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Approximations of Optimal Calibration Experimental Designs Using Gaussian Influence Diagrams †

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ABSTRACT

A measuring instrument must be calibrated for accurate inferences of an unknown quantity. Bayesian calibration designs with respect to squared error loss based on a linear model are discussed in Kim and Barlow [1992]. In this paper, we consider approximations of the optimal calibration designs using the idea of Gaussian influence diagrams. The approximation is evaluated by means of numerical calculations, where it is compared with the exact values from the numerical integration.

KEYWORDS: Bayesian calibration design, influence diagram, linear model, near-optimal

1. INTRODUCTION

A linear calibration problem consists of two experiments — the future measuring experiments and the calibration experiments. Based on a linear model, one wishes to make inference on a future (true) x_f from the observation of future $\mathbf{y_f}$. To this end, the information on the parameters $(\boldsymbol{\alpha}, \boldsymbol{\beta})$ of the linear model is obtained from the calibration experiments [or, "training" data set $(x_i, \mathbf{y_i})$, $i = 1, 2, .., n$] in the form

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of the posterior distribution of $(\boldsymbol{\alpha}, \boldsymbol{\beta})$ which depends on the design vector $\mathbf{x} = (x_1, \ldots, x_n)'$. Our interest is to find an optimal design vector $\mathbf{x}$ with respect to some loss function.

The calibration inference problem is discussed in the literature. Hoadley [1970] considers univariate calibration and justifies the inverse estimator as a posterior mean for x_f with a t prior density. Brown [1982] generalized Hoadley's results with a multivariate setup. Racine-Poon [1988] considers Bayesian nonlinear calibration, where an approximation method is proposed for posterior distribution of x_f . Optimal design for linear regression model is discussed in Chaloner [1984], in which the Bayesian optimal design for estimating linear combination of the regression parameters and a geometric interpretation of optimal one-point designs are given.

Optimal calibration designs are discussed in Barlow, Mensing and Smiriga [1991], where they use Bayesian approach with univariate formulation. Kim and Barlow [1992] consider the multivariate linear calibration and investigate the optimal design with respect to squared error loss. They suggest the optimal calibration design as a conjecture, based on the observation of information gained from the calibration experiments along with the results of numerical calculations.

Howard and Matheson [1984] developed influence diagrams as a modelling tool for decision problems, and Barlow [1987] discussed the operations in the influence diagrams. An algorithm to solve Bayesian decision problems using influence diagram manipulations was developed by Shachter [1986]. Shachter and Kenley [1989] introduce the concept of the Gaussian influence diagrams and discuss the procedure to make decisions with quadratic value function for the univariate case.

In Section 2, we describe the calibration experimental designs based on a linear model and the Bayesian decision analysis for optimal design is summarized. In Section 3, the Gaussian influence diagrams are introduced and the arc reversal theorem is presented. The idea of the Gaussian influence diagrams are applied to the calibration problem in Section 4, where we obtain a near-optimal calibration design. Numerical results are given to demonstrate the structure of the expected loss and the approximation.

2. DESIGNING THE CALIBRATION EXPERIMENTS

Consider a linear model for the calibration and future experiments

$$\mathbf{Y} = \mathbf{1}\boldsymbol{\alpha}' + (\mathbf{x} - x_0\mathbf{1})\boldsymbol{\beta}' + \mathbf{E} \tag{2.1}$$

$$\mathbf{y_f} = \boldsymbol{\alpha} + (x_f - x_0)\boldsymbol{\beta} + \boldsymbol{\epsilon}_f \ , \tag{2.2}$$

where x_f is a scalar, $\boldsymbol{\alpha}, \boldsymbol{\beta}$, $\mathbf{y_f}$ and $\boldsymbol{\epsilon}_f$ are q-vectors, and $\mathbf{Y}$ and $\mathbf{E}$ are $(n \times q)$ matrices. The results of n calibration experiments consists of $\mathbf{x}(n \times 1)$ and $\mathbf{Y}(n \times q)$. The center

of the model is x_0 , which is a prior mean of x_f . The error vectors $\boldsymbol{\epsilon}_i$ are assumed to be independent and distributed as $N_q(\mathbf{0}, \boldsymbol{\Gamma})$ given $\boldsymbol{\Gamma}$. The error covariance matrix, $\boldsymbol{\Gamma}$, is assumed to be known. We also assume that x_f is independent of $(\boldsymbol{\alpha}, \boldsymbol{\beta}, \mathbf{x}, \mathbf{Y})$, and that $\mathbf{y_f}$ is independent of $(\mathbf{x}, \mathbf{Y})$ given $(\boldsymbol{\alpha}, \boldsymbol{\beta})$. x_f is independent of $(\mathbf{x}, \mathbf{Y})$ since the calibration experiment provides no information on x_f . We judged x_f is $N(x_0, {\sigma_0}^2)$ and $\begin{pmatrix} \boldsymbol{\alpha} \\ \boldsymbol{\beta} \end{pmatrix}$ is $N_{2q}\left[\begin{pmatrix} \mathbf{a} \\ \mathbf{b} \end{pmatrix}, \begin{bmatrix} \mathbf{D_a} & \mathbf{0} \\ \mathbf{0} & \mathbf{D_b} \end{bmatrix}\right]$, a priori. The loss function considered in this paper is a squared error loss, *i.e.*, $\ell(d, x_f) = (d - x_f)^2$. It is also assumed that the set Ω of feasible experimental designs is bounded.

Under the squared error loss, the Bayes estimator of x_f is the posterior mean $E(x_f|\mathbf{y_f}, \mathbf{Y}, \mathbf{x})$, and the posterior risk after observing $\mathbf{y_f}$ is the posterior variance $Var(x_f|\mathbf{y_f}, \mathbf{Y}, \mathbf{x})$. At the time of the decision regarding the experimental design, we do not know $\mathbf{y_f}$ nor the test result $\mathbf{Y}$. Therefore, the overall expected loss $R(\mathbf{x})$ is the preposterior risk:

$$R(\mathbf{x}) = E_{\mathbf{Y}|\mathbf{x}} E_{\mathbf{y_f}|\mathbf{Y},\mathbf{x}}[Var(x_f|\mathbf{y_f}, \mathbf{Y}, \mathbf{x})] \ . \tag{2.3}$$

We must minimize $R(\mathbf{x})$ with respect to $\mathbf{x} = (x_1, ..., x_n)'$.

Kim and Barlow [1992] characterized the structure of the expected loss function $R(\mathbf{x})$. They show that $R(\mathbf{x})$ depends on $\mathbf{x}$ only through n, $\bar{x} - x_0 = \sum_{i=1}^{n}(x_i - x_0)/n$ and ${s_x}^2 = \sum_{i=1}^{n}(x_i - x_0)^2/n$ using the argument of sufficient statistics. It is also shown that $R(\mathbf{x})$ is symmetric in $\bar{x} - x_0$ for fixed n and s_x , so that the design space can be reduced from an n-dimensional space to a smaller one:

$$\Xi_n = \{(\bar{x} - x_0, s_x);\ |\bar{x} - x_0| \leq s_x\} \ ,$$

for fixed n. The posterior distribution of x_f given $(\mathbf{y_f}, \mathbf{Y}, \mathbf{x})$ is derived:

$$\begin{aligned} & p(x_f|\mathbf{y_f}, \mathbf{Y}, \mathbf{x}) \\ & \quad \propto p(\mathbf{y_f}|x_f, \mathbf{Y}, \mathbf{x}) p(x_f) \\ & \quad \propto \left|2\pi(\mathbf{A}\mathbf{S}^{-1}\mathbf{A}' + \boldsymbol{\Gamma})\right|^{-1/2} \exp\{-1/2\,((x_f - x_0)^2/{\sigma_0}^2 \\ & \quad + [\mathbf{y_f} - \boldsymbol{\mu}_\alpha - (x_f - x_0)\boldsymbol{\mu}_\beta]'(\mathbf{A}\mathbf{S}^{-1}\mathbf{A}' + \boldsymbol{\Gamma})^{-1}[\mathbf{y_f} - \boldsymbol{\mu}_\alpha - (x_f - x_0)\boldsymbol{\mu}_\beta]\ )\ \}, \end{aligned} \tag{2.4}$$

where $\boldsymbol{\mu}_\alpha, \boldsymbol{\mu}_\beta$ and $\mathbf{S}^{-1}$ are the parameters of the posterior distribution of $(\boldsymbol{\alpha}, \boldsymbol{\beta})$ which is given in Kim and Barlow [1992]. As $\mathbf{A} = [\mathbf{I}\ (x_f - x_0)\ \mathbf{I}]$ depends on x_f , this distribution cannot be normal. This non-normality of posterior x_f makes the problem even harder, and we need a numerical $(2q + 1)$ nested integration to calculate $R(\mathbf{x})$ for a given $\mathbf{x}$. It is suggested that the structure of $R(\mathbf{x})$ is following: *For $n > 1$, $R(\mathbf{x}) = R_n(\bar{x} - x_0,\ s_x)$ is decreasing in s_x and increasing in $|\bar{x} - x_0|$ for others fixed.* Details can be found in Kim and Barlow [1992].

3. GAUSSIAN INFLUENCE DIAGRAMS

An influence diagram is a directed acyclic graph with nodes representing variables (probabilistic or decision), and arcs meaning possible statistical dependencies or informations available at the time of decisions. Associated with each probabilistic node in an influence diagram is a conditional probability function. Given the network structure for the influence diagram together with conditional probabilities of the nodes, there exists a unique joint distribution corresponding to the random quantities in the diagram. The influence diagram is called Gaussian if this joint probability distribution is multivariate normal.

Let N be a set of integers $\{1, ..., n\}$ which correspond to vector valued variables $\mathbf{x_1}, \ldots, \mathbf{x_n}$. The conditioning variables for $\mathbf{x_j}$ have indices in the set $C(j) \subseteq N$, *i.e.*, "$i \in C(j)$" means that $\mathbf{x_i}$ is a conditioning variable for $\mathbf{x_j}$, or that $\mathbf{x_i}$ is a direct predecessor of $\mathbf{x_j}$. We will follow the Shachter and Kenley's [1989] convention that if J is a set of nodes then $\mathbf{x_J}$ denotes the vector of variables indexed by J stacked columnwise. Thus in this convention, $\mathbf{x_{C(j)}}$ is the vector of the conditioning variables for $\mathbf{x_j}$.

In the Gaussian influence diagram, $\mathbf{x_N}$ has a multivariate normal distribution charachterized by mean $\boldsymbol{\mu}_N = \mathbf{E}(\mathbf{x_N})$ and covariance matrix $\boldsymbol{\Sigma}_{\mathbf{NN}}$. Applying the general results on the partition of multivariate normal vectors (see for example, Press [1982, p73]), we have that $\mathbf{x_j}$ given $\mathbf{x_{C(j)}}$ is distributed multivariate normal with mean

$$\mathbf{E}[\mathbf{x_j}|\mathbf{x_{C(j)}}] = \boldsymbol{\mu}_j + \boldsymbol{\Sigma}_{\mathbf{jC(j)}}\boldsymbol{\Sigma}_{\mathbf{C(j)C(j)}}^{-1}[\mathbf{x_{C(j)}} - \boldsymbol{\mu}_{C(j)}] \ , \tag{3.1}$$

and covariance matrix

$$\mathbf{V_j} = Var[\mathbf{x_j}|\mathbf{x_{C(j)}}] = \boldsymbol{\Sigma}_{\mathbf{jj}} - \boldsymbol{\Sigma}_{\mathbf{jC(j)}}\boldsymbol{\Sigma}_{\mathbf{C(j)C(j)}}^{-1}\boldsymbol{\Sigma}_{\mathbf{C(j)j}} \ ,$$

where $\mathbf{x_j}$ is $(n_j \times 1)$, $\boldsymbol{\mu}_j$ is the (unconditional) mean of $\mathbf{x_j}$, and $\boldsymbol{\Sigma}_{\cdot\cdot}$ is the corresponding submatrix of $\boldsymbol{\Sigma}_{\mathbf{NN}}$. If we let $\boldsymbol{\Sigma}_{\mathbf{jC(j)}}\boldsymbol{\Sigma}_{\mathbf{C(j)C(j)}}^{-1} = \left[\mathbf{B}'_{1j} \ \ \mathbf{B}'_{2j} \ldots \mathbf{B}'_{mj}\right]$, where m is the number of variables in $\mathbf{x_{C(j)}}$, the second term in (3.1) becomes

$$\boldsymbol{\Sigma}_{\mathbf{jC(j)}}\boldsymbol{\Sigma}_{\mathbf{C(j)C(j)}}^{-1}[\mathbf{x_{C(j)}} - \boldsymbol{\mu}_{C(j)}] = \sum_{k \in C(j)} \mathbf{B}'_{kj}(\mathbf{x_k} - \boldsymbol{\mu}_k) \ .$$

Therefore, the conditional distribution of $\mathbf{x_j}$ given $\mathbf{x_{C(j)}}$ is characterized by the unconditional mean $\boldsymbol{\mu}_j$, conditional covariance matrix $\mathbf{V_j}$, and coefficient matrix $\mathbf{B}'_{kj}$. The conditional mean of $\mathbf{x_j}$ given $\mathbf{x_{C(j)}}$ is :

$$\mathbf{E}[\mathbf{x_j}|\mathbf{x_{C(j)}}] = \boldsymbol{\mu}_j + \sum_{k \in C(j)} \mathbf{B}'_{kj}(\mathbf{x_k} - \boldsymbol{\mu}_k) \ , \tag{3.2}$$

which is expressed in terms of $\boldsymbol{\mu}_j$ and $\mathbf{B}'_{kj}$. If the conditional distribution is specified by its conditional mean and conditional covariance matrix, the coefficient matrix $\mathbf{B}'_{kj}$ can be derived by differentiating the conditional mean (3.2) with respect to $\mathbf{x_k}$ as :

$$\mathbf{B}'_{kj} = \begin{cases} \frac{\partial}{\partial \mathbf{x_k}'} \mathbf{E}[\mathbf{x_j}|\mathbf{x_{C(j)}}] & \text{if } k \in C(j) \\ 0 & \text{otherwise .} \end{cases} \tag{3.3}$$

Also $\boldsymbol{\mu}_j$ can be found from (3.2) by :

$$\boldsymbol{\mu}_j = \mathbf{E}[\mathbf{x_j}|\mathbf{x_{C(j)}} = \boldsymbol{\mu}_{C(j)}] \, . \tag{3.4}$$

In the Bayesian analysis, the key operation is to apply the Bayes' Theorem to calculate the posterior distribution. This corresponds to the reversal of arc to calculate the new conditional distribution in the influence diagram analysis. For jointly normal variables, the new conditional distribution is also normal, so that new conditional covariance matrices and coefficient matrices are sufficient for specifying their new conditional distributions. Shachter and Kenley [1989] has summarized the updating formula when all the variables x_j are scalar valued. Theorem 1, which is proved in Kim [1988], is the multivariate version of the result of Shachter and Kenley [1989].

Theorem 1. (Arc Reversal) Suppose node $i \in C(j)$ and no other directed path exists from i to j. Then we have

$$E[\mathbf{x_j}|\mathbf{x_K}] = \boldsymbol{\mu}_j + \sum_{k \in K} [\mathbf{B}'_{kj} + \mathbf{B}'_{ij}\mathbf{B}'_{ki}](\mathbf{x_k} - \boldsymbol{\mu}_k), \tag{3.5}$$

and

$$Var(\mathbf{x_j}|\mathbf{x_K}) = \mathbf{V}_j + \mathbf{B}'_{ij}\mathbf{V}_i\mathbf{B}_{ij}, \tag{3.6}$$

where $K = [C(i) \cup C(j)] \setminus \{i\}$. If $\mathbf{V}_j + \mathbf{B}'_{ij}\mathbf{V}_i\mathbf{B}_{ij}$ is nonsingular and if we denote $\tilde{\mathbf{B}}_{ij}$ the new coefficient matrix for the arc from node i to node j, then we have

$$Var(\mathbf{x_i}|\mathbf{x_j}, \mathbf{x_K}) = \mathbf{V}_i - \tilde{\mathbf{B}}'_{ji}\mathbf{B}'_{ij}\mathbf{V}_i, \tag{3.7}$$

and

$$E[\mathbf{x_i}|\mathbf{x_j}, \mathbf{x_K}] = \boldsymbol{\mu}_i + \tilde{\mathbf{B}}'_{ji}(\mathbf{x_i} - \boldsymbol{\mu}_i) + \sum_{k \in K} \tilde{\mathbf{B}}'_{ki}(\mathbf{x_k} - \boldsymbol{\mu}_k), \tag{3.8}$$

where

$$\tilde{\mathbf{B}}'_{ji} = \mathbf{V}_i\mathbf{B}_{ij}[\mathbf{V}_j + \mathbf{B}'_{ij}\mathbf{V}_i\mathbf{B}_{ij}]^{-1}, \tag{3.9}$$

and

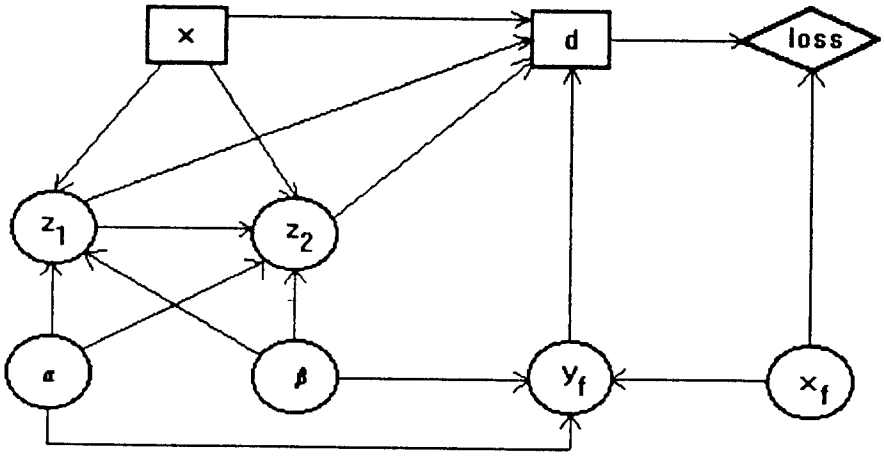
$$\tilde{\mathbf{B}}'_{ki} = \mathbf{B}'_{ki} - \tilde{\mathbf{B}}'_{ji}[\mathbf{B}'_{kj} + \mathbf{B}'_{ij}\mathbf{B}'_{ki}]. \tag{3.10}$$

As we see in Theorem 1, no integration is necessary to reverse an arc, and only one matrix inversion is required in (3.9), computing the new coefficient matrix $\tilde{\mathbf{B}}'_{ji}$. Theorem 1 also explains the operation of "integrating out" a variable, *i.e.*, finding a predictive distribution.

Corollary 2. (Node Removal) Suppose $i \in C(j)$ and j is the only successor node of i. Then with the notation of Theorem 1, the conditional distribution of $\mathbf{x_j}$ given $\mathbf{x_K}$, after integrating out $\mathbf{x_i}$, is normal with mean (3.5) and covariance matrix (3.6).

4. APPROXIMATIONS FOR A NEAR-OPTIMAL DESIGN

In this section, we apply the idea of the Gaussian influence diagrams to the calibration problem to find a near-optimal design. Since our underlying model is linear, we have to approximate some of the parameters in the resulting diagram, for our problem to satisfy the joint normality. Whenever the conditional covariance matrix $\mathbf{V}_j$ or the arc coefficient $\mathbf{B}'_{kj}$ depends on any of the variables, we approximate the parameter. No approximation, however, is necessary for the parameters that depends on the design $\mathbf{x}$. This is because the design is the preexperimental decision so that $\mathbf{x}$ can be considered constant during the probability manipulation and other decision making stages. Figure 1 shows the standard influence diagram for the calibration problem.



$$y_f = \alpha + (x_f - x_0)\beta + \epsilon$$

$$x_f \sim N(x_0, \sigma_0^2) \quad ; \quad \alpha \sim N_0(a, D_\alpha) \quad ; \quad \beta \sim N_0(b, D_\beta)$$

$$y_f | x_f, \alpha, \beta \sim N_0(\alpha + (x_f - x_0)\beta, \Gamma)$$

$$z_2 | z_1, x, \alpha, \beta \sim N_0(\mu_2 + (\bar{x} - x_0)(z_1 - \mu_1), \Sigma(x_i - \bar{x})^2 \Gamma)$$

Figure 1. Influence diagram for calibration problem

To construct the Gaussian influence diagram for the calibration problem, we need to assess (unconditional) mean $\boldsymbol{\mu}_j$ and conditional covariance matrix $\mathbf{V}_j$ for each node, and coefficient matrix $\mathbf{B}'_{kj}$ for each arc. Using the equations (3.2) through (3.4), we can find the conditional means, coefficient matrix and unconditional means for the Gaussian influence diagram. After two approximations on $\mathbf{B}'_{x_f y_f}$ and $\mathbf{B}'_{\beta y_f}$, we can have a multivariate Gaussian influence diagram for the calibration problem. Since every arc reversal involves a matrix inversion and the matrices to be inverted depend on $\mathbf{x}$, the resulting expected loss should be a complicated function of matrices which depend on $\mathbf{x}$, even though no integration is necessary. Rather than trying to minimize this complicated function of matrices, we will work on the univariate problem in this section.

4.1 A near optimal design for the univariate case

If all the variables are scalar, then there is a significant simplification in updating the parameters. Figure 2 shows the Gaussian influence diagram in this case. The experimental design $\mathbf{x}$ has been removed from the diagram and will be considered later to minimize the expected loss. For the univariate case, σ^2 is the error variance ($\boldsymbol{\Gamma}$), and ${\sigma_a}^2$ and ${\sigma_b}^2$ are the prior variances of α and β($\mathbf{D}_a$ and $\mathbf{D}_b$), respectively.

Since α and β are not observable, we must find the posterior distribution of (α, β)

and integrate out into y_f . However, the exact posterior distribution of (α, β), which is bivariate normal, is available, so that we can derive the distribution of y_f given $(z_1, z_2, \mathbf{x})$ rather than working directly on the diagram. Table 1 gives the parameters of the posterior distribution of (α, β) for the univariate calibration, which are derived in Barlow, Mensing and Smiriga [1991]. The utilization of the exact posterior distribution should reduce the amount of error due to the approximation. Figure 3 is the Gaussian influence diagram after removing (α, β), where we approximate the parameters for the first time. The distribution of (z_1, z_2) given $\mathbf{x}$ is

Table 1. Parameters of the Posterior Distribution of (α, β) given y and x for univariate calibration

$$\mu_\alpha = a + \frac{(\sum e_i)[\sum(x_i - x_0)^2 + \sigma^2/{\sigma_b}^2] - [\sum(x_i - x_0)][e_i(x_i - x_0)]}{(n + \sigma^2/{\sigma_a}^2)[\sum(x_i - x_0)^2 + \sigma^2/{\sigma_b}^2] - [\sum(x_i - x_0)]^2}$$

$$\mu_\beta = b + \frac{(n + \sigma^2/{\sigma_b}^2)[\sum e_i(x_i - x_0)] - [\sum(x_i - x_0)](\sum e_i)}{(n + \sigma^2/{\sigma_a}^2)[\sum(x_i - x_0)^2 + \sigma^2/{\sigma_b}^2] - [\sum(x_i - x_0)]^2}$$

$$\sigma_\alpha = \frac{\sigma^2[\sum(x_i - x_0)^2 + \sigma^2/{\sigma_b}^2]}{(n + \sigma^2/{\sigma_a}^2)[\sum(x_i - x_0)^2 + \sigma^2/{\sigma_b}^2] - [\sum(x_i - x_0)]^2}$$

$$\sigma_\beta = \frac{\sigma^2(n + \sigma^2/{\sigma_a}^2)}{(n + \sigma^2/{\sigma_a}^2)[\sum(x_i - x_0)^2 + \sigma^2/{\sigma_b}^2] - [\sum(x_i - x_0)]^2}$$

$$cov(\alpha, \beta) = \frac{-\sigma^2 \sum(x_i - x_0)}{(n + \sigma^2/{\sigma_a}^2)[\sum(x_i - x_0)^2 + \sigma^2/{\sigma_b}^2] - [\sum(x_i - x_0)]^2}$$

where

$$e_i = y_i - a - b(x_i - x_0)$$

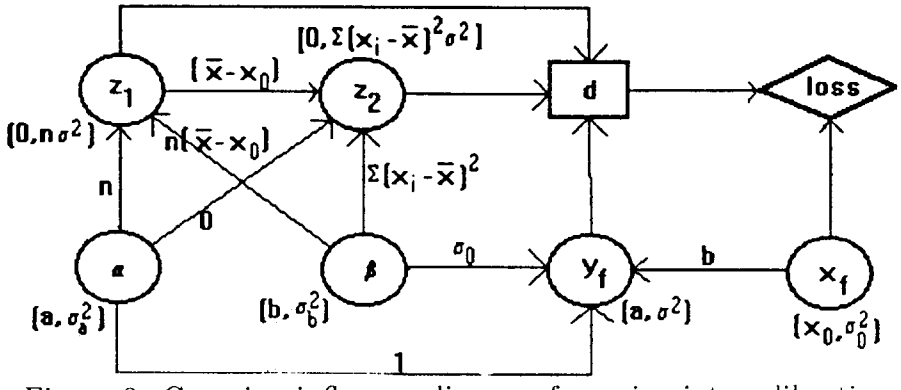


Figure 2. Gaussian influence diagram for univariate calibration

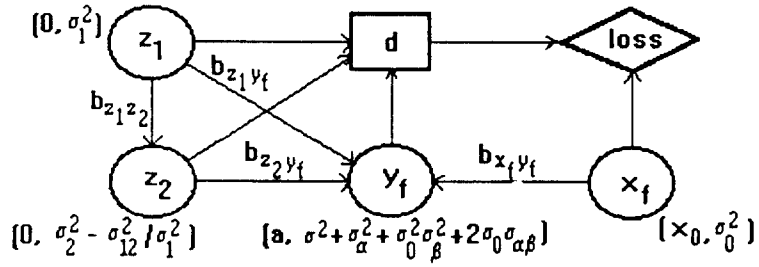


Figure 3. Starting Gaussian influence diagram

$$N\left[\binom{0}{0},\ \begin{pmatrix}\sigma_1{}^2 & \sigma_{12}\\ \sigma_{12} & \sigma_2{}^2\end{pmatrix}\right] ,$$

where

$$\begin{aligned}\sigma_1{}^2 &= n^2\sigma_a{}^2 + n^2(\bar{x}-x_0)^2\sigma_b{}^2 + n\sigma^2\\ \sigma_2{}^2 &= n^2(\bar{x}-x_0)^2\sigma_a{}^2 + n^2(s_x{}^2)^2\sigma_b{}^2 + ns_x{}^2\sigma^2\\ \sigma_{12} &= n^2(\bar{x}-x_0)\sigma_a{}^2 + n^2(\bar{x}-x_0)s_x{}^2\sigma_b{}^2 + n(\bar{x}-x_0)\sigma^2.\end{aligned}$$

It follows that the conditional variances of z_1 and z_2 in Figure 3 are

$$\begin{aligned}v_{z_1} &= Var(z_1) = \sigma_1{}^2 ,\\ v_{z_2} &= Var(z_2|z_1,x) = \sigma_2{}^2 - \sigma_{12}{}^2/\sigma_1{}^2 .\end{aligned}$$

And the arc coefficient is

$$b_{z_1z_2} = \sigma_{12}\ \sigma_1{}^2 .$$

The distribution of y_f given $(z_1, z_2, x_f, \mathbf{x})$ is normal with

$$E[y_f|z_1,z_2,x_f,\mathbf{x}] = \mu_\alpha + \mu_\beta(x_f - x_0), \tag{4.1}$$

and

$$Var(y_f|z_1,z_2,x_f,\mathbf{x}) = \sigma^2 + \sigma_\alpha^2 + \sigma_\beta^2(x_f-x_0)^2 + 2\sigma_{\alpha\beta}(x_f-x_0), \tag{4.2}$$

where μ_α, μ_β, σ_α^2, σ_β^2 and $\sigma_{\alpha\beta} = Cov(\alpha,\beta)$ are the parameters of the posterior distribution of (α,β) given $(z_1, z_2, \mathbf{x})$ which are summarized in Table 1. If we let D be the common denominator of the above parameters :

$$D = (n + \sigma^2/\sigma_a{}^2)(ns_x{}^2 + \sigma^2/\sigma_b{}^2) - n^2(\bar{x}-x_0)^2 ,$$

then the arc coefficients are :

$$b_{z_1 y_f} = [n{s_x}^2 + \sigma^2/{\sigma_b}^2 - n(x - x_0)(x_f - x_0)]/D \tag{4.3}$$

$$b_{z_2 y_f} = [-n(\bar{x} - x_0) + n(x_f - x_0) + (x_f - x_0)\sigma^2/{\sigma_a}^2]/D \tag{4.4}$$

$$b_{x_f y_f} = \mu_\beta. \tag{4.5}$$

Since (4.2) through (4.5) involve x_f or μ_β , we approximate them by :

$$v_{y_f} \approx \sigma^2 + \sigma_\alpha^2 + \sigma_\beta^2 {\sigma_0}^2 + 2\sigma_{\alpha\beta}\sigma_0 \tag{4.2.a}$$

$$b_{z_1 y_f} \approx [n{s_x}^2 + \sigma^2/{\sigma_b}^2 - n(x - x_0)\sigma_0]/D \tag{4.3.a}$$

$$b_{z_2 y_f} \approx [-n(\bar{x} - x_0) + n\sigma_0 + \sigma_0\sigma^2/{\sigma_a}^2]/D \tag{4.4.a}$$

$$b_{x_f y_f} \approx b. \tag{4.5.a}$$

Note that the above four are the only approximations we made. We lose some information from the calibration experiment by approximating the posterior mean, μ_β , of β by the prior mean b. However, since the loss function will be averaged against the experimental result and we keep using the posterior variance of β in the analysis, the information lost by this approximation will not be significant. The approximation of $x_f - x_0$ by σ_0 may change the sign as $x_f - x_0$ can take negative values while σ_0 is always positive. The effect of it will be discussed later in this section.

The decision d in Figure 3 can be made easily from the result of the Bayesian decision analysis. The optimal decision d^* with respect to a squared error loss is the posterior mean of x_f given $(y_f, z_1, z_2, \mathbf{x})$, and the expected loss is the posterior variance. Using the univariate results of Theorem 1 for arc reversal, we have

$$\begin{aligned} E_{x_f}[(d^* - x_f)^2 | y_f, z_1, z_2, \mathbf{x}] &= Var(x_f | y_f, z_1, z_2, \mathbf{x}) \\ &= v_{x_f} v_{y_f}/(v_{y_f} + b_{x_f y_f} v_{x_f}) \ . \end{aligned} \tag{4.6}$$

Since the expected loss, (4.6), does not depend on y_f, z_1 or z_2, the approximated overall expected loss $R^2(\mathbf{x})$ is

$$\begin{aligned} R^2(\mathbf{x}) &= v_{x_f} v_{y_f}/(v_{y_f} + b_{x_f y_f} v_{x_f}) \\ &= \left(\frac{1}{{\sigma_0}^2} + \frac{b^2}{\sigma^2 + \sigma_\alpha^2 + {\sigma_0}^2\sigma_\beta^2 + 2\sigma_0\sigma_{\alpha\beta}} \right)^{-1} , \end{aligned} \tag{4.7}$$

where σ_α^2, σ_β^2 and $\sigma_{\alpha\beta}$, which depend on $\mathbf{x}$, are the posterior variances and covariance

of α and β. Notice that $R^2(\mathbf{x})$ is not symmetric about $\bar{x} - x_0 = 0$, while $R(\mathbf{x})$ should be so (see Barlow, Mensing and Smiriga [1991]). In the proof of the symmetric property of $R(\mathbf{x})$, $\sigma_{\alpha\beta}$ which depends on $\bar{x} - x_0$ is multiplied by $x_f - x_0$, so that $R(\mathbf{x})$ depends on $\bar{x} - x_0$ only through $(\bar{x} - x_0)^2$. But in $R^2(\mathbf{x})$, $\sigma_{\alpha\beta}$ is multiplied by σ_0 which is the approximation for $x_f - x_0$. As we pointed out earlier, this approximation changes the sign when $x_f - x_0$ is negative, and it is why $R^2(\mathbf{x})$ is not symmetric.

Minimizing $R^2(\mathbf{x})$ is equivalent to minimizing

$$\sigma_\alpha^2 + {\sigma_0}^2\sigma_\beta^2 + 2\sigma_0\sigma_{\alpha\beta} \ . \tag{4.8}$$

If we substitute σ_α^2, σ_β^2 and $\sigma_{\alpha\beta}$ from Table 1 for the posterior distribution of (α, β), the optimization becomes to minimize $f_n(\bar{x} - x_0, s_x)$ over the region $|\bar{x} - x_0| \leq s_x$, where:

$$f_n(\bar{x} - x_0, s_x) = \frac{\sigma^2[{s_x}^2 - 2\sigma_0(x - x_0) + \sigma_0^2 + \sigma^2/n\sigma_0^2 + \sigma_0^2\sigma^2/n\sigma_a^2]}{n[(1 + \sigma^2/n\sigma_a^2)s_x^2 - (\bar{x} - x_0)^2 + (1 + \sigma^2/n\sigma_a^2)(\sigma^2/n\sigma_b^2)]}. \tag{4.9}$$

For fixed $n \geq 2$, as a function of $\bar{x} - x_0$ and ${s_x}^2$, $f_n(\bar{x} - x_0, s_x)$ is convex in the region $|\bar{x} - x_0| \leq s_x$. For a given s_x fixed, it has a minimum at $\bar{x} - x_0 = \sigma_0(1 + \sigma^2/n{\sigma_a}^2)$. And it is decreasing in s_x for fixed $\bar{x} - x_0$ except that it is constant in s_x for $\bar{x} - x_0 = \sigma_0(1 + \sigma^2/n{\sigma_a}^2)$. Therefore, the minimum occurs at $\bar{x} - x_0 = \sigma_0(1 + \sigma^2/n{\sigma_a}^2)$ with any value of feasible s_x. Notice that the quantity $\sigma_0(1 + \sigma^2/n{\sigma_a}^2)$ is positive unless $\sigma_0 = 0$. Considering the symmetry of $R(\mathbf{x})$, this approximation should be accurate for large n and small σ_0 and σ, in which case $\sigma_0(1 + \sigma^2/n{\sigma_a}^2)$ is close to zero. The reason for the symmetry of $R^2(\mathbf{x})$ is the possible sign changes due to the approximation on the parameters of the influence diagram. Although $R^2(\mathbf{x})$ has the drawback of asymmetry, it generally supports the conjecture on the optimal designs that Kim and Barlow [1992] suggested, that is, both $R(\mathbf{x})$ and $R^2(\mathbf{x})$ are nonincreasing in s_x and having smaller values for small $|\bar{x} - x_0|$.

4.2 Numerical Results

In this section, we consider three different situations of prior variance of α and β, and investigate the approximation $R^2(\mathbf{x})$ given in (4.7). The values of $R^2(\mathbf{x})$ for different designs $\mathbf{x}$ are calculated and they are compared with the values of $R(\mathbf{x})$. Kim and Barlow [1992] calculated $R(\mathbf{x})$ for the univariate case using three-nested subroutine of numerical integration. Table 2 shows $R^2(\mathbf{x})$ along with $R(\mathbf{x})$ for the three situations.

Table 2. Calculated values of $R(x)$ and $R^2(x)$
Each cell showing $R(x)$ and $R^2(x)$
$n = 5 \quad \sigma = 1 \quad x_0 = 0 \quad \sigma_0 = 1 \quad a = 1 \quad b = 1$

(a) $\sigma_a = 2 \quad \sigma_b = 0.1$ Minimum $R^2(x)$ occurs at $\bar{x} - x_0 = 1.05$

			s_x			
$\bar{x} - x_0$	0	0.5	1	2	3	4
−4						0.574002
						0.585630
−3					0.562813	0.558813
					0.571942	0.565020
−2				0.554207	0.552745	0.551454
				0.560257	0.557026	0.554149
−1			0.548788	0.548519	0.548205	0.547914
			0.551268	0.550269	0.549074	0.547967
−0.5		0.547393	0.547370	0.547293	0.547199	0.547110
		0.547972	0.547812	0.547269	0.546615	0.546004
0	0.546989	0.546925	0.546919	0.546904	0.546873	0.546849
	0.545553	0.545527	0.545455	0.545208	0.544911	0.544633
0.5		0.547393	0.547370	0.547293	0.547199	0.547110
		0.544049	0.544028	0.543959	0.543876	0.543797
1			0.548788	0.548519	0.548205	0.547914
			0.543483	0.543482	0.543482	0.543481
2				0.554207	0.552745	0.551454
				0.545162	0.544829	0.544536
3					0.562813	0.558813
					0.550409	0.548660
4						0.574002
						0.558794

(b) $\sigma_a = 1 \quad \sigma_b = 1.2$ Minimum $R^2(x)$ occurs at $\bar{x} - x_0 = 1.2$

	s_x					
$\bar{x} - x_0$	0	0.5	1	2	3	4
−4						0.613591
						0.714716
−3					0.614979	0.547321
					0.726849	0.591881
−2				0.620941	0.543306	0.533559
				0.745688	0.585345	0.560966
−1			0.656282	0.541469	0.531688	0.528587
			0.770992	0.578064	0.555082	0.547631
−0.5		0.707189	0.568045	0.535755	0.529702	0.527567
		0.772196	0.615090	0.559236	0.547841	0.543767
0	0.735003	0.615367	0.557760	0.534188	0.529094	0.527244
	0.722736	0.626998	0.573065	0.548530	0.543077	0.541086
0.5		0.707189	0.568045	0.535755	0.529702	0.527567
		0.606855	0.553532	0.542121	0.540079	0.539369
1			0.656282	0.541469	0.531688	0.528587
			0.542302	0.538819	0.538604	0.538539
2				0.620941	0.543306	0.533559
				0.560828	0.541700	0.539935
3					0.614979	0.547321
					0.590373	0.549297
4						0.613591
						0.608578

(c) $\sigma_a = 0.1$ $\sigma_b = 2$ Minimum $R^2(x)$ occurs at $\bar{x} - x_0 = 21$

			s_x			
$\bar{x} - x_0$	0	0.5	1	2	3	4
−4						0.407711
						0.506919
−3					0.409482	0.407632
					0.509761	0.506477
−2				0.414412	0.409337	0.407578
				0.517301	0.508986	0.506088
−1			0.438494	0.414052	0.409254	0.407547
			0.551268	0.515590	0.508335	0.505743
−0.5		0.508839	0.437832	0.413966	0.409233	0.407538
		0.634662	0.547812	0.514902	0.508048	0.505585
0	0.848897	0.505219	0.437027	0.413937	0.409227	0.407536
	0.833597	0.626335	0.545455	0.514305	0.507783	0.505436
0.5		0.508839	0.437832	0.413966	0.409233	0.407538
		0.625619	0.544028	0.513789	0.507537	0.505295
1			0.438494	0.414052	0.409254	0.407547
			0.543483	0.513346	0.507310	0.505161
2				0.414412	0.409337	0.407578
				0.512657	0.506904	0.504913
3					0.409482	0.407632
					0.506555	0.504688
4						0.407711
						0.504484

For all three cases, we have fixed the error variance (σ^2), the prior mean (x_0) and variance ($\sigma_0{}^2$) of x_f and the prior means (a and b) of α and β, as shown in the table. As to the calculation of $R(\mathbf{x})$, the number of grid points in one numerical integration is 80. The selection of $n = 5$ is arbitrary, but when n is large, $R(\mathbf{x})$ is small and has little variation. The choice of σ and σ_0 are not major factors for the comparison. The three cases are (a) $\sigma_a = 2$, $\sigma_b = 0.1$; $(b)\sigma_a = 1$, $\sigma_b = 1.2$; and $(c)\sigma_a = 0.1$, $\sigma_b = 2$.

The case (a) represents the situation where there is little uncertainty in β, the case (c) represents little uncertainty in α, and (b) in between them. The case (a) gives better approximation than (c) because the posterior mean of β, μ_β, has been replaced by the prior mean, b, in the assessment of the coefficients of the Gaussian influence diagram. Since we have, a priori, more information about β for the case (a), the effect of the replacing μ_β should be smaller, hence $R^2(\mathbf{x})$ is more accurate for case (a). Near-optimal designs using $R^2(\mathbf{x})$ are consistent with the result obtained in the previous section for all three cases, namely the designs with $\bar{x} - x_0 = \sigma_0(1+\sigma^2/n\sigma_a{}^2)$. Specifically, they are $\bar{x} - x_0 = 1.05$ for (a), $\bar{x} - x_0 = 1.2$ for (b) and $\bar{x} - x_0 = 21$ for (c). As mentioned in the previous section, both $R(\mathbf{x})$ and $R^2(\mathbf{x})$ are nonincreasing in s_x and having smaller values for small $|\bar{x} - x_0|$.

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