Biometrika (1984), 71, 2, pp. 381-5
Printed in Great Britain

Minimizing the maximum variance of the difference between two estimated responses

BY S. HUDA AND RAHUL MUKERJEE
Division of Theoretical Statistics and Mathematics, Indian Statistical Institute, Calcutta, India

SUMMARY

Minimization of the variance of the difference between estimated responses at two points maximized over all pairs of points in the design space is taken as the criterion for selecting designs. Optimal designs under the criterion are derived for second-order polynomial models when the design spaces are spherical.

Some key words: Optimal design; Response surface; Rotatable design; Second-order model.

1. INTRODUCTION

It has been recognized in recent years that even in response surface designs the response at individual locations may not always be the main interest (Herzberg, 1967; Atkinson, 1970; Hader & Park, 1978; Box & Draper, 1980). Often the difference between estimated responses at two points may be of greater interest. If the possibility of bias in the assumed model (Box & Draper, 1959) is excluded, then in such situations the designs minimizing the variance of the difference maximized over all pairs of points in the design space may be preferable to others. In this paper the optimal designs under this minimax criterion are derived for second-order polynomial regression in spherical regions.

Consider the design set-up where the k quantitative factors $x_1, \ldots, x_k$ take values in the k-ball $\mathscr{X} = \{x = (x_1, \ldots, x_k); \Sigma x_i^2 \leqslant R^2\}$ and the expected value of the observation $y(x)$ at point x is given by

$$E\{y(x)\} = f'(x)\beta = \beta_0 + \sum_{i=1}^{k} \beta_i x_i + \sum_{i=1}^{k} \sum_{j=1}^{i} \beta_{ij} x_i x_j, \tag{1}$$

a polynomial of degree two. It is assumed that the observations are uncorrelated and have a common variance σ^2 which without loss of generality is taken to be unity. A design ξ is a probability measure on $\mathscr{X}$. The design is of order two if it allows the estimation of all the parameters in (1). If N experiments are performed according to ξ then

$$N \operatorname{cov}(\hat{\beta}) = M^{-1}(\xi), \quad N \operatorname{var}\{\hat{y}(x)\} = f'(x) M^{-1}(\xi) f(x),$$

where $\hat{\beta}$ is the least squares estimator of β, $\hat{y}(x)$ is the corresponding estimated response at x and $M(\xi) = \int f(x) f'(x) \xi(dx)$ is the information matrix of ξ.

2. THE OBJECTIVE FUNCTION

It can be shown that for polynomial regression in spherical regions, the optimal designs under the type of criterion considered are also rotatable (Kiefer, 1960). Hence only rotatable designs (Box & Hunter, 1957) need be considered. For a second-order design ξ the conditions for rotatability are

$$\int x_i^2\,\xi(dx) = \lambda_2,\quad \int x_i^4\,\xi(dx) = 3\int x_i^2 x_j^2\,\xi(dx) = 3\lambda_4 \quad (i \neq j),\quad \lambda_4 > k(k+2)^{-1}\lambda_2^2,$$

and all other moments up to order four are zero.

Herzberg (1967) showed that, for a rotatable design, the variance of the difference between estimated responses at two points depends on the distances of the points from the centre and the angle subtended by the points at the centre. Herzberg (1967) also showed that for a second-order rotatable design,

$$N\,\mathrm{var}\{\hat{y}(z)-\hat{y}(x)\} = \lambda_2^{-1} r_1 + (2\lambda_4)^{-1}[r_2^2 - \{(k+2)\lambda_4 - k\lambda_2^2\}^{-1} \times (\lambda_4 - \lambda_2^2)(\rho_x^2 - \rho_z^2)^2], \quad (2)$$

where

$$\rho_x^2 = \Sigma x_i^2,\quad \rho_z^2 = \Sigma z_i^2,\quad r_j^2 = (\rho_x^{2j} + \rho_z^{2j} - 2\rho_x^j \rho_z^j \cos^j\theta),\quad \theta = \cos^{-1}\{\Sigma x_i z_i (\rho_x \rho_z)^{-1}\}.$$

Hence, our objective is to find

$$\min_{\lambda_2,\lambda_4} \max V(\lambda_2, \lambda_4, \rho_x, \rho_z, \theta),$$

where the maximum is over $\rho_x, \rho_z \in [0, R]$, $\theta \in [0, \pi]$ and where $V(\lambda_2, \lambda_4, \rho_x, \rho_z, \theta)$ is the right-hand side of (2). Without loss of generality, in what follows, we assume that $R = 1$. Then $\lambda_2 < k^{-1}$ and $\lambda_4 \leqslant \lambda_2(k+2)^{-1}$, equality being achieved if the design is supported at the centre and the surface of the k-ball only.

3. The minimax solution

Equation (2) may be rewritten as

$$V(\lambda_2, \lambda_4, \rho_x, \rho_z, \theta) = \lambda_2^{-1} r_1 + [2\lambda_4\{(k+2)\lambda_4 - k\lambda_2^2\}]^{-1}\{(k+1)\lambda_4 - (k-1)\lambda_2^2\} \times (\rho_x^2 - \rho_z^2)^2 + \lambda_4^{-1}\rho_x^2\rho_z^2(1-\cos^2\theta),$$

from which it is readily seen that for fixed λ_2 and any ρ_x, ρ_z and θ the variance function is strictly decreasing in λ_4. Therefore, we only need to consider the designs with $\lambda_4 = \lambda_2(k+2)^{-1}$. For these designs, writing

$$V(\lambda_2, \rho_x, t, \theta) = V\{\lambda_2, \lambda_2(k+2)^{-1}, \rho_x, \rho_z, \theta\}$$

where $\rho_z = t\rho_x$, we get

$$V(\lambda_2, \rho_x, t, \theta) = (2\lambda_2)^{-1}\{2\rho_x^2(1+t^2-2t\cos\theta) + 2\rho_x^4 t^2(k+2)(1-\cos^2\theta) + \rho_x^4(1-t^2)^2(k+1)\} + (1-k\lambda_2)^{-1}\rho_x^4(1-t^2)^2. \quad (3)$$

From (3) it can be seen that for any fixed λ_2 and any t, θ the value of $V(\lambda_2, \rho_x, t, \theta)$ is maximized by making ρ_x as large as possible. Therefore, we can take $\rho_x = 1$ and rewrite the specifications as

$$\min_{\lambda_2} \max V(\lambda_2, t, \theta),$$

where the maximum is over $t \in [0, 1]$, $\theta \in [0, \pi]$ and where $V(\lambda_2, t, \theta)$ is given by the right-hand side of (3) with $\rho_x = 1$.

Partial derivatives $\partial V(\lambda_2, t, \theta)/\partial\theta$ and $\partial^2 V(\lambda_2, t, \theta)/\partial\theta^2$ show that $\theta = 0$ always gives a minimum and $\theta = \pi$ gives a maximum when $0 \leqslant t \leqslant (k+2)^{-1}$. For $(k+2)^{-1} < t \leqslant 1$, the maximum is at $\theta = \cos^{-1}[-\{t(k+2)\}^{-1}]$ and $\theta = \pi$ is a minimum. Therefore, writing $V(\lambda_2, t)$ for $V(\lambda_2, t, \theta)$ maximized with respect to θ, we have that

$$V(\lambda_2, t) = \begin{cases} V_1(\lambda_2, t) = (2\lambda_2)^{-1}\{2(1+t)^2 + (k+1)(1-t^2)^2\} \\ \qquad + (1-k\lambda_2)^{-1}(1-t^2)^2 & (0 \leqslant t \leqslant (k+2)^{-1}), \\ V_2(\lambda_2, t) = (2\lambda_2)^{-1}[2\{1+(k+3)t^2\} + (k+1)(1-t^2)^2] \\ \qquad + \{(k+2)\lambda_2\}^{-1} + (1-k\lambda_2)^{-1}(1-t^2)^2 & ((k+2)^{-1} < t \leqslant 1). \end{cases}$$

The problem, therefore, is to find the λ_2 which minimizes $V(\lambda_2)$, the value of $V(\lambda_2, t)$ maximized with respect to t. The solution is given by the following lemma, the proof of which is provided in the Appendix.

LEMMA 1. *For $k \geqslant 2$ the variance function $V(\lambda_2)$ is minimized by λ_2^* which is the root of the equation*

$$\lambda_2[2C + \lambda_2^{-1}(10 - C^{-1}) + 2C\{1 - 2(\lambda_2 C)^{-1}\}^{3/2}] = 4(k+3)^2(k+2)^{-1}, \qquad (4)$$

where $C = (k+1)(2\lambda_2)^{-1} + (1-k\lambda_2)^{-1}$

The roots of (4) provide the moments of designs optimal for minimizing the maximum variance of the difference between two estimated responses. Numerical solutions of (4) can be quickly found and the first row of Table 1 gives these for $k = 2$ to $k = 10$. Like the D-optimal designs our optimal designs put all the mass at the centre and the surface of the k-ball. The moments of these designs are fairly close to those of the D-optimal designs. However, the latter designs put slightly greater mass at the surface. The opposite holds when $k = 1$ as shown in the London Ph.D. thesis of S. Huda.

The designs obtained seem to perform well when judged by the more usual criteria. As an example, the D-efficiencies of these 'minimax' designs are given in the second row of Table 1, which shows that the efficiencies are always greater than 0·99. The efficiency at 0·9910 is a minimum for $k = 2$, then strictly increases and reaches 0·9998 for $k = 10$.

The performance of various designs under the criterion introduced may be judged by taking as a measure of efficiency the ratios of the maximum variance of the difference for these designs to that of the optimal designs. The third row of Table 1, for example, provides the efficiencies of the D-optimal designs under the criterion. As expected, the D-optimal designs perform well but not so well as our optimal designs do under the D-optimality criterion, particularly for small values of k. Hence, if the differences between estimated responses are of greater interest than estimated responses at individual locations, other things being equal, it is better to use the designs derived here.

Table 1. *Value of λ_2^* for optimal design for minimizing maximum variance; D-efficiency E_k of minimax design; efficiency e_k of D-optimal design*

	$k = 2$	$k = 3$	$k = 4$	$k = 5$	$k = 6$	$k = 7$	$k = 8$	$k = 9$	$k = 10$
λ_2^*	0·4396	0·3083	0·2371	0·1924	0·1618	0·1396	0·1227	0·1094	0·0987
E_k	0·9910	0·9959	0·9979	0·9988	0·9993	0·9995	0·9996	0·9998	0·9998
e_k	0·9477	0·9731	0·9841	)·9900	0·9933	0·9948	0·9961	0·9972	0·9978

Two figures are provided to illustrate the behaviour of the variance function. Figure 1 shows $V(\lambda_2, t)$ for some typical values of λ_2 close to the optimal value λ_2^*. There is a local maximum at $t_0(\lambda_2) < (k+2)^{-1}$. The overall maximum occurs at $t_0(\lambda_2)$ for $\lambda_2 > \lambda_2^*$ and at the boundary point $t = 1$ for $\lambda_2 < \lambda_2^*$, while for $\lambda_2 = \lambda_2^*$ the values at these two points are equal.

Figure 2 shows that $V_2(\lambda_2)$, the maximum value of $V_2(\lambda_2, t)$ for $t \in ((k+2)^{-1}, 1]$, is strictly decreasing in λ_2 while $V_1(\lambda_2)$, the maximum value of $V_1(\lambda_2, t)$ for $t \in [0, (k+2)^{-1}]$, has a single minimum. The optimal value λ_2^* of λ_2 as given by Lemma 1 corresponds to the point of intersection of the curves corresponding to $V_1(\lambda_2)$ and $V_2(\lambda_2)$.

Herzberg (1967) suggested that λ_2 and λ_4 should be taken as large as possible without violating the constraint $\lambda_4 > k\lambda_2^2(k+2)^{-1}$. However, this prescription may be misleading. Our results show that λ_4 should have the value at its upper bound and also λ_2 should be increased but only up to the optimal value λ_2^*. Any design with λ_2 too close to the bound k^{-1} would result in too large a value for $V_1(\lambda_2)$ and hence $V(\lambda_2)$ as seen in Fig. 2.

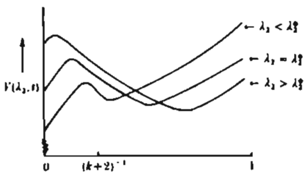

Fig. 1. A rough sketch of $V(\lambda_2, t)$ for some typical values of λ_2 close to λ_2^*.

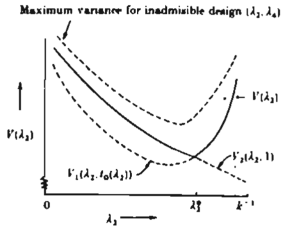

Fig. 2. A rough sketch of $V(\lambda_2)$.

4. COMMENTS

The optimal designs derived here are not necessarily exact, i.e. discrete. However, many discrete designs have moments close to those of the optimal designs. Using the criterion under consideration the performance of some discrete designs has been investigated. For example, in two dimensions the design with one centre point and seven equally spaced points on the unit circle has maximum variance 14·2857. For the optimal design the maximum variance is 14·2119, giving the discrete design an efficiency of 99·48%. Similarly, the four-dimensional design consisting of two centre points and the vertices of a 'cube + cross-polytope' inscribed on the unit sphere was found to have 97·34% efficiency.

If differences in response at points close together are of greater interest then the approach adopted by Atkinson (1970) may be more suitable.

We are grateful to Professor D. R. Cox for suggesting the problem, to Dr Bikas K. Sinha for his active interest in the work and to the referee for helpful comments.

Appendix

Proof of Lemma 1

For t in $[0, 1]$, $V_2(\lambda_2, t)$ is convex in t with a single minimum which is in $[0, (k+2)^{-1}]$ if and only if $\lambda_2 \leqslant (2k+3)\{(k+2)(2k+1)\}^{-1} = \bar{\lambda}_2$. Also $V_2(\lambda_2, t) \geqslant V_1(\lambda_2, t)$ for t in $[0, 1]$. Hence if $\lambda_2 \leqslant \bar{\lambda}_2$, it follows that

$$V(\lambda_2) = V_2(\lambda_2, 1) = (k+3)^2\{(k+2)\lambda_2\}^{-1}$$

since

$$\max\{V_2(\lambda_2, 0), V_2(\lambda_2, (k+2)^{-1})\} \leqslant V_2(\lambda_2, 1).$$

For $\lambda_2 > \bar{\lambda}_2$,

$$V(\lambda_2) = \max[V_2\{\lambda_2, (k+2)^{-1}\}, V_2(\lambda_2, 1), V_1\{\lambda_2, t_0(\lambda_2)\}]$$
$$= \max[V_2(\lambda_2, 1), V_1\{\lambda_2, t_0(\lambda_2)\}],$$

where

$$t_0(\lambda_2) = \tfrac{1}{2}[1 - \{1 - 2(\lambda_2 C)^{-1}\}^{\frac{1}{2}}]$$

is the maximum of $V_1(\lambda_2, t)$ in $[0, (k+2)^{-1}]$.

Hence, because

$$V_1\{\lambda_2, t_0(\lambda_2)\} = \tfrac{1}{4}[2C + \lambda_2^{-1}(10 - C^{-1}) + 2C\{1 - 2(\lambda_2 C)^{-1}\}^{3/2}],$$

$V_1\{\bar{\lambda}_2, t_0(\bar{\lambda}_2)\} < V_2(\bar{\lambda}_2, 1)$ and $V_2(\lambda_2, 1)$ is decreasing in λ_2,

$$\min_{\lambda_2} V(\lambda_2) = \min_{\lambda_2 > \bar{\lambda}_2} \max[V_2(\lambda_2, 1), V_1\{\lambda_2, t_0(\lambda_2)\}]. \tag{A1}$$

Since for $k \geqslant 3$ and t in $[0, (k+2)^{-1}]$, $V_1(\lambda_2, t)$ is increasing in λ_2 provided $\lambda_2 > \bar{\lambda}_2$ and $t_0(\lambda_2)$ is in $[0, (k+2)^{-1}]$, it follows that $V_1\{\lambda_2, t_0(\lambda_2)\}$ is increasing in λ_2 for $\lambda_2 > \bar{\lambda}_2$. Also $V_2(\lambda_2, 1)$ is decreasing in λ_2. Hence by (A1) and the detailed expressions for $V_1\{\lambda_2, t_0(\lambda_2)\}$, $V_2(\lambda_2, 1)$, the lemma follows. Elementary considerations establish the result for $k = 2$.

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[*Received March* 1983. *Revised December* 1983]