Metrika (2005) 61: 157–168
DOI 10.1007/s001840400329

Metrika

Optimal allocation of measurements in a linear calibration process

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Received October 2003

Abstract. A problem of allocation of measurements for a linear calibration process is considered in this article. It is assumed that a total of N measurements are made some of which may be measurements on two distinct standards, while the remaining measurements are on m different unknown specimens. We discuss allocation of the N measurements for the two standards and m unknown specimens based on A-optimality criterion, which is applied to asymptotic variances of maximum likelihood estimators for the true values of unknown specimens. It can be shown that the optimal allocation depends on the true values of unknown specimens. Hence, the user may resort to locally or Bayesian A-optimal measurement designs. Some practical solution is presented. Furthermore, the impact of prior on the allocation is also discussed.

Key words: Calibration model, A-optimality criterion, measurement design, Bayesian design.

1 Introduction

A measurement process is typically subject to errors which are generally classified as systematic, random and a combination of both. Random errors are defined to have a zero expected value and systematic errors are defined to be due to biases in the measurement process. It is very common that the instrument is considered to have a linear systematic error in which the measured value of an unknown specimen ("*unknown*" for short) is described by the model

$$y_i = \alpha + \beta\tau + \epsilon_i, \tag{1.1}$$

where α and β are parameters of the systematic error; τ represents the true value of the unknown being measured; and ϵ_i represents the random error.

Since "*standards*" have known true values, the errors associated with the measurement process are observed whenever a standard is measured. Therefore, the known standards are always used to estimate parameters of the errors.

The calibration problem for estimation procedure has been extensively studied. The main results can be found in Fuller (1987) and Brown (1993). Literature pertaining to calibration problems involving allocation of the measurements appears to begin with Pepper (1973). He discussed measurement designs for the process described by an additive model of the form $y_i = \tau + (b_i + \eta_i)$, where the quantity $(b_i + \eta_i)$ represents the random error. b_i's arise from a random walk process and η_i's are identical and independent normal random variables with common mean 0 and variance σ_η^2. Perng and Tong (1977) considered the linear calibration model of (1.1). They presented a sequential procedure, observing either standard or unknown at each time, for optimal allocation of measurements for interval estimation of one single unknown so that coverage probability is maximized. More recently, Liao, Taylor and Iyer (2000) discussed optimum balanced designs for the simple additive model $y_i = \tau + e_i$, where e_i's arise from a first order autoregressive process (AR(1)).

As in many practical situations, the linear calibration model of (1.1) is required to estimate the actual concentration of an analyte in a specimen for a given response in various measurement processes. One of the examples described in Hunter and Lamboy (1981) is given below.

Example 1.1. A chemist wants to establish a calibration line to use in measuring the amount of molybdenum in specimens sent to an analytical laboratory. Table 1.1 is the real data.

Figure 1.1. gives a plot of the known amount of molybdenum against the measured amount of molybdenum, which is quite linear on this scale.

We thus consider the linear calibration model of (1.1) with random errors being assumed to be identical and independent normal random variables with common mean 0 and variance σ^2. Note that the normality of the random errors is in practice a reasonable assumption. It is well known that variance of LSE (least square estimator) of slope parameter in the simple regression model is minimized by putting equal proportion of trials at the two end points of the design region. See Atkinson and Donev (1992). Therefore, for both practical and theoretical considerations, we focus on the optimal allocation of N measurements for two standards and m unknowns in this study. The following example of a practical situation provides a setting to motivate this study.

Table 1.1. The real data for the calibration process of the amount of molybdenum

The known amount of molybdenum	1.0	1.0	2.0	2.0	3.0	3.0	4.0	4.0	5.0	5.0
The measured amount of molybdenum	1.8	1.6	3.1	2.6	3.6	3.4	4.9	4.2	6.0	5.9
The known amount of molybdenum	6.0	6.0	7.0	7.0	8.0	8.0	9.0	9.0	10.0	10.0
The measured amount of molybdenum	6.8	6.9	8.2	7.3	8.8	8.5	9.5	9.5	10.6	10.6

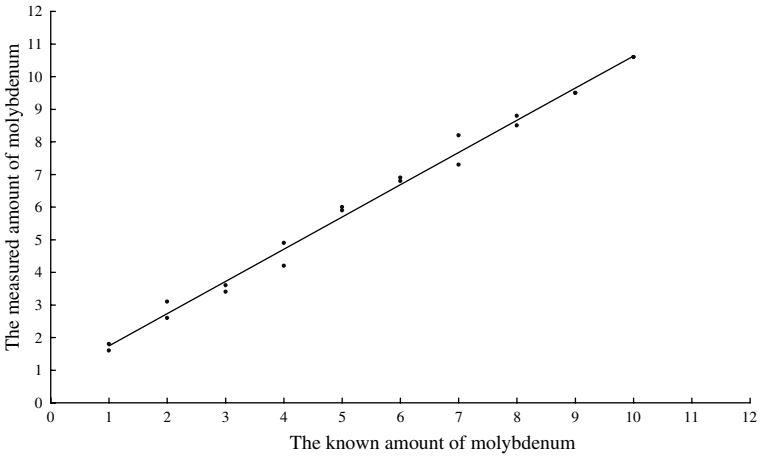

Fig. 1.1. The known amount of molybdenum versus the measured amount of molybdenum. The points represent the measured values, the solid line is the linear calibration model estimated by least square estimation

Example 1.2 A chemistry laboratory may be requested to analyze water samples from different sources. The small quantity of some toxic substance like cadmium in the water samples is highly concerned. Suppose for the used measurement instrument AAS (Atomic Absorption Spectroscopy), a chemist knows that the relationship between τ, the actual amount of a toxic substance (concentration of cadmium) present in water samples and y_i, the measured value (absorption) is given by the regression function described by equation (1.1). Typically, a set of standard solutions with predetermined concentrations can be prepared in order to estimate the parameters associated with the errors of measurement process. Before conducting the measurements, the chemist needs a "good" approach to allocating standards and unknown specimens from different sources within a fixed total number of measurements.

In the next section, we formulate the problem of interest. In Section 3, we present maximum likelihood estimation for the parameters in model (1.1). Section 4 provides some practical locally A-optimal measurement designs. Section 5 investigates Bayesian A-optimal measurement designs and the impact of prior on the designs.

2 The problem of interest

Let the number of measurements on two distinct standards S_0 and S_1 be denoted by a_0 and a_1, respectively, and the number of measurements on unknown U_j is denoted by n_j, for $j = 1, 2, \ldots, m$. Thus, the total number of measurements is $N = a_0 + a_1 + \sum_{j=1}^{m} n_j$. Moreover, let x_0 and x_1 be the known true values of standards S_0 and S_1, respectively, and τ_j denote the true value of unknown U_j, for $j = 1, 2, \ldots, m$. Define indicator functions $\delta_i^{S_k}$ and $\delta_i^{U_j}$ by

$$\delta_i^{S_k} = \begin{cases} 1 & \text{if } k \in \{0,1\} \text{ and observation } i \text{ is of standard } S_k, \\ 0 & \text{otherwise,} \end{cases}$$

and

$$\delta_i^{U_j} = \begin{cases} 1 & \text{if } j \in \{1,2,\ldots,m\} \text{ and observation } i \text{ is of unknown } U_j, \\ 0 & \text{otherwise.} \end{cases}$$

Then, model (1.1) can be rewritten as

$$y_i = \alpha + \beta(\delta_i^{S_0} x_0 + \delta_i^{S_1} x_1 + \sum_{j=1}^{m} \delta_i^{U_j} \tau_j) + \epsilon_i, \quad \text{for } i = 1,2,\ldots,N. \tag{2.1}$$

The random errors ϵ_i's are now assumed to be independent and identically distributed with $N(0,\sigma^2)$. This paper is concerned with obtaining optimal allocation of S_0, S_1, U_1, $U_2,\ldots,U_m$ such that τ_1, $\tau_2,\ldots,\tau_m$ can be estimated most efficiently. In particular, we consider A-optimality criterion according to which the average asymptotic variance of MLEs of τ_j's is minimized.

3 Maximum likelihood estimation

The log-likelihood function corresponding to the observed data of (2.1) is given by

$$l = -\frac{N}{2} log(2\pi) - \frac{N}{2} log(\sigma^2) - \frac{1}{2\sigma^2} \sum_{i=1}^{N} [y_i - \alpha - \beta(\delta_i^{S_0} x_0 + \delta_i^{S_1} x_1 + \sum_{j=1}^{m} \delta_i^{U_j} \tau_j)]^2, \tag{3.1}$$

from which the following likelihood estimators are derived.

$$\hat{\alpha} = \bar{y} - \hat{\beta}\bar{x}, \tag{3.2}$$

$$\hat{\beta} = \frac{\sum_{i=1}^{N} \delta_i^{S_0}(y_i - \bar{y})(x_0 - \bar{x}) + \sum_{i=1}^{N} \delta_i^{S_1}(y_i - \bar{y})(x_1 - \bar{x})}{a_0(x_0 - \bar{x})^2 + a_1(x_1 - \bar{x})^2}, \tag{3.3}$$

$$\hat{\tau}_j = \frac{\bar{y}_j - \hat{\alpha}}{\hat{\beta}}, \quad \text{for } j = 1,2,\ldots,m, \tag{3.4}$$

where $\bar{y} = \frac{1}{a_0+a_1}(\sum_{i=1}^{N} \delta_i^{S_0} y_i + \sum_{i=1}^{N} \delta_i^{S_1} y_i)$, $\bar{x} = \frac{a_0 x_0 + a_1 x_1}{a_0 + a_1}$ and $\bar{y}_j = \frac{1}{n_j} \sum_{i=1}^{N} \delta_i^{U_j} y_i$, for $j = 1,2,\ldots,m$.

Clearly, the MLE for τ_j given in (3.4) is the well known classical estimator computed from $\hat{\alpha}$ of (3.2) and $\hat{\beta}$ of (3.3), which only depend on the observed data of S_0 and S_1.

Computing the second derivatives of log-likelihood function (3.1) with respect to parameters α, β, τ_1, $\tau_2,\ldots,\tau_m$, σ^2 and taking expectation, we can obtain the Fisher information matrix. By using the standard properties of partitioned matrices (Graybill, 1983), we then invert the Fisher information to obtain the asymptotic covariance matrix of MLEs for τ_j's, which are of primary interest, as follows.

$$Var(\hat{\boldsymbol{\tau}}) = \{v_{jk}\},\ j = 1, 2, \ldots, m;\ k = 1, 2, \ldots, m,$$

where $\hat{\boldsymbol{\tau}} = [\hat{\tau}_1, \hat{\tau}_2, \ldots, \hat{\tau}_m]'$ and

$$v_{jk} = \begin{cases} \frac{\sigma^2}{\beta^2}\left[\frac{1}{n_j} + \frac{a_0(x_0-\tau_j)^2 + a_1(x_1-\tau_j)^2}{a_0 a_1 (x_0-x_1)^2}\right] & \text{if } j = k, \\ \frac{\sigma^2}{\beta^2}\left[\frac{a_0(x_0-\tau_j)(x_0-\tau_k) + a_1(x_1-\tau_j)(x_1-\tau_k)}{a_0 a_1 (x_0-x_1)^2}\right] & \text{if } j \neq k. \end{cases} \tag{3.5}$$

The details of the derivation are given in Appendix.

4 Locally A-optimal measurement design

It is easy to see that an explicit expression for the trace of covariance matrix $Var(\hat{\boldsymbol{\tau}})$ is given by

$$Trace[Var(\hat{\boldsymbol{\tau}})] = \frac{\sigma^2}{\beta^2}\left[\sum_{j=1}^{m}\frac{1}{n_j} + \frac{1}{a_1}\sum_{j=1}^{m}\frac{(x_0-\tau_j)^2}{(x_0-x_1)^2} + \frac{1}{a_0}\sum_{j=1}^{m}\frac{(x_1-\tau_j)^2}{(x_0-x_1)^2}\right].$$

Let $\theta_0 = \sum_{j=1}^{m}\frac{(x_0-\tau_j)^2}{(x_0-x_1)^2}$ and $\theta_1 = \sum_{j=1}^{m}\frac{(x_1-\tau_j)^2}{(x_0-x_1)^2}$. Also let $b_0 = a_0/N$, $b_1 = a_1/N$ and $r_j = n_j/N$, for $j = 1, 2, \ldots, m$. To obtain A-optimal measurement designs for estimating τ_j's, we need to minimize the following objective function

$$f(b_0, b_1, r_1, r_2, \ldots, r_m, \theta_0, \theta_1) = \frac{\theta_1}{b_0} + \frac{\theta_0}{b_1} + \sum_{j=1}^{m}\frac{1}{r_j}, \tag{4.1}$$

subject to the constraint

$$b_0 + b_1 + \sum_{j=1}^{m} r_j = 1. \tag{4.2}$$

For given values of θ_0 and θ_1, by using a Lagrange multiplier, we have the following optimal allocation of measurements for the standards and unknowns

$$b_0^* = \frac{\sqrt{\theta_1}}{\sqrt{\theta_0} + \sqrt{\theta_1} + m},$$
$$b_1^* = \frac{\sqrt{\theta_0}}{\sqrt{\theta_0} + \sqrt{\theta_1} + m}$$

and

$$r_j^* = \frac{1}{\sqrt{\theta_0} + \sqrt{\theta_1} + m}, \quad \text{for } j = 1, 2, \ldots, m.$$

Clearly, the values of b_0^*, b_1^*, r_1^*, $r_2^*, \ldots, r_m^*$ depend on parameters $\tau_1, \tau_2, \ldots, \tau_m$. Hence, the problem of allocation cannot be solved unless one has prior information on these parameters. We first consider the following strategy so as to obtain a locally A-optimal measurement design. In practice, according to knowledge of the user, it may be possible to designate standards S_0 and S_1 such that the range $[x_0, x_1]$ is large enough to cover the true values of unknowns. Then a very natural estimate for τ_j is the average of x_0 and x_1, i.e. letting

Table 4.1. The locally A-optimal measurement designs for $\tau_j = (x_0 + x_1)/2$, for $j = 1, 2, \ldots, m$; and $1 \leq m \leq 5$

m	b^*	r_j^*
1	0.250	0.500
2	0.207	0.293
3	0.183	0.211
4	0.167	0.167
5	0.155	0.138

$$\tau_j = \frac{x_0 + x_1}{2}, \quad \text{for } j = 1, 2, \ldots, m. \tag{4.3}$$

Substituting the values of (4.3) in θ_0 and θ_1, we have $\theta_0 = \theta_1 = m/4$. Thus, for fixed m, the values of b_0^*, b_1^* and r_j^* can be determined. Table 4.1 displays some locally A-optimal measurement designs based on this strategy. Note that we use b^* to denote both b_0^* and b_1^* in the table since their values are equal.

To evaluate how good the locally A-optimal designs of Table 4.1 are in estimating the true values of unknowns, the following simulation study is carried out. In the simulation study, we consider the two cases that $m = 1$ and $m = 2$. The values of parameters are set as follows. $x_0 = 0$, $x_1 = 1$, $\alpha = 0.2$, $\beta = 0.4$ and $\sigma = 0.1$; $N = 20, 40, 60, 80, 100$; for the case that $m = 1$, τ_1 ranges from 0.1 to 1.5 in steps of 0.2; for the case that $m = 2$, the pair of values (τ_1, τ_2) range from 0.25 to 1.5 in steps of 0.2. Since the classical estimator of τ_j does not have a finite expectation or a finite variance, the median and interquartile range (IQR) of the estimated τ_j's are reported from 5000 simulated data sets for each given parameter combination. Table 4.2 displays the simulation results for the case that $m = 1$.

It has shown that the locally A-optimal measurement design performs very satisfactory accuracy in estimation, based on the reported medians, for all the cases considered even the value of τ_1 occurs outside the range $[x_0, x_1]$. But it may only perform great precision in estimation, based on the reported IQRs, for the large sample size cases with $N \geq 40$. Notice that the minimum

Table 4.2. Simulation results for the case that $m = 1$

τ_1		$N = 20$	$N = 40$	$N = 60$	$N = 80$	$N = 100$
0.1	Median	0.1002	0.1014	0.0991	0.1004	0.1002
	IQR	0.1720	0.1262	0.1003	0.0868	0.0775
0.3	Median	0.3002	0.2996	0.2991	0.3011	0.3002
	IQR	0.1586	0.1082	0.0896	0.0778	0.0716
0.5	Median	0.4995	0.5000	0.4987	0.5006	0.5016
	IQR	0.1517	0.1080	0.0869	0.0759	0.0673
0.7	Median	0.7003	0.7010	0.6985	0.6994	0.7003
	IQR	0.1578	0.1132	0.0931	0.0796	0.0711
0.9	Median	0.9019	0.8965	0.8991	0.9011	0.8990
	IQR	0.1747	0.1226	0.1007	0.0881	0.0779
1.1	Median	1.1023	1.0981	1.1036	1.1027	1.0998
	IQR	0.1954	0.1392	0.1173	0.0989	0.0896
1.3	Median	1.3019	1.3023	1.3004	1.3001	1.3005
	IQR	0.2325	0.1663	0.1320	0.1142	0.1037
1.5	Median	1.5024	1.4972	1.4979	1.4993	1.5016
	IQR	0.2697	0.1824	0.1484	0.1281	0.1202

Table 4.3. Simulation results for the case that $m = 2$

			$N = 20$		$N = 40$		$N = 60$		$N = 80$		$N = 100$	
τ_1	τ_2		$\hat{\tau}_1$	$\hat{\tau}_2$	$\hat{\tau}_1$	$\hat{\tau}_2$	$\hat{\tau}_1$	$\hat{\tau}_2$	$\hat{\tau}_1$	$\hat{\tau}_2$	$\hat{\tau}_1$	$\hat{\tau}_2$
0.25	0.25	Median	0.2502	0.2461	0.2494	0.2519	0.2511	0.2531	0.2500	0.2498	0.2496	0.2494
		IQR	0.1893	0.1956	0.1312	0.1326	0.1103	0.1129	0.0969	0.0954	0.0845	0.0886
	0.50	Median	0.2509	0.5002	0.2519	0.4984	0.2513	0.4999	0.2497	0.4996	0.2522	0.5005
		IQR	0.1954	0.1814	0.1359	0.1287	0.1101	0.1024	0.0953	0.0883	0.0865	0.0797
	0.75	Median	0.2514	0.7502	0.2476	0.7469	0.2512	0.7513	0.2512	0.7495	0.2535	0.7510
		IQR	0.1943	0.1949	0.1353	0.1381	0.1101	0.1115	0.0996	0.0978	0.0863	0.0861
	1.00	Median	0.2517	1.0036	0.2480	0.9980	0.2521	0.9964	0.2485	0.9998	0.2504	1.0016
		IQR	0.1961	0.2217	0.1350	0.1536	0.1102	0.1254	0.0959	0.1069	0.0854	0.0982
	1.25	Median	0.2478	1.2428	0.2495	1.2526	0.2505	1.2557	0.2502	1.2482	0.2494	1.2521
		IQR	0.1946	0.2539	0.1388	0.1811	0.1084	0.1472	0.0954	0.1227	0.0874	0.1120
	1.50	Median	0.2464	1.5019	0.2498	1.4993	0.2510	1.4989	0.2493	1.5002	0.2478	1.4990
		IQR	0.1918	0.3046	0.1388	0.2165	0.1113	0.1732	0.0926	0.1476	0.0873	0.1321
0.50	0.50	Median	0.5004	0.5013	0.5002	0.4996	0.5019	0.5050	0.5004	0.5003	0.4996	0.5008
		IQR	0.1873	0.1854	0.1313	0.1314	0.1032	0.1064	0.0904	0.0914	0.0827	0.0815
	0.75	Median	0.4980	0.7475	0.4982	0.7508	0.4997	0.7510	0.4998	0.7499	0.4995	0.7515
		IQR	0.1879	0.1896	0.1281	0.1347	0.1045	0.1125	0.0943	0.0951	0.0810	0.0851
	1.00	Median	0.4988	0.9972	0.5010	1.0000	0.5000	0.9995	0.4995	1.0000	0.5011	1.0009
		IQR	0.1848	0.2136	0.1310	0.1578	0.1044	0.1273	0.0924	0.1095	0.0807	0.0965
	1.25	Median	0.5003	1.2552	0.5021	1.2461	0.4995	1.2483	0.5002	1.2527	0.4994	1.2528
		IQR	0.1838	0.2524	0.1293	0.1841	0.1043	0.1475	0.0889	0.1263	0.0818	0.1168
	1.50	Median	0.5015	1.5006	0.4983	1.4979	0.4998	1.4989	0.5000	1.5001	0.4998	1.4997
		IQR	0.1813	0.3018	0.1284	0.2207	0.1073	0.1778	0.0892	0.1508	0.0802	0.1366
0.75	0.75	Median	0.7516	0.7509	0.7481	0.7513	0.7479	0.7501	0.7483	0.7498	0.7482	0.7483
		IQR	0.1995	0.1974	0.1368	0.1333	0.1101	0.1086	0.0971	0.0940	0.0842	0.0846
	1.00	Median	0.7513	0.9958	0.7515	1.0018	0.7529	1.0034	0.7525	1.0030	0.7509	1.0017
		IQR	0.1935	0.2191	0.1364	0.1515	0.1124	0.1272	0.0992	0.1112	0.0867	0.0970
	1.25	Median	0.7476	1.2492	0.7490	1.2501	0.7510	1.2487	0.7497	1.2516	0.7499	1.2490
		IQR	0.1931	0.2613	0.1373	0.1805	0.1122	0.1473	0.0933	0.1272	0.0860	0.1128

Table 4.3 (contd.)

			$N = 20$		$N = 40$		$N = 60$		$N = 80$		$N = 100$	
τ_1	τ_2		$\hat{\tau}_1$	$\hat{\tau}_2$	$\hat{\tau}_1$	$\hat{\tau}_2$	$\hat{\tau}_1$	$\hat{\tau}_2$	$\hat{\tau}_1$	$\hat{\tau}_2$	$\hat{\tau}_1$	$\hat{\tau}_2$
	1.50	Median	0.7521	1.4990	0.7487	1.5010	0.7481	1.4970	0.7498	1.5030	0.7506	1.5016
		IQR	0.1878	0.3004	0.1341	0.2132	0.1108	0.1726	0.0956	0.1498	0.0872	0.1337
1.00	1.00	Median	0.9986	1.0001	1.0001	1.0025	1.0016	1.0018	1.0007	0.9997	1.0007	1.0039
		IQR	0.2180	0.2271	0.1571	0.1551	0.1243	0.1242	0.1113	0.1085	0.0979	0.0960
	1.25	Median	1.0034	1.2518	1.0017	1.2490	0.9987	1.2495	1.0017	1.2511	1.0010	1.2506
		IQR	0.2251	0.2527	0.1548	0.1790	0.1260	0.1469	0.1073	0.1267	0.0974	0.1113
	1.50	Median	0.9986	1.4986	1.0015	1.5011	0.9998	1.4986	0.9991	1.4985	0.9984	1.4989
		IQR	0.2193	0.3145	0.1522	0.2132	0.1273	0.1744	0.1094	0.1462	0.0955	0.1338
1.25	1.25	Median	1.2500	1.2491	1.2524	1.2537	1.2499	1.2509	1.2529	1.2524	1.2484	1.2525
		IQR	0.2654	0.2631	0.1789	0.1810	0.1458	0.1472	0.1294	0.1289	0.1121	0.1109
	1.50	Median	1.2483	1.4978	1.2489	1.4993	1.2514	1.5022	1.2517	1.5039	1.2503	1.5015
		IQR	0.2578	0.3041	0.1925	0.2146	0.1504	0.1705	0.1302	0.1496	0.1123	0.1357
1.50	1.50	Median	1.4935	1.4946	1.4959	1.4943	1.4989	1.4995	1.4982	1.5004	1.4991	1.4995
		IQR	0.2908	0.2974	0.2147	0.2140	0.1709	0.1717	0.1440	0.1484	0.1336	0.1368

IQR occurs at $\tau_1 = 0.5$ for any N, this is because that the used design is the locally A-optimal design for $\tau_1 = 0.5$. However, for any given N, the design proposed is likely to be robust to the value of τ_1 provided it is not much larger than x_1. Therefore, when there is no prior information available on the true value of unknown, the design proposed can be a practical choice. Similar results can be found for the case that $m = 2$ in Table 4.3.

5. Bayesian A-optimal measurement design

It is well known that optimal designs for non-linear models like model (2.1) depend on the values of unknown parameters. In this section, instead of locally A-optimal designs, a prior for $\tau_1, \tau_2, \ldots, \tau_m$ will be incorporated into the objective function of (4.1) to yield Bayesian A-optimal designs. We refer Atkinson and Donev (1992) for a general theory regarding the Bayesian design.

It is assumed that τ_j's are uncorrelated random variables with common and known mean x_τ and variance s_τ^2. Notice that only the first and second moments of τ_j's are required, there is no specified distribution. Then the objective function for the allocation obtained from taking expectation of (4.1) over this prior is given by

$$E_{\theta_0,\theta_1}[f(b_0, b_1, r_1, r_2, \ldots, r_m, \theta_0, \theta_1)] = \frac{m[(x_1 - x_\tau)^2 + s_\tau^2]}{b_0(x_0 - x_1)^2} + \frac{m[(x_0 - x_\tau)^2 + s_\tau^2]}{b_1(x_0 - x_1)^2} + \sum_{j=1}^{m} \frac{1}{r_j}.$$

Similarly, under the constraint of (4.2), we have the following optimal allocation of measurements for the standards and unknowns

$$b_0^* = \frac{1}{\sqrt{\frac{(x_0-x_\tau)^2+s_\tau^2}{(x_1-x_\tau)^2+s_\tau^2}} + \sqrt{\frac{m(x_0-x_1)^2}{(x_1-x_\tau)^2+s_\tau^2}} + 1},$$

$$b_1^* = \frac{1}{\sqrt{\frac{(x_1-x_\tau)^2+s_\tau^2}{(x_0-x_\tau)^2+s_\tau^2}} + \sqrt{\frac{m(x_0-x_1)^2}{(x_0-x_\tau)^2+s_\tau^2}} + 1}$$

and

$$r_j^* = \frac{1}{\sqrt{\frac{m[(x_0-x_\tau)^2+s_\tau^2]}{(x_0-x_1)^2}} + \sqrt{\frac{m[(x_1-x_\tau)^2+s_\tau^2]}{(x_0-x_1)^2}} + m}, \quad \text{for } j = 1, 2, \ldots, m.$$

To investigate how the prior affects the allocation, we calculate b_0^*, b_1^* and r_j^* for some given values of x_τ and s_τ. Without loss of generality, let $x_0 = 0$ and $x_1 = 1$. The results are displayed in Table 5.1.

It is of interest to see that the allocation of standards S_0 and S_1 is highly related to x_τ. For a fixed s_τ, the value of b_0^* (b_1^*) increases as the distance between x_τ and x_0 (x_1) decreases. This is fairly reasonable because the user would like to give more weight to the standard whose value may be closer to

Table 5.1. Bayesian A-optimal measurement designs for x_τ being from 0.1 to 1.7 in steps of 0.2; s_τ from 0.1 to 0.5 in steps of 0.2; and $1 \leq m \leq 3$

x_τ	s_τ	m	b_0^*	b_1^*	r_j^*	x_τ	s_τ	b_0^*	b_1^*	r_j^*	x_τ	s_τ	b_0^*	b_1^*	r_j^*
0.1	0.1	1	0.442	0.069	0.489	0.3	0.1	0.349	0.156	0.494	0.5	0.1	0.252	0.252	0.495
		2	0.368	0.057	0.287			0.290	0.130	0.290			0.209	0.209	0.291
		3	0.326	0.051	0.208			0.257	0.115	0.210			0.185	0.185	0.210
	0.3	1	0.419	0.140	0.442		0.3	0.348	0.194	0.457		0.3	0.269	0.269	0.462
		2	0.354	0.118	0.264			0.293	0.163	0.272			0.226	0.226	0.274
		3	0.317	0.106	0.193			0.261	0.145	0.198			0.201	0.201	0.199
	0.5	1	0.405	0.201	0.394		0.5	0.352	0.239	0.409		0.5	0.293	0.293	0.414
		2	0.349	0.173	0.239			0.301	0.204	0.247			0.250	0.250	0.250
		3	0.315	0.156	0.176			0.271	0.184	0.182			0.225	0.225	0.184
0.7	0.1	1	0.156	0.349	0.494	0.9	0.1	0.069	0.442	0.489	1.1	0.1	0.063	0.492	0.445
		2	0.130	0.290	0.290			0.057	0.368	0.287			0.053	0.415	0.266
		3	0.115	0.257	0.210			0.051	0.326	0.208			0.047	0.371	0.194
	0.3	1	0.194	0.348	0.457		0.3	0.140	0.419	0.442		0.3	0.129	0.464	0.407
		2	0.163	0.293	0.272			0.118	0.354	0.264			0.110	0.397	0.246
		3	0.145	0.261	0.198			0.106	0.317	0.193			0.099	0.358	0.181
	0.5	1	0.239	0.352	0.409		0.5	0.201	0.405	0.394		0.5	0.188	0.445	0.368
		2	0.204	0.301	0.247			0.173	0.349	0.239			0.163	0.386	0.226
		3	0.184	0.271	0.182			0.156	0.315	0.176			0.148	0.350	0.167
1.3	0.1	1	0.121	0.498	0.382	1.5	0.1	0.169	0.499	0.332	1.7	0.1	0.207	0.499	0.293
		2	0.104	0.430	0.233			0.149	0.439	0.206			0.185	0.445	0.185
		3	0.094	0.389	0.172			0.136	0.401	0.154			0.171	0.411	0.139
	0.3	1	0.154	0.484	0.363		0.3	0.187	0.491	0.321		0.3	0.218	0.495	0.287
		2	0.134	0.421	0.223			0.165	0.434	0.200			0.195	0.442	0.181
		3	0.122	0.382	0.165			0.152	0.398	0.150			0.180	0.409	0.137
	0.5	1	0.196	0.468	0.336		0.5	0.215	0.481	0.304		0.5	0.237	0.488	0.275
		2	0.172	0.411	0.209			0.191	0.427	0.191			0.213	0.438	0.175
		3	0.157	0.376	0.156			0.176	0.393	0.144			0.197	0.406	0.132

the true values of unknowns. Another interesting result is that the value of r_j^* decreases as s_τ increases. This implies that when the variation of unknowns gets large, the precision in estimation of systematic errors can become more desirable.

6. Concluding remarks

The results discussed in Sections 4 and 5 can be easily extended to the case that a cost constraint is considered in the measurement process. Suppose that each measurement of standards S_0 and S_1 cost c_0 and c_1 dollars, respectively, and each measurement of any unknowns costs c dollars. Moreover, the total cost is assumed to be budgeted within B dollars. The problem thus turns out to be in determination of a_0, a_1 and n_j, for $j = 1, 2, \ldots, m$, such that the objective function

$$f(a_0, a_1, n_1, n_2, \ldots, n_m, \theta_0, \theta_1) = \frac{\theta_1}{a_0} + \frac{\theta_0}{a_1} + \sum_{j=1}^{m} \frac{1}{n_j},$$

is minimized subject to the constraint

$$c_0 a_0 + c_1 a_1 + c \sum_{j=1}^{m} n_j \leq B.$$

Similarly, we can obtain the following optimal allocation for the budget being exactly equal to B dollars.

$$a_0^* = \frac{B\sqrt{\theta_1}}{\sqrt{c_0}(\sqrt{c_1\theta_0} + \sqrt{c_0\theta_1} + m\sqrt{c})},$$

$$a_1^* = \frac{B\sqrt{\theta_0}}{\sqrt{c_1}(\sqrt{c_1\theta_0} + \sqrt{c_0\theta_1} + m\sqrt{c})}$$

and

$$n_j^* = \frac{B}{\sqrt{c}(\sqrt{c_1\theta_0} + \sqrt{c_0\theta_1} + m\sqrt{c})}, \quad \text{for } j = 1, 2, \ldots, m.$$

In practice, a_0, a_1 and n_j can be taken to be the largest integers less than or equal to a_0^*, a_1^* and n_j^*, respectively. Obviously, the optimal allocation still depends on τ_1, $\tau_2, \ldots, \tau_m$. Therefore, the user still needs to use locally or Bayesian A-optimal measurements designs.

In this paper, we investigate construction of A-optimal measurement designs under the assumption that measurement errors are independent and have a homogenous variance in the linear calibration process. It is not uncommon to encounter situations where the measurements are serially correlated (Liao et al. 2000) or the variance of the measurement depends on its true value (Rocke and Lorenzato 1995). Certainly, the optimal allocation problem for the linear calibration process involving heterogeneous variances or correlated errors can become more complicated. We are currently investigating this interesting issue.

Appendix

The derivation of Equations (3.2), (3.3), (3.4) and (3.5)

After differentiating the log-likelihood of (3.1) with respect to α, β and τ_j, for $j = 1, 2, \ldots, m$, we have the following.

$$\sum_{i=1}^{N} y_i - N\hat{\alpha} - \left(a_0 x_0 + a_1 x_1 + \sum_{j=1}^{m} n_j \hat{\tau}_j\right)\hat{\beta} = 0, \tag{A.1}$$

$$\left(x_0 \sum_{i=1}^{N} \delta_i^{S_0} y_i + x_1 \sum_{i=1}^{N} \delta_i^{S_1} y_i + \sum_{j=1}^{m} n_j \bar{y}_j \hat{\tau}_j\right) - \left(a_0 x_0 + a_1 x_1 + \sum_{j=1}^{m} n_j \hat{\tau}_j\right)\hat{\alpha}$$
$$- \left(a_0 x_0^2 + a_1 x_1^2 + \sum_{j=1}^{m} n_j \hat{\tau}_j^2\right)\hat{\beta} = 0, \tag{A.2}$$

$$n_j\bar{y}_j - n_j\hat{\alpha} - n_j\hat{\tau}_j\hat{\beta} = 0, \quad \text{for } j = 1, 2, \ldots, m. \tag{A.3}$$

Clearly, Equation (3.4) results from (A.3). Then, we substitute (A.3) in (A.1) and (A.2) to yield

$$(a_0 + a_1)\hat{\alpha} + (a_0x_0 + a_1x_1)\hat{\beta} = \sum_{i=1}^{N} \delta_i^{S_0} y_i + \sum_{i=1}^{N} \delta_i^{S_1} y_i, \tag{A.4}$$

$$(a_0x_0 + a_1x_1)\hat{\alpha} + (a_0x_0^2 + a_1x_1^2)\hat{\beta} = x_0 \sum_{i=1}^{N} \delta_i^{S_0} y_i + x_1 \sum_{i=1}^{N} \delta_i^{S_1} y_i. \tag{A.5}$$

Finally, solving (A.4) and (A.5), we have Equations (3.2) and (3.3). Moreover, the expectation of the second derivatives of the log-likelihood are given by

$$-E\left[\frac{\partial^2 l}{\partial\alpha^2}\right] = \frac{1}{\sigma^2}N, \qquad -E\left[\frac{\partial^2 l}{\partial\alpha\partial\beta}\right] = \frac{1}{\sigma^2}(a_0x_0 + a_1x_1 + \textstyle\sum_{j=1}^{m} n_j\tau_j),$$
$$-E\left[\frac{\partial^2 l}{\partial\alpha\partial\tau_j}\right] = \frac{1}{\sigma^2}(n_j\beta), \qquad -E\left[\frac{\partial^2 l}{\partial\alpha\partial\sigma^2}\right] = 0,$$
$$-E\left[\frac{\partial^2 l}{\partial\beta^2}\right] = \frac{1}{\sigma^2}(a_0x_0^2 + a_1x_1^2 + \textstyle\sum_{j=1}^{m} n_j\tau_j^2), \qquad -E\left[\frac{\partial^2 l}{\partial\beta\partial\tau_j}\right] = \frac{1}{\sigma^2}(n_j\beta\tau_j),$$
$$-E\left[\frac{\partial^2 l}{\partial\beta\partial\sigma^2}\right] = 0, \qquad -E\left[\frac{\partial^2 l}{\partial\tau_j^2}\right] = \frac{1}{\sigma^2}(n_j\beta^2),$$
$$-E\left[\frac{\partial^2 l}{\partial\tau_j\partial\sigma^2}\right] = 0, \qquad -E\left[\frac{\partial^2 l}{\partial(\sigma^2)^2}\right] = \frac{N}{2\sigma^4}.$$

These elements constitute the Fisher information matrix. Then Equation (3.5) follows by some algebra calculations.

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