uniformly smaller average squared error in the range of the controlled variable. This note presents some results obtained when using these procedures for extrapolation. Situations are shown to exist in extrapolation in which the Classical Method is superior to the Inverse Method.

CALIBRATION

Consider the problem of calibrating an instrument, say a pressure gauge, when the gauge response is known to be a linear function of the pressure. To calibrate this gauge, one subjects it to two or more known pressures. Using these pressures and the corresponding gauge markings, the gauge is calibrated so that it may be used to determine a future unknown pressure by reading the calibrated marking.

Let us say that in the calibrating experiment we have obtained responses (gauge markings)

$$y_i = \alpha + \beta x_i + \epsilon_i \qquad i = 1, 2, 3, \cdots, N \tag{1}$$

to the controlled variables x_i (the pressures) where α and β are unknown parameters, and where the ϵ_i are independent identically distributed errors with zero means. The Classical method for using these data to estimate an unknown pressure, X, as a function of a gauge marking, Y, is given by

$$\hat{X}_{CL} = \frac{Y - a}{b} \tag{2}$$

where

$$b = \frac{\sum_{i=1}^{N} (x_i - \bar{x}) y_i}{\sum_{i=1}^{N} (x_i - \bar{x})^2} \tag{3}$$

and

$$a = \bar{y} - b\bar{x} \tag{4}$$

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and where

$$\bar{x} = \frac{1}{N}\sum_{i=1}^{N} x_i \quad \text{and} \quad \bar{y} = \frac{1}{N}\sum_{i=1}^{N} y_i \,.$$

The Inverse method for estimating the same unknown pressure from the same gauge marking is given by

$$\hat{X}_{IN} = c + dY \tag{5}$$

where

$$d = \frac{\sum_{i=1}^{N} (x_i - \bar{x})y_i}{\sum_{i=1}^{N} (y_i - \bar{y})^2} \tag{6}$$

and

$$c = \bar{x} - d\bar{y}. \tag{7}$$

Extrapolation

This article is not a plea for extrapolation, nor should it be used as a justification for extrapolation. However, sometimes one must extrapolate even though he would prefer not to. If this is the case, then which method should one use, the Classical or the Inverse Method of calibration?

This note is an extension of an earlier article (Krutchkoff, 1967), and to avoid repetition, should be considered in conjunction with it. In the original article the range of observation was taken (without loss in generality) to be zero to unity, results were also given for extra-polations at $X = 1.2$ and $X = 2$. Other results quoted there for $X = 5$ and $X = 10$ were incorrectly labeled and were merely independent repetitions of the $X = 2$ column. This author has extended the results of all ten tables to the points $X = 3, 4, 5, 6, 7, 8, 9, 10$. In all but three situations the Inverse Method gave a uniformly smaller average squared error than the Classical Method. In Table X, where there was an ignored quadratic

Table 1
(an extension of Table X of Krutchkoff, 1967)
Comparison Between Classical and Inverse Methods of Calibration: The Effect of a Negative Quadratic Term

	$\alpha = 0$ $\beta = .5$ $\sigma = .1$ Design: $3(x = .15)$, $3(x = .85)$							
	$X=3$	$X=4$	$X=5$	$X=6$	$X=7$	$X=8$	$X=9$	$X=10$
$\theta = -.05$								
AV. $(\hat{X} - X)^2$ CL.	1.141	2.383	5.338	10.96	21.15	37.89	63.63	101.4
STD. ERR.	.189	.162	.236	.18	.16	.10	.05	.1
AV. $(\hat{X} - X)^2$ IN.	2.201	3.269	7.298	14.26	25.32	41.98	65.74	98.41
STD. ERR.	.007	.014	.023	.03	.04	.04	.04	.05
RATIO	.950	.729	.732	.779	.835	.903	.968	1.03

TABLE 2
(an extension of Table V of Krutchkoff, 1967)
Comparison Between Classical and Inverse Methods of Calibration: Effect of the Number of Observations at each Design Point

$\alpha = 0 \quad \beta = .5 \quad \sigma = .1$	$X=3$	$X=4$	$X=5$	$X=6$	$X=7$	$X=8$	$X=9$	$X=10$
$5(x = 0)$								
$5(x = 1)$								
AV. $(\hat{X} - X)^2$ CL.	.163	.283	.432	.620	.850	1.11	1.43	1.76
STD. ERR.	.003.	.005	.008	.012	.016	.022	.028	.034
AV. $(\hat{X} - X)^2$ IN.	.170	.303	.469	.689	.945	1.24	1.60	1.99
STD. ERR.	.002	.003	.005	.007	.010	.013	.017	.021
RATIO	.957	.934	.921	.900	.899	.892	.895	.889
$10(x = 0)$								
$10(x = 1)$								
AV. $(\hat{X} - X)^2$ CL.	.100	.151	.226	.310	.422	.551	.681	.849
STD. ERR.	.002	.002	.004	.005	.007	.009	.011	.014
AV. $(\hat{X} - X)^2$ IN.	.154	.272	.427	.624	.860	1.12	1.44	1.79
STD. ERR.	.002	.003	.004	.006	.008	.010	.013	.016
RATIO	.647	.556	.529	.498	.490	.490	.472	.475

	$X=2$	$X=3$	$X=4$	$X=5$	$X=6$	$X=7$	$X=8$	$X=9$	$X=10$
$20(x = 0)$									
$20(x = 1)$									
AV. $(\hat{X} - X)^2$ CL.	.0522	.0685	.0962	.1313	.1724	.2279	.2865	.3619	.4378
STD. ERR.	.0007	.0010	.0015	.0020	.0027	.0035	.0043	.0056	.0067
AV. $(\hat{X} - X)^2$ IN.	.0742	.1496	.2624	.4143	.6046	.8369	1.101	1.396	1.747
STD. ERR.	.0009	.0014	.0023	.0033	.0046	.0060	.008	.010	.012
RATIO	.704	.458	.367	.317	.285	.272	.260	.259	.251
$50(x = 0)$									
$50(x = 1)$									
AV. $(\hat{X} - X)^2$ CL.	.0437	.0515	.0610	.0747	.0936	.1118	.1364	.1632	.1917
STD. ERR.	.0006	.0007	.0009	.0011	.0014	.0016	.0020	.0023	.0028
AV. $(\hat{X} - X)^2$ IN.	.0717	.1491	2603	.4162	.6056	.8348	1.089	1.408	1.745
STD. ERR.	.0008	.0014	.0020	.0027	.0030	.0047	.0058	.0073	.0087
RATIO	.610	.345	.234	.180	.155	.134	.125	.116	.110

term $\theta = -.05$, the Classical Method gave the smaller average squared error. Those results are given here in Table 1. The other situations in which the Classical Method gave the smaller average squared error were in Table V with five or more observations at each design point. These are reported in Table 2. These results indicate that as the number of observations taken at the design points increases, the Classical Method's average squared error decreases faster than does the average squared error for the Inverse Method. Thus, in extrapolation, if one can take a sufficient number of observations during calibration, he can be protected against the large average squared errors which occur for the smaller values of β. How many observations should be taken, of course, will depend on several things including the size of σ, the truncation value for b, and the minimum size of β for which one wants protection. From Table 2 we can conclude that five observations will be sufficient for $\sigma = .1$, trunction at .001 and β as low as .5.

Does taking more observations effect the results obtained within the range (i.e., $0 \leq X \leq 1$)? The values used in Tables I–X were rerun with fifty observations at each design point. The results were not significantly altered. The conclusions stated in the original article remained unchanged for X values in the calibration range.

Reference

Krutchkoff, R. G., "Classical and Inverse Regression Methods of Calibration." *Technometrics*, *9*, 425–439.

Reference

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