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Choice of Statistical Calibration Procedures When the Standard Measurement is Also Subject to Error†

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ABSTRACT

This paper considers a statistical calibration problem in which the standard as well as the nonstandard measurement is subject to error. Since the classical approach cannot handle this situation properly, a functional relationship model with additional feature of prediction is proposed. For the analysis of the problem four different approaches-two estimation techniques (ordinary and grouping least squares) combined with two prediction methods (classical and inverse prediction)-are considered. By Monte Carlo simulation the performance of each approach is assessed in terms of the probability of concentration. The simulation results indicate that the ordinary least squares with inverse prediction is generally preferred in interpolation while the grouping least squares with classical prediction turns out to be better in extrapolation.

1. Introduction

Statistical calibration is the most widely used technique for achieving compatibility between different measurement methods. Due to this popularity as well as its interesting statistical properties, the calibration problem has received a wide concern not only from statisticians but also from practictioners in many scientific fields.

The classical theory of calibration is based upon the assumption that the standard or reference measurement is always free from errors (e.g., see Williams, 1959). However, in virtually all situatuions one is likely to face the problem of uncertainties in the standard as well as in the nonstandard measurement due to internal and external sources of errors in the measuring processes. Thus from a realistic point of view the classical assumption

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needs to be relaxed, and more meaningful calibration procedures must be developed.

Any statistical calibration consists of the following two procedures. That is, in a calibration experiment the relationship between the standard(x) and nonstandard measurement(y) is determined yielding a calibration equation, and given y in the future the corresponding x is predicted using the calibration equation. In classical calibration, regression of y on x determines the calibration equation, which is then used in reverse to predict x for given y. This paper presents a functional relationship model which explicitly considers errors in both measurenents. For the estimation of the relationship ordinary and grouping least squares estimation techniques are considered, and for prediction the classical and inverse methods are examined. By Monte Carlo simulation the above approaches are compared in terms of the probability of concentration which is the probability that an estimator is within a specified distance from its true value.

2. A Predictive Functional Relationship Model

For a calibration experiment when both measurements are subject to error the following model is proposed.

$$\left.\begin{aligned} x_{ij}&=\xi_i+\delta_{ij}\\ y_{ij}&=\eta_i+\varepsilon_{ij}\end{aligned}\right\}\begin{matrix} i=1,2,\ldots,n\\ j=1,2,\ldots,m\end{matrix} \tag{1}$$

$$\eta_i=\alpha+\beta\xi_i \quad i=1,2,\ldots,n \tag{2}$$

where ξ_i and η_i respectively represent the unobservable, true standard and nonstandard measurements, and α and β are unknown constants. The random measurement errors δ_{ij} and ε_{ij} are assumed to be distributed as

$$\begin{pmatrix}\delta_{ij}\\ \varepsilon_{ij}\end{pmatrix}\sim BVN\left\{\begin{pmatrix}0\\0\end{pmatrix},\ \begin{bmatrix}\sigma_\delta^2 & 0\\ 0 & \sigma_\varepsilon^2\end{bmatrix}\right\} \tag{3}$$

where σ_δ and σ_ε are unknown. We further assume that error vectors are independent for all i and j.

By symmetry, the relationship (2) can be written in another form as follows.

$$\xi_i=\alpha'+\beta'\eta_i,\ i=1,2,\ldots,n \tag{4}$$

where $\alpha'=-\alpha/\beta$ and $\beta'=1/\beta$.

The model described in (1) and (2) or (1) and (4) is commonly called an errors-in-variables model(EVM) in the literature. The EVM is further classified into functional and structural model according as ξ (and hence η) is fixed and random, respectively

(Kendall and Stuart, 1973). In this paper ξ is assumed to be fixed.

Statistical problems in *EVM* have been investigated by many authors with their major concerns being the estimation of the unknown coefficients of the relationship. For instance, least squares or generalized least squares estimation was considered by Sprent(1966), Richardson and Wu(1970), Gleser(1981), Dahm and Fuller(1981) among others. Those who considered the maximum likelihood estimation include Villegas(1961), Dolby and Lipton(1972), Fuller(1980), Gallo(1982), Amemiya and Fuller(1984), Isogawa(1985), etc. For a survey of estimation methods for the *EVM* we refer the reader to Kendall and Stuart(1973), Madansky(1959), Moran(1971), or Anderson(1976).

Since least squares estimation is widely used in practice this paper considers the ordinary least squares(*OLS*) and the grouping least squares(*GRLS*) estimation methods. In passing, it is worth noting that analytic results are available for these types of estimation (e.g., see Richarson and Wu, 1970). Unfortunately, however, such analytic results cannot be directly applied to the present calibration problem since it involves one further step-prediction.

Before defining the *OLS* and *GRLS* estimators of the unknown parameters, we first define

$$S_{pq}=\sum_{i=1}^{n}\sum_{j=1}^{m}(p_{ij}-\bar{\bar{p}})(q_{ij}-\bar{\bar{q}})$$

$$S_{\bar{p}\bar{q}}=\sum_{i=1}^{n}(\bar{p}_i-\bar{\bar{p}})(\bar{q}_i-\bar{\bar{q}})$$

where $\bar{\bar{p}}$ and $\bar{\bar{q}}$ represent the grand means of all p_{ij} and q_{ij}, respectively. Similarly, $\bar{p}_i$ and $\bar{q}_i$ are respectively the i-th group means of p_{ij} and q_{ij}, $j=1, 2, \ldots, m$. Then, the *OLS* estimators of β, α, β', α' are respectively given by

$$b_{OLS}=S_{xy}/S_{xx} \tag{5}$$

$$a_{OLS}=\bar{y}-b_{OLS}\bar{x} \tag{6}$$

$$b'_{OLS}=S_{xy}/S_{yy} \tag{7}$$

$$a'_{OLS}=\bar{\bar{x}}-b'_{OLS}\bar{y} \tag{8}$$

Similaly, the *GRLS* estimators of β, α, β', and α' are given by

$$b_G=S_{\bar{x}\bar{y}}/S_{\bar{x}\bar{x}} \tag{9}$$

$$a_G=\bar{y}-b_G\bar{\bar{x}} \tag{10}$$

$$b'_G=S_{\bar{x}\bar{y}}/S_{\bar{y}\bar{y}} \tag{11}$$

$$a'_G=\bar{\bar{x}}-b'_G\bar{y} \tag{12}$$

In the future suppose a nonstandard measurement y_f is obtained for an unknown η_f.

That is,

$$y_f=\eta_f+\varepsilon_f \tag{13}$$

where

$$\varepsilon_f\sim N(0,\ \sigma_\varepsilon^2) \tag{14}$$

Then, based upon relationship (2), the corresponding ξ_f is estimated as

$$\hat{\xi}_{fc}=(y_f-a)/b \tag{15}$$

where a and b are either the *OLS* or *GRLS* estimators of α and β, respectively. If relationship (4) is used, ξ_f is predicted as

$$\hat{\xi}_{fI}=a'+b'y_f \tag{16}$$

where a' and b' respectively represent either the *OLS* or *GRLS* estimators of α' and β'. We will subsequently call $\hat{\xi}_{fc}$ and $\hat{\xi}_{fI}$ the classical and inverse predictor, respectively.

In this paper the following four approaches are compared by Monte Carlo simulation.

Approach 1: *OLS* Estimation and Classical Prediction

Approach 2: *OLS* Estimation and Inverse Prediction

Approach 3: *GRLS* Estimation and Classical Prediction

Approach 4: *GRLS* Estimation and Inverse Prediction

The performance of each approach is evaluated in terms of the probability of concentration which is defined by

$$PC(\xi_f, w)=Pr\{|\hat{\xi}_f-\xi_f|\leqq w\} \tag{17}$$

where $\hat{\xi}_f$ is an estimator of ξ_f obtained by one of the above four approaches, and w is a given positive constant. By Monte Carlo simulation PC is estimated by calculating the relative frequency that $|\hat{\xi}_f-\xi_f|\leqq w$ occurs.

3. Design of the Simulation Experiment

The layout of the simulation experiment is illustrated in Figure 1. Without loss of generality, the range of ξ in the calibration experiment is taken as $[0, 1]$. The values of other parameters included in the simulation are as follows.

$\alpha=0$ (equivalently, $\alpha'=0$)

$\beta=1$ (equivalently, $\beta'=1$)

$\sigma_\delta=0.001,\ 0.1$ (0.1% and 10% of the range of ξ)

$\sigma_\varepsilon/\sigma_\delta=0.1,\ 1,\ 10,\ 100$

$(n, m)=(2,6),\ (2,12),\ (6,2),\ (6,4)$

$$\xi_i=\begin{cases}0, 1 \text{ for } n=2\\ 0,\ 0.2,\ 0.4,\ 0.6,\ 0.8,\ 1.0 \text{ for } n=6\end{cases}$$

$$\xi_f=\begin{cases}0.6,\ 0.8,\ 1.0 \text{ for interpolation}\\ 2,\ 5,\ 10 \text{ for extrapolation}\end{cases}$$

In addition, the following w values were used.

$w=0.0001,\ 0.0003,\ 0.0005,\ 0.001$ for Runs 1~8

$w=0.001,\ 0.003,\ 0.005,\ 0.01$ for Runs 9~12

$w=0.01,\ 0.03,\ 0.05,\ 0.1$ for Runs 13~24

$w=0.1,\ 0.2,\ 0.3,\ 0.4$ for Runs 25~32

Different w values were used for better comparisons of the approaches by avoiding unnecessarily large or small PC values.

β	σ_δ	$\sigma_\varepsilon/\sigma_\delta$	$n=2$		6	
			$m=6$	12	2	4
1	0.001	0.1	1	2	3	4
		1	5	6	7	8
		10	9	10	11	12
		100	13	14	15	16
	0.1	0.1	17	18	19	20
		1	21	22	23	24
		10	25	26	27	28
		100	29	30	31	32

Figure 1. Layout of the Simulation Experiment (Cells contain the run numbers).

It may seem restrictive that the value of β was fixed to 1. However, it can be shown that many other cases are implicitly considered in the simulation study. That is, consider the transformation, $y_{ij}^*=cy_{ij}$. Then, the model described in Eqs. (1) and (2) can be rewritten as

$$x_{ij}=\xi_i+\delta_{ij}$$

$$y_{ij}^*=\eta_i^*+\varepsilon_{ij}^*$$

$$\eta_i^*=\alpha^*+\beta^*\xi_i$$

where $\eta_i^*=c\eta_i$, $\varepsilon_{ij}^*=c\varepsilon_{ij}$, $\alpha^*=c\alpha$, and $\beta^*=c\beta$. Thus, we can expect that the cases obtainable through the above transformation give essentially the same results. For instance,

the case where $\beta=10$, $\sigma_\delta=0.001$, and $\sigma_\varepsilon/\sigma_\delta=10$ can be obtained from Run 5 ($\beta=1$, $\sigma_\delta=0.001$, $\sigma_\varepsilon/\sigma_\delta=1$) with $c=10$.

For interpolation the only ξ_f values considered are 0.6, 0.8, 1.0 since *PC* values at ξ_f and $1-\xi_f$ must be the same theoretically due to the symmetry of ξ_i values.

The normal random deviates were generated by *IMSL* subroutine *GGNML* which generates the standard normal random deviates from *UNIFORM*(0, 1) by inverse transformation. Each simulation run involves 5,000 trials, and for all the four approaches *PC* values were calculated for all ξ_f and w. All the computation was done on a *IBM* 3031.

4. Discussion of the results

In case of interpolation (i.e., prediction is made at $\xi_f \in[0, 1]$), we observe the following.

i) For runs 1-12, all four approaches give very close *PC* values (refer to Table 1).

ii) For runs 17-20, *PC* values for Approaches 2, 3, and 4, are similar (refer to Table 2).

iii) For runs 13-16, 21, and 22, Approach 2 is slightly better than the others (refer to Table 3).

iv) For runs 25 and 26, *PC* values for Approach 2 are substantially higher than those of others (refer to Table 4).

v) For runs 23 and 24, Approach 2 is better at $\xi_f=0.6$, 0.8, while approach 4 is slightly preferred at $\xi_f=1$ (refer to Table 5).

vi) For runs 29 and 30, Approach 2 is better at $\xi_f=0.6$, 0.8, while Approach 3 and 4 give slightly larger *PC* values at $\xi_f=1$ (refer to Table 6).

vii) For runs 27, 28, 31, and 32, Approach 2 is better at $\xi_f=0.6$, and Approach 4 is preferred at $\xi_f=1$ (refer to Table 7).

The above results indicate that Approach 2 is preferred in most situations except the cases in v), vi), and vii) where Approach 2 perform better in the region close to the middle of the experimental range while Approach 4 is preferred otherwise. In general, predictions are made more frequently in the middle of the range, and therefore, the results in v), vi), and vii) do not necessarily indicate that Approach 2 is inferior to others. When the relative importance of ξ_f is known, some weighted *PC* values may be used to measure the overall performance. For instance, suppose the weight function for ξ_f is normal with mean 0.5 (center of the experimental region) and standard deviation 1/6 (i.e., 6 standard deviations covers the range of the experimental region). For each ξ_f

Table 1. *PC* Values for Run 1.

ξ_f	w	Approaches			
		1	2	3	4
0.6	0.0001	0.2450	0.2456	0.2456	0.2456
	0.0003	0.6666	0.6668	0.6668	0.6668
	0.0005	0.8888	0.8886	0.8886	0.8886
	0.001	0.9986	0.9986	0.9986	0.9986
0.8	0.0001	0.2266	0.2260	0.2260	0.2260
	0.0003	0.6056	0.6058	0.6058	0.6058
	0.0005	0.8456	0.8450	0.8450	0.8450
	0.001	0.9944	0.9944	0.9944	0.9944
1	0.0001	0.1742	0.1746	0.1746	0.1746
	0.0003	0.5166	0.5152	0.5152	0.5152
	0.0005	0.7592	0.7588	0.7588	0.7588
	0.001	0.9814	0.9812	0.9812	0.9812
2	0.0001	0.0800	0.0806	0.0806	0.0806
	0.0003	0.2466	0.2466	0.2468	0.2468
	0.0005	0.4090	0.4082	0.4082	0.4082
	0.001	0.7106	0.7100	0.7100	0.7100
5	0.0001	0.0286	0.0282	0.0284	0.0284
	0.0003	0.0892	0.0922	0.0924	0.0924
	0.0005	0.1482	0.1480	0.1480	0.1480
	0.001	0.2880	0.2882	0.2880	0.2880
10	0.0001	0.0116	0.0112	0.0110	0.0110
	0.0003	0.0416	0.0406	0.0406	0.0406
	0.0005	0.0704	0.0714	0.0714	0.0714
	0.001	0.1390	0.1396	0.1396	0.1396

Table 2. *PC* Values for Run 20.

ξ_f	w	Approaches			
		1	2	3	4
0.6	0.01	0.3014	0.3260	0.3266	0.3264
	0.03	0.7598	0.7956	0.7922	0.7964
	0.05	0.9450	0.9608	0.9598	0.9606
	0.1	0.9996	1.0000	0.9998	1.0000
0.8	0.01	0.1990	0.2624	0.2624	0.2600
	0.03	0.5546	0.6846	0.6864	0.6852
	0.05	0.8068	0.9072	0.8982	0.9070
	0.1	0.9942	0.9994	0.9990	0.9994
1	0.01	0.1328	0.2022	0.2010	0.1998
	0.03	0.3774	0.5640	0.5564	0.5660
	0.05	0.6068	0.8016	0.7976	0.8014
	0.1	0.9412	0.9900	0.9908	0.9898
2	0.01	0.0396	0.0890	0.0856	0.0890
	0.03	0.1226	0.2540	0.2462	0.2544
	0.05	0.2064	0.4144	0.3986	0.4132
	0.1	0.4206	0.7050	0.6982	0.7034
5	0.01	0.0146	0.0330	0.0316	0.0328
	0.03	0.0438	0.0900	0.0890	0.0912
	0.05	0.0688	0.1476	0.1522	0.1492
	0.1	0.1376	0.2964	0.2836	0.2942
10	0.01	0.0048	0.0152	0.0150	0.0112
	0.03	0.0184	0.0376	0.0430	0.0392
	0.05	0.0324	0.0678	0.0728	0.0678
	0.1	0.0664	0.1422	0.1404	0.1418

Table 3. *PC* Values for Run 15.

ξ_f	w	Approaches			
		1	2	3	4
0.6	0.01	0.0746	0.0770	0.0748	0.0746
	0.03	0.2234	0.2392	0.2234	0.2310
	0.05	0.3626	0.3830	0.3626	0.3732
	0.1	0.6596	0.6964	0.6596	0.6748
0.8	0.01	0.0798	0.0756	0.0796	0.0764
	0.03	0.2192	0.2268	0.2190	0.2238
	0.05	0.3592	0.3706	0.3594	0.3628
	0.1	0.6458	0.6732	0.6456	0.6584
1	0.01	0.0758	0.0742	0.0760	0.0694
	0.03	0.2088	0.2152	0.2088	0.2120
	0.05	0.3426	0.3464	0.3428	0.3482
	0.1	0.6226	0.6322	0.6226	0.6256
2	0.01	0.0506	0.0462	0.0498	0.0500
	0.03	0.1446	0.1236	0.1452	0.1406
	0.05	0.2418	0.2028	0.2412	0.2340
	0.1	0.4592	0.4062	0.4588	0.4544
5	0.01	0.0212	0.0134	0.0210	0.0202
	0.03	0.0622	0.0448	0.0620	0.0534
	0.05	0.1040	0.0772	0.1038	0.0966
	0.1	0.2030	0.1478	0.2028	0.1984
10	0.01	0.0104	0.0062	0.0094	0.0100
	0.03	0.0328	0.0190	0.0330	0.0300
	0.05	0.0558	0.0316	0.0560	0.0518
	0.1	0.1062	0.0658	0.1062	0.0986

Table 4. *PC* Values for Run 26.

ξ_f	w	Approaches			
		1	2	3	4
0.6	0.1	0.0756	0.3348	0.0760	0.0760
	0.2	0.1460	0.6198	0.1502	0.1502
	0.3	0.2176	0.7938	0.2248	0.2248
	0.4	0.2866	0.8956	0.2968	0.2968
0.8	0.1	0.0792	0.1756	0.0826	0.0826
	0.2	0.1528	0.3604	0.1568	0.1568
	0.3	0.2234	0.5952	0.2312	0.2312
	0.4	0.2932	0.7748	0.3016	0.3016
1	0.1	0.0772	0.0766	0.0826	0.0826
	0.2	0.1472	0.1730	0.1544	0.1544
	0.3	0.2206	0.2996	0.2256	0.2256
	0.4	0.2798	0.4780	0.2912	0.2912
2	0.1	0.0682	0.0004	0.0680	0.0680
	0.2	0.1306	0.0014	0.1370	0.1370
	0.3	0.1964	0.0028	0.2016	0.2016
	0.4	0.2062	0.0056	0.2634	0.2684
5	0.1	0.0366	0.0	0.0354	0.0354
	0.2	0.0820	0.0	0.0714	0.0714
	0.3	0.1212	0.0	0.1124	0.1124
	0.4	0.1602	0.0	0.1540	0.1540
10	0.1	0.0210	0.0	0.0220	0.0220
	0.2	0.0434	0.0	0.0446	0.0446
	0.3	0.0630	0.0	0.0664	0.0664
	0.4	0.0814	0.0	0.0820	0.0820

Table 5. *PC* Values for Run 24.

ξ_f	w	Approaches			
		1	2	3	4
0.6	0.01	0.0752	0.0868	0.0830	0.0828
	0.03	0.2180	0.2544	0.2302	0.2368
	0.05	0.3496	0.4008	0.3686	0.3790
	0.1	0.6344	0.7028	0.6614	0.6732
0.8	0.01	0.0646	0.0758	0.0722	0.0780
	0.03	0.1968	0.2338	0.2174	0.2258
	0.05	0.3234	0.3742	0.3510	0.3588
	0.1	0.6024	0.6656	0.6396	0.6488
1	0.01	0.0602	0.0734	0.0698	0.0742
	0.03	0.1842	0.2114	0.2088	0.2182
	0.05	0.3132	0.3518	0.3398	0.3522
	0.1	0.5774	0.6269	0.6298	0.6400
2	0.01	0.0406	0.0374	0.0508	0.0462
	0.03	0.1146	0.1184	0.1504	0.1468
	0.05	0.1880	0.1912	0.2406	0.2408
	0.1	0.3660	0.3780	0.4524	0.4552
5	0.01	0.0142	0.0150	0.0182	0.0188
	0.03	0.0464	0.0440	0.0554	0.0626
	0.05	0.0746	0.0750	0.0962	0.0986
	0.1	0.1368	0.1534	0.1936	0.2004
10	0.01	0.0074	0.0050	0.0086	0.0108
	0.03	0.0190	0.0192	0.0258	0.0306
	0.05	0.0314	0.0330	0.0464	0.0490
	0.1	0.0624	0.0714	0.0904	0.0962

Table 6. *PC* Values for Run 30.

ξ_f	w	Approaches			
		1	2	3	4
0.6	0.1	0.0250	0.4522	0.0236	0.0236
	0.2	0.0510	0.8516	0.0498	0.0498
	0.3	0.0758	0.9498	0.0758	0.0758
	0.4	0.1022	0.9800	0.1008	0.1008
0.8	0.1	0.0242	0.0384	0.0240	0.0240
	0.2	0.0472	0.1232	0.0510	0.0510
	0.3	0.0738	0.4916	0.0778	0.0778
	0.4	0.1006	0.8712	0.1040	0.1040
1	0.1	0.0222	0.0064	0.0212	0.0212
	0.2	0.0450	0.0184	0.0480	0.0480
	0.3	0.0700	0.0462	0.0748	0.0748
	0.4	0.0928	0.1350	0.0980	0.0980
2	0.1	0.0212	0.0	0.0208	0.0208
	0.2	0.0412	0.0	0.0426	0.0426
	0.3	0.0618	0.0	0.0634	0.0634
	0.4	0.0784	0.0	0.0820	0.0820
5	0.1	0.0074	0.0	0.0074	0.0074
	0.2	0.0118	0.0	0.0140	0.0140
	0.3	0.0204	0.0	0.0214	0.0214
	0.4	0.0278	0.0	0.0316	0.0316
10	0.1	0.0030	0.0	0.0036	0.0036
	0.2	0.0054	0.0	0.0068	0.0068
	0.3	0.0080	0.0	0.0092	0.0092
	0.4	0.0102	0.0	0.0110	0.0110

Table 7. *PC* Values for Run 28.

ξ_f	w	Approaches			
		1	2	3	4
0.6	0.1	0.0740	0.4702	0.0788	0.2244
	0.2	0.1492	0.8214	0.1558	0.4236
	0.3	0.2218	0.9416	0.2382	0.5738
	0.4	0.2898	0.9806	0.3108	0.6854
0.8	0.1	0.0694	0.0834	0.0770	0.1578
	0.2	0.1438	0.2530	0.1520	0.3076
	0.3	0.2080	0.5996	0.2264	0.4736
	0.4	0.2826	0.8826	0.2996	0.6150
1	0.1	0.0778	0.0164	0.0786	0.1168
	0.2	0.1454	0.0450	0.1512	0.2306
	0.3	0.2138	0.1284	0.2236	0.3576
	0.4	0.2796	0.3110	0.2914	0.4810
2	0.1	0.0570	0.0	0.0592	0.0294
	0.2	0.1144	0.0	0.1180	0.0618
	0.3	0.1648	0.0	0.1794	0.0974
	0.4	0.2212	0.0004	0.2336	0.1422
5	0.1	0.0292	0.0	0.0276	0.0058
	0.2	0.0548	0.0	0.0544	0.0140
	0.3	0.0826	0.0	0.0836	0.0190
	0.4	0.1122	0.0	0.1124	0.0238
10	0.1	0.0148	0.0	0.0102	0.0008
	0.2	0.0294	0.0	0.0248	0.0034
	0.3	0.0440	0.0	0.0368	0.0052
	0.4	0.0578	0.0	0.0510	0.0074

Table 8. Weighted *PC* Values for Run 28

w	Weighted *PC*			
	Approach 1	2	3	4
0.1	0.0731	0.3802	0.0784	0.2084
0.2	0.1480	0.6873	0.1549	0.3957
0.3	0.2187	0.8554	0.2354	0.5487
0.4	0.2881	0.9489	0.3081	0.6671

(=0, 0.2, 0.4, 0.6, 0.8, 1) the corresponding weight is given by the area under the nomal curve between $\xi_f-0.1$ and $\xi_f+0.1$. Applying these weights to *PC* values of run 28 yields the weighted *PC* values as shown in Table 8. We note that the weighted *PC* value of Approach 2 is higher than the others for each w.

Figure 2 summarizes the results for extrapolation. It appears that Approach 3 is generally preferred to others.

To study the design effect the following runs were compared.

Runs $(4k+1)$ and $(4k+3)$ for $k=0, 1, \ldots, 7$.

Runs $(4r+2)$ and $(4r+4)$ for $r=0, 1, \ldots, 7$.

β	σ_δ	$\sigma_\varepsilon/\sigma_\delta$	$n=2$		6	
			$m=6$	12	2	4
1	0.001	0.1	·	·	·	·
		1	·	·	·	·
		10	·	·	·	·
		100	1, 3, 4	1, 3, 4	1, 3, 4	1, 3, 4
	0.1	0.1	2, 3, 4	2, 3, 4	2, 3, 4	2, 3, 4
		1	3, 4	3, 4	3, 4	3, 4
		10	1, 3, 4	1, 3, 4	1, 3	1, 3
		100	1, 3, 4	1, 3, 4	1, 3	1, 3

Figure 2. Better Approaches in Extrapolation ('·' represents no marked difference in *PC* values).

For the first group, the total number of observations (N) are 12, and for the second, 24. For interpolation, when Approach 2 is used we observe the following.

i) Design with $n=2$ is better when k, $r=0$, 4, $k=1$, and $r=2$.

ii) When $r=3$, design with $n=2$ is better at $\xi_f=1$, while design with $n=6$ is preferred otherwise.

iii) When k, $r=5,6,7$, $k=2,3$, and $r=1$, design with $n=2$ is better at $\xi_f=0.8$, 1.0 while design with $n=6$ is preferred otherwise.

For extrapolation, using Approach 3, it is found that designs with $n=2$ are better than designs with $n=6$. One exception is that when $k=7$ design with $n=6$ is better at $\xi_f=2$ while design with $n=2$ is preferred otherwise.

The above results indicate that when both variables are subject to error designs with $n=2$ (extreme-point design) are not necessarily optimal.

5. Conclusions

A predictive functional relationship model is proposed for the calibration problem when both measurements are subject to error. Monte Carlo simulation results indicate that for interpolation the *OLS* estimation combined with inverse prediction (Approach 2) is generally preferred especially in the region close to the middle of the experimental range. For extrapolation the *GRLS* estimation with classical prediction (Approach 3) performs

better than others as a whole. It is also found that the classical extreme-point design is not necessarily optimal for the given problem. A fruitful area of future research may include analytic investigation of the behavior of the *PC* as a function of the parameters involved. Other estimation techniques (e.g., maximum likelihood or generalized least squares estimation) may be considered for comparisons with *OLS* and *GRLS* methods.

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