Chapter 2

OPTIMAL DESIGNS FOR THE EVALUATION OF AN EXTREMUM POINT

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Abstract This paper studies the optimal experimental design for the evaluation of an extremum point of a quadratic regression function of one or several variables. Experimental designs which are locally optimal for arbitrary dimension k among all approximate designs are constructed (although for $k > 1$ an explicit form proves to be available only under a restriction on the location of the extremum point). The result obtained can be considered as an improvement of the last step of the well-known Box-Wilson procedure.

Introduction

Let us consider the problem of optimal design for estimating the point of extremum — $\beta_2/2\beta_3$ in the quadratic regression model

$$y_i = \beta_1 + \beta_2 x_i + \beta_3 x_i^2 + \varepsilon_i,\ i = 1, \ldots, n,$$

where y_i is the result of an observation at point $x_i \in [-1, 1]$ and $\{\varepsilon_i\}$ are i.i.d. random values such that $E\varepsilon_i = 0$ and $E\varepsilon_i^2 = 1$.

This problem is a nonlinear one. There exist a few standard approaches to such problems: sequential, minimax, Bayesian and locally optimal. All these approaches have been implemented for the above model. Ford and Silvey (1980) and Müller and Pötscher (1992) considered sequential procedures, Mandal (1978), Chaloner (1989), Mandel and Heiligers (1992), Müller (1995) and Müller and Pazman (1998) studied the problem from Bayesian or minimax points of view.

Locally optimal designs were considered by Fedorov and Müller (1997). The authors of that paper investigated also the multivariate regression model. They suggested to use a known reparametrization of the problem that allows to obtain a convenient representation of the information matrix (the reparametrization was also used by Chatterjee and Mandal (1981), Buonaccorsi and Iyer (1986) and others).

The present paper can be considered as a further development of this approach. We consider the multivariate quadratic regression model on the hypercube $[-1,1]^k$. We find, analytically, locally optimal designs for this model under a restriction on the location of the extremum point. More precisely, our analytical solution is appropriate if the extremum point belongs to the hypercube $[-1/2,1/2]^k$.

This problem can be considered as part of a more general problem, that of extremum point evaluation for a function of general form. To be specific, we will consider estimation of the minimum point. Investigation of this problem was initiated in the well-known paper by Box and Wilson (1951). The approach to the problem, elaborated in that paper, is based on the combination of the steepest descent technique with methods of planning factorial experiments. Box and Wilson suggested that experiments be performed in the vicinity of a certain basic point, according to a complete or fractional factorial design from which a linear model can be built using the resulting observations. If this model proves to be adequate, it gives an unbiased estimate of the function gradient. A few test steps are then performed in the direction of the antigradient until a decrease in the measured values of the function is observed. The last successful point is taken as a new basic point and so on. In the vicinity of an extremum point the linear model will be inadequate and, when this occurs, a quadratic model can be built for the final estimation of location of the extremum point.

A review of some other approaches to this general problem can be found in Pronzato and Walter (1993).

The analytical solution elaborated in the present paper can be used to optimize the last stage of the Box–Wilson procedure. The formal outline of the problem is given in Sections 1 and 2. Further, in Section 3, we formulate our basic results. A short discussion is given in Section 4. Proofs of the basic results are concentrated in the Appendix.

1. PRELIMINARY OUTLINE OF THE PROBLEM

Consider a quadratic function of several variables:

$$\eta(x) = \eta(x, A, \beta, \gamma) = x^T A x + \beta^T x + \gamma, \tag{2.1}$$

where A is a positive definite $k \times k$ matrix, β is a k dimensional vector, γ is a real number. This function attains, as is well known, its minimal value equal to $c = \gamma - \beta^T A^{-1}\beta/4$ at the point $x = x^* = b = -\frac{1}{2}A^{-1}\beta$.

Suppose the function can only be measured with a random error at design points x belonging to the hypercube $\mathcal{X} = [-1,1]^k$. More precisely, let the experimental results at the design points $x_{(i)}$, $i = 1,2,\ldots,n$, $x_{(i)} \in \mathcal{X}$ be described by the equation

$$y_i = \eta(x_{(i)}, A, \beta, \gamma) + \varepsilon_i, \quad i = 1,2,\ldots,n, \tag{2.2}$$

where $\{\varepsilon_i\}$ are random errors such that $E\varepsilon_i = 0$, $E\varepsilon_i\varepsilon_j = 0$ $i \neq j$, $E\varepsilon_i^2 = \sigma^2$, $i,j = 1,2,\ldots,n$.

Elements of the matrix A and of the vector β as well as γ are unknown. It is required to construct an estimate of the vector $x^* = b$ and to find an optimal (in a sense to be yet defined) experimental design

$$\xi = \{x_{(1)},\ldots,x_{(n)}; m_1,\ldots,m_n\},$$

where $x_{(i)} \in \mathcal{X}$ and $m_i > 0$ are respectively the design point and the proportion of the total number of available experiments to be performed at that design point, for $i = 1,2,\ldots,n$, with $\sum_{i=1}^n m_i = 1$.

2. THE APPROACH TO THE PROBLEM

Rewrite the regression function in the form

$$\bar{\eta}(x,\theta) = (x-b)^T A(x-b) + c, \tag{2.3}$$

where

$$\begin{aligned} \theta &= (b_1,\ldots,b_k,a_{11},\ldots,a_{kk},a_{12},\ldots,a_{1k},a_{23},\ldots,a_{k-1k},c)^T, \\ b &= -\frac{1}{2}A^{-1}\beta,\ c = \gamma - \beta^T A^{-1}\beta/4. \end{aligned}$$

This function depends on parameters $b_1,\ldots,b_k$ in a nonlinear way. We apply to our case well-known results for nonlinear models.

Let $\xi = \{x_{(1)},\ldots,x_{(n)}; m_1,\ldots,m_n\}$ be an experimental design. Consider the matrix

$$M(\xi) = \left(\sum_{l=1}^n \frac{\partial\bar{\eta}(x_{(l)},\theta)}{\partial\theta_i}\frac{\partial\bar{\eta}(x_{(l)},\theta)}{\partial\theta_j} m_{(l)}\right)_{i,j=1}^r,$$

$r = k + k(k+1)/2 + 1$.

An immediate calculation gives

$$M(\xi) = \begin{pmatrix} 2A & 0 \\ 0 & I \end{pmatrix} \bar{M}(\xi) \begin{pmatrix} 2A & 0 \\ 0 & I \end{pmatrix},$$

where I is the identity matrix,

$$\begin{aligned}\bar{M}(\xi) &= \bar{M}(\xi, b) = \sum_{l=1}^{n} f(x_{(l)}) f^T(x_{(l)}) m_l, \\ f(x) &= f(x, b) = \big((b_1 - x_1), \ldots, (b_k - x_k), (x_1 - b_1)^2, \ldots, (x_k - b_k)^2, \\ &\quad (x_1 - b_1)(x_2 - b_2), \ldots, (x_{k-1} - b_{k-1})(x_k - b_k), 1\big)^T .\end{aligned}$$

Note that for $n = r$ we have $\det \bar{M}(\xi, b) = \det \bar{M}(\xi, 0)$. This can be verified through the equality $\bar{M}(\xi, b) = F^T F$, where $F = \big(\sqrt{m_j} f_i(x_{(j)})\big)_{i,j=1}^{r}$ and linear transformations of columns of the matrix F. Then, with $n \geq r$, the Binet-Cauchy formula states that $\det \bar{M}(\xi, b) \neq 0$ for an arbitrary b if $\det \bar{M}(\xi, 0) \neq 0$.

An arbitrary design ξ will be called a *nonsingular* design if $\det \bar{M}(\xi, 0) \neq 0$. From the above remark we have $\det \bar{M}(\xi, b) \neq 0$ for an arbitrary vector b if the design ξ is a nonsingular design.

Consider the (nonlinear) least squares estimate of the vector θ for the regression function (2.3):

$$\hat{\theta} = \arg\min_{\theta} \sum_{l=1}^{N} \big(\bar{\eta}(x_{(l)}, \theta) - y_l\big)^2 . \tag{2.4}$$

Since $\bar{\eta}(x, \theta) = \eta(x, A, \beta, \gamma)$ we have $\hat{b} = -\frac{1}{2}\bar{A}^{-1}\bar{\beta}$, where $\bar{A}$ is the matrix consisting of least squares estimates of elements of the matrix A in the linear regression function $\eta(x, A, \beta, \gamma)$ under the equation (2.2) and $\bar{\beta}$ is the similar estimate for β. Thus the construction of the estimate $\hat{\theta}$ is easy.

At the same time we have the following proposition:

Proposition 2.1. *Let ξ be an arbitrary nonsingular design and $\hat{\theta}$ be determined by (2.4), where $y_1, \ldots, y_N$ are results obtained from Nm_j experiments at point $x_{(j)}$, $j = 1, \ldots, n$. Then $\hat{\theta}$ is a strongly consistent estimate for θ and with $N \to \infty$ the vector $\sqrt{N}(\hat{\theta} - \theta)$ has asymptotically the normal distribution with zero expectation and the covariance matrix $\mathcal{D}_{\hat{\theta}} = \sigma^2 M^{-1}(\xi)$.*

This proposition is a particular case of results obtained in Jennrich (1969).

Rewrite the matrix $\bar{M}(\xi)$ in the block form

$$\bar{M}(\xi) = \begin{pmatrix} M_1 & M_2^T \\ M_2 & M_3 \end{pmatrix},$$

where M_1 is a $k \times k$ matrix. Let

$$M_s = M_s(\xi) = M_1 - X^T M_3 X,$$

where $X = M_3^{-1} M_2$ if the matrix M_3 is nonsingular and X is an arbitrary solution of the equation $M_3 X = M_2$ otherwise. It is known (Karlin & Studden, 1966, §10.8) that M_s does not depend on the choice of the solution.

Let $\xi = \alpha\xi_1 + (1-\alpha)\xi_2$, where ξ_1 is a nonsingular design and ξ_2 is an arbitrary design, $0 < \alpha < 1$. Then the covariance matrix of $\sqrt{N}(\hat{b} - b)$, where $\hat{b}$ is the nonlinear least squares estimate of the vector b, takes the form

$$\mathcal{D}_{\hat{b}}(\xi) = \frac{\sigma^2}{4} A^{-1} M_s^{-1}(\xi) A^{-1}.$$

Definition 2.1. *Any design ξ_2 minimizing the magnitude*

$$\lim_{\alpha \to 0} \det \mathcal{D}_{\hat{b}}(\xi) = \left(\frac{\sigma^2}{4}\right)^k (\det A)^{-2} \det M_s^{-1}(\xi_2, b)$$

for a fixed value $b = b^{(0)}$ will be called a locally optimal design for estimating an extremum point of the regression function (2.1). Note that the locally optimal design depends on b and does not depend on the true values of A and c.

It is evident that for large N the majority of experiments should be performed in accordance with a locally optimal design where $b^{(0)}$ is the current estimate of the vector b.

The problem of finding locally optimal designs is equivalent to the problem $\det M_s(\xi, b) \to \max_\xi$, where the maximum is taken over all (approximate) designs and $b = b^{(0)}$. The remainder of the paper considers the solution of this problem.

3. BASIC RESULTS

Let k be an arbitrary natural number and $b = b^{(0)} \in \mathrm{Int}[-1,1]^k$. Consider all hyperparallelepipeds with centre at the point b inscribed in the hypercube $[-1,1]^k$ and take the maximal one. Let ξ^* be the experimental design that consists of all vertices of this hyperparallelepiped with equal weights, $m_l = 1/n, l = 1, \ldots, n, n = 2^k$.

Our basic result is the following theorem:

Theorem 1. *For an arbitrary k, the design ξ^* described above is a locally optimal design for estimation of an extremum point of the regression function (2.1) if and only if $|b_i| \le \frac{1}{2}, i = 1, 2, \ldots, k$.*

The result of Theorem 1 for the case $k = 2$ is illustrated in Fig. 2.1.

The exact analytical solution given by Theorem 1 allows us to study the efficiency of the locally optimal design. This design is more accurate than the usual D-optimal design for the estimation of all parameters of the regression function (2.1). For example, suppose $b = (\frac{1}{2}, \ldots, \frac{1}{2})^T$. In this case we need s_k times less observations to receive the same accurancy under dimension k, where $s_1 = 1.5$, $s_2 \approx 1.78$, $s_3 \approx 2.08$, $s_4 \approx 2.38$, $s_5 \approx 2.68$. We see that the efficiency of the locally optimal design increases with k.

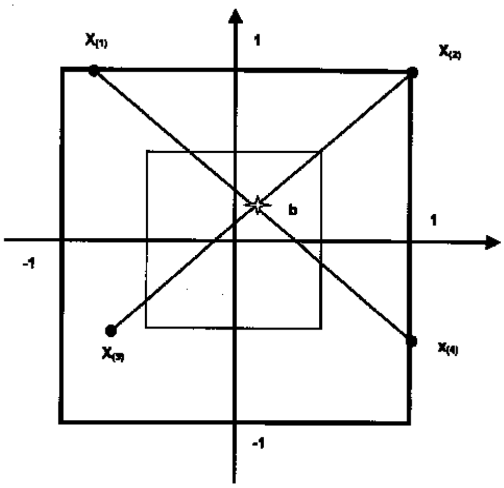

Figure 2.1 Points of the design ξ^* for $k = 2$.

Note that the design ξ^* corresponds to the full factorial design. For $k \geq 4$ it is possible to construct a locally optimal design with the number of points less than 2^k. Assume that $k \geq 4$. Let ν be a natural number such that

$$2^{\nu-1} \geq k, \ \nu \leq k. \tag{2.5}$$

Let $z_{(1)}, \dots, z_{(n)}, n = 2^\nu$ be distinct vertices of the hypercube $[-1, 1]^\nu$. Assign to the number $j = \nu + 1, \dots, k$ a vector $(j_1, \dots, j_\alpha)$ whose components are distinct numbers from the set $\{1, \dots, \nu\}$, with α an odd number, $\alpha \geq 3$. The assignment is such that distinct vectors correspond to distinct numbers, which is possible since the number of the distinct vectors equals

$$\sum_{i=2}^{[\nu/2]} C_\nu^{2i-1} = 2^{\nu-1} - \nu \geq k - \nu.$$

Introduce the vectors $\tilde{z}_{(i)} = (\tilde{z}_{(i)1}, \dots, \tilde{z}_{(i)k})^T$, $i = 1, 2, \dots, n$,

$$\begin{aligned} \tilde{z}_{(i)j} &= z_{(i)j}, \ j = 1, \dots, \nu, \\ \tilde{z}_{(i)j} &= z_{(i)j_1} \dots z_{(i)j_\alpha}, \ j = \nu + 1, \dots, k. \end{aligned}$$

Now consider the vectors $x_{(i)} = (x_{(i)1}, \dots, x_{(i)k})^T$, $i = 1, \dots, n$, which are vertices of the hyperparallelepiped described above and correspond to the vectors $\tilde{z}_{(i)}$ in such a way that $\text{sign}(x_{(i)j} - b_j) = \text{sign}(\tilde{z}_{(i)j})$, $i = 1, \dots, n = 2^\nu$, $j = 1, \dots, k$. Let

$$\xi^+ = \{x_{(1)}, \dots, x_{(n)}; \frac{1}{n}, \dots, \frac{1}{n}\}.$$

Theorem 2. *If $b \in [-1/2, 1/2]^k$, and $k \geq 4$, then ξ^+ is a locally optimal design for the estimation of an extremum point of the function (2.1).*

Note that with k satisfying the inequality (2.5) we can construct a locally optimal design ξ^+ with $n = 2^\nu$ distinct points. Let ν^* be the minimal number satisfying (2.5) for a given k, and set $n^*(k) = 2^\nu$. It seems important that when k increases the corresponding value $n^*(k)$ increases very slowly. For example, with $5 \leq k \leq 10$ we have $n^*(k) = 16$.

4. DISCUSSION

Consider the results obtained in the context of the Box-Wilson procedure. It is evident that at the last stage of this procedure we have already a rough estimate of the extremum point and it is only necessary to make it more exact.

If the extremum point lies rather far from the boundary of the design region, it is reasonable to use the design $\alpha\xi_1 + (1-\alpha)\xi_2$, where ξ_1 is the usual D-optimal design and ξ_2 is the locally optimal design given by Theorem 1. It can be shown that the asymptotically best value of α is $\alpha = \alpha^*/\sqrt{N}$, where α^* does not depend on N.

However the calculation of α^* is reasonably combined in practice with the elaboration of a sequential procedure . This problem exceeds the scope of the present article and will be considered elsewhere. If the extremum point is close to the boundary, or outside the design region, our approach can also be applied. However, in this case, Theorem 1 does not give a locally optimal design. This also will be the subject of further study.

5. APPENDIX

Proof of Theorem 1

Introduce the notation $f^{(1)}(x) = f^{(1)}(x,b)$, $f^{(2)}(x) = f^{(2)}(x,b)$,

$$\begin{aligned}
f^{(1)}(x,b) &= (b_1 - x_1, \ldots, b_k - x_k)^T, \\
f^{(2)}(x,b) &= \big((x_1-b_1)^2, \ldots, (x_k-b_k)^2\ , \\
&\quad (x_1-b_1)(x_2-b_2), \ldots, (x_{k-1}-b_{k-1})(x_k-b_k), 1\big)^T\ , \\
d_s(x,\xi,X) &= \left(f^{(1)}(x) - X^T f^{(2)}(x)\right)^T M_s^{-1}(\xi)\left(f^{(1)}(x) - X^T f^{(2)}(x)\right).
\end{aligned}$$

Note that for a fixed $b = b^{(0)}$, the matrix $\bar{M}(\xi)$ coincides with the information matrix for the linear regression function $\bar{\theta}^T f(x,b)$. Therefore a locally optimal design for estimation of an extremum point of the regression function (2.1) is a truncated D-optimal design for estimation of the first k parameters of the regression function $\bar{\theta}^T f(x,b)$ and *vice versa*. We can apply the corresponding equivalence theorem from Karlin & Studden, 1966, §10.8, which we reformulate in a form convenient for our purpose:

Lemma 5.1. *The following definitions are equivalent:*

1) a design $\tilde{\xi}$ *maximizes* $\det M_s(\xi)$,

2) there exists a matrix X *such that*

$$M_3(\tilde{\xi})X = M_2(\tilde{\xi}), \quad \max_x d_s(x, \tilde{\xi}, X) = k.$$

Besides, if one of these conditions is fulfilled then $d_s(\tilde{x}_{(i)}, \tilde{\xi}, X) = k$, $(i = 1, \ldots, n)$ *where* $\tilde{x}_{(i)}, i = 1, \ldots, n$ *are the points of the design* $\tilde{\xi}$.

Consider now the design ξ^*. Due to the symmetry properties of the hypercube, we can restrict consideration to the case $b \in [0,1]^k$. It is easy to verify that

$$\begin{aligned} M_1(\xi^*) &= \operatorname{diag}\{(1-b_1)^2, \ldots, (1-b_k)^2\},\ M_2 = 0,\ M_s = M_1, \\ M_3 &= M_3(\xi^*) = \begin{pmatrix} G_1^T G_1 & 0 & G_1^T \\ 0 & G_2 & 0 \\ G_1 & 0 & 1 \end{pmatrix}, \end{aligned}$$

where

$$\begin{aligned} G_1 &= ((1-b_1)^2, \ldots, (1-b_k)^2) \text{ is a row vector, and} \\ G_2 &= 4 \operatorname{diag}\{(1-b_1)^2(1-b_2)^2, \ldots, (1-b_{k-1})^2(1-b_k)^2\} \end{aligned}$$

is a diagonal matrix of size $k(k-1)/2 \times k(k-1)/2$.

Let

$$X^T = \left(\operatorname{diag}\left\{ \frac{1}{2(1-b_1)}, \ldots, \frac{1}{2(1-b_k)} \right\}, O, \left(-\frac{1-b_1}{2}, \ldots -\frac{1-b_k}{2} \right)^T \right),$$

where O is the zero matrix of size $k \times k(k-1)/2$. Then

$$M_3 X = M_2 = 0 \tag{2.6}$$

and

$$d_s(x, \xi^*, X) = \sum_{i=1}^{k} s_i^2(x_i),$$

where

$$s_i(x_i) = \frac{(x_i + 1 - 2b_i)^2 - 2(1-b_i)^2}{2(1-b_i)^2}.$$

The function $s_i(x_i)$ is a quadratic polynomial and $s_i'(x_i) = 0$ with $x_i = 2b_i - 1$. Since for $b_i \in [0, 1/2]$ we have

$$s_i^2(1) = 1,\ s_i^2(2b_i - 1) = 1,\ s_i^2(-1) = \left(1 - \frac{2b_i}{(1-b_i)^2}\right)^2 \le 1,$$

then $\max_{x_i \in [-1,1]} s_i^2(x_i) = 1$ and $\max_{x \in [-1,1]^k} d(x, \xi^*, X) = k$. Therefore, from Lemma 5.1, the design ξ^* is a locally optimal design under the condition $b \in [0, 1/2]^k$.

Now let $1 \geq b_i > 1/2$ for some $i = i^*$. Suppose that ξ^* is a locally optimal design. An arbitrary solution of equation (2.6) has the form

$$X^T = (W^T \vdots O \vdots V),$$

where $W = (w_{ij})_{i,j=1}^k$ is an arbitrary matrix, O is the zero matrix of size $k \times k(k-1)/2$ and

$$V = \left(-\sum_{i=1}^k w_{i1}(1-b_i)^2, \ldots, -\sum_{i=1}^k w_{ik}(1-b_i)^2 \right)^T.$$

Therefore the function $d_s(x, \xi^*, X)$ is of the form

$$\sum_{i=1}^k \left\{ \left(b_i - x_i - \sum_{j=1}^k w_{ji} \left[(x_j - b_j)^2 - (1-b_j)^2 \right] \right)^2 / (1-b_i)^2 \right\}.$$

For an arbitrary $j = 1, \ldots, k$, consider the points $x_{(1)} = (2b_1 - 1, \ldots, 2b_k - 1)$ and $x_{(2)} = (2b_1 - 1, \ldots, 2b_{j-1} - 1, 1, 2b_{j+1} - 1, \ldots, 2b_k - 1)$. From Lemma 5.1 $d_s(x, \xi^*, X)'_{x_i} = 0$ for $x = x_{(1)}$ and arbitrary $i = 1, \ldots, k$ and for $x = x_{(2)}$ and $i \neq j$. From this it follows that $w_{ij} = 0$ for $i \neq j$ and $w_{ii} = 1/(2(1-b_i))$. Therefore, $d_s(x, \xi^*) > k$ at the point $\bar{x} = (\bar{x}_1, \ldots, \bar{x}_k)^T$, where $\bar{x}_i = -|b_i|/b_i$, $i = i^*$ and $\bar{x}_i = 2b_i - 1$ otherwise. This contradicts our supposition. Hence, in this case, ξ^* is not a locally optimal design. ■

Proof of Theorem 2

It was shown in the proof of Theorem 1 that the conditions

$$\begin{aligned} M_1(\xi) &= \operatorname{diag}\{(1-|b_1|)^2, \ldots, (1-|b_k|)^2\}, \\ M_2(\xi) &= O \end{aligned} \tag{2.7}$$

are sufficient for local optimality of the design ξ if $b \in [-1/2, 1/2]^k$. Now let $\alpha = 1, \ldots, \nu, j_1, \ldots, j_\nu \in \{1, \ldots, \nu\}$, $n = 2^\nu$. Introduce vectors $w_{(j_1, \ldots, j_\alpha)} \in \mathcal{R}^n$ by the formula

$$w_{(j_1, \ldots, j_\alpha)i} = z_{(i)j_1} \ldots z_{(i)j_\alpha}, \ i = 1, \ldots, n.$$

It is easy to check that all these vectors are orthogonal to the vector $(1, \ldots, 1)$. Therefore,

$$\sum_{i=1}^n z_{(i)j_1} \ldots z_{(i)j_\alpha} = 0, \ \alpha = 1, \ldots, \nu,$$

if $\alpha = 1$ or $\alpha \geq 2$ and at least two of the numbers $j_1, \ldots, j_\alpha$ are distinct.

From these relationships we can verify by an immediate calculation that conditions (2.7) are satisfied for the design $\xi = \xi^+$. ■

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