Biometrika (1985), 72, 1, pp. 173–8
Printed in Great Britain

Minimax second- and third-order designs to estimate the slope of a response surface

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Summary

Designs for estimating the slope of a response surface are considered. Minimization of the variance of the estimated slope maximized over all points in the factor space is taken as the optimality criterion. Optimal designs under the minimax criterion are derived for second- and third-order polynomial regression over spherical regions.

Some key words: Optimal design; Rotatable design; Second-order design; Slope of a response surface; Third-order design.

1. Introduction

In recent years it has been recognized that even in response surface designs often the difference between estimated responses at two points may be of greater interest rather than the response at individual locations. Herzberg (1967) and Box & Draper (1980) derived forms of variance function for the difference when the design used is rotatable. Huda & Mukerjee (1984) obtained optimal second-order designs for spherical regions under the criterion of minimizing the variance maximized over all pairs of points.

If differences at points close together in the factor space are involved, the estimation of the local slope of the response surface becomes important. The pioneering work in this area is by Atkinson (1970) and the problem has subsequently been taken up by many other researchers (Ott & Mendenhall, 1972; Murthy & Studden, 1972; Myres & Lahoda, 1975; Hader & Park, 1978).

Clearly, the mean squared error of the estimated slope at a point depends on the point and some of the above mentioned authors indicate the construction of optimal designs that minimize the mean squared error, averaged over the factor space with respect to a suitable weight measure. The present paper, on the other hand, considers a different criterion, namely minimizing the variance of the estimated slope maximized over all points in the factor space, and constructs optimal designs under this minimax criterion for second- and third-order polynomial regressions over spherical regions.

2. Minimax second-order designs

Suppose that 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 that the expected value of the observation $y(x)$ at point x is

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

a second-degree polynomial. The observations are assumed to be uncorrelated and homoscedastic, the common variance being, without loss of generality, taken to be unity. A design ξ, which is a probability measure on $\mathscr{X}$, is of order two if it allows the estimation of all the parameters in (1). If N experiments are performed according to ξ then $N\operatorname{cov}(\hat{\beta}) = M^{-1}(\xi)$, where $\hat{\beta}$ is the least squares estimator of β and $M(\xi) = \int f(x)f'(x)\xi(dx)$ is the information matrix of ξ.

It can be shown that for polynomial regression in spherical regions, optimal designs under the present type of criterion are symmetric (Kiefer, 1960). Hence, restricting to symmetric designs, we observe that for a second-order design ξ the conditions for symmetry are

$$\int x_i^2\,\xi(dx) = \alpha_2, \quad \int x_i^4\,\xi(dx) = \alpha_4, \quad \int x_i^2 x_j^2\,\xi(dx) = \alpha_{22} \quad (i \neq j),$$
$$\alpha_2 > 0, \quad \alpha_4 > \alpha_{22} > 0, \quad \alpha_4 + (k-1)\alpha_{22} > k\alpha_2^2, \tag{2}$$

and all other moments up to order four are zero.

If $y(x)$ denotes the estimated response at $x \in \mathscr{X}$, the vector of estimated slopes along the factor axes is given by

$$d\hat{y}/dx = (\partial\hat{y}/\partial x_1, \ldots, \partial\hat{y}/\partial x_k)'.$$

Then arranging the elements in β in the order

$$\beta = (\beta_0, \beta_1, \ldots, \beta_k, \beta_{11}, \ldots, \beta_{kk}, \beta_{12}, \ldots, \beta_{k-1,k})',$$

it can be shown that $d\hat{y}/dx = H\hat{\beta}$, where

$$H = [0, I_k, 2\operatorname{diag}(x_1, \ldots, x_k), H^*].$$

Here the matrix H^* may be computed easily but the details of H^* are not required for our purpose and it is enough to observe that H^* is such that the diagonal elements of $H^*H^{*\prime}$ are

$$\sum_{j \neq i=1}^{k} x_j^2 \quad (i = 1, \ldots, k).$$

One can now obtain the covariance matrix of dy/dx and consider the variance of the estimated slope averaged over all directions. Following Atkinson (1970), this is equivalent to considering the trace of the covariance matrix and the minimax design will be that which minimizes this trace maximized over all points in $\mathscr{X}$. Since

$$N\operatorname{cov}(d\hat{y}/dx) = \operatorname{cov}(H\hat{\beta}) = HM^{-1}(\xi)H',$$

if one computes $M^{-1}(\xi)$ under (2) and observes the structure of H, it follows, after some simplification, that the trace of this covariance matrix is

$$\alpha_2^{-1}k + [4(\alpha_4 - \alpha_{22})^{-1}\{1 - D(\alpha_{22} - \alpha_2^2)\} + \alpha_{22}^{-1}(k-1)]\rho_x^2, \tag{3}$$

where

$$\rho_x^2 = \sum_{i=1}^{k} x_i^2, \quad D = \{\alpha_4 + (k-1)\alpha_{22} - k\alpha_2^2\}^{-1}.$$

Note that (3) is a function only of ρ_x^2 even though the design has been assumed to be only symmetric and not necessarily rotatable.

If, without loss of generality, the radius R of the spherical design region is taken as unity, then noting that the coefficient of ρ_x^2 in (3) is nonnegative, it follows that (3) is maximum over the factor space when $\rho_x^2 = 1$ and this maximum, after some rearrangement of terms, can be expressed as

$$\alpha_2^{-1} k + \alpha_{22}^{-1}(k-1) + 4k^{-1}(\alpha_4 - \alpha_{22})^{-1}(k-1) + 4k^{-1} D, \tag{4}$$

where $0 < \alpha_2 < k^{-1}, \alpha_4 > \alpha_{22} > 0, k\alpha_2^2 < \alpha_4 + (k-1)\alpha_{22} \leqslant \alpha_2$. For fixed α_2 and α_{22}, clearly (4) is decreasing in α_4 and is a minimum when $\alpha_4 = \alpha_2 - (k-1)\alpha_{22}$, in which case (4) becomes

$$\alpha_2^{-1} k + \alpha_{22}^{-1}(k-1) + 4k^{-1}(\alpha_2 - k\alpha_{22})^{-1}(k-1) + 4(k\alpha_2)^{-1}(1-k\alpha_2)^{-1}, \tag{5}$$

with $0 < \alpha_2 < k^{-1}, 0 < \alpha_{22} \leqslant \alpha_2(k+2)^{-1}$. Simple differentiation shows that for fixed α_2, expression (5) is a minimum with respect to α_{22} when $\alpha_{22} = (k+2)^{-1}\alpha_2$, and if this is substituted in (5) the resulting expression, as a function of α_2, is a minimum when $\alpha_2 = \{k + 2(k+4)^{-\frac{1}{2}}\}^{-1} = \alpha_{20}$, say.

Thus for the minimax design $\alpha_2 = \alpha_{20}$ as stated above, and

$$\alpha_{22} = (k+2)^{-1}\alpha_{20}, \quad \alpha_4 = 3(k+2)^{-1}\alpha_{20}.$$

Since then $\alpha_4 = 3\alpha_{22}$, the minimax design is rotatable (Box & Hunter, 1957). In fact, like the D-optimal designs, the optimal designs under the minimaxity criterion put the entire mass at the centre and on the surface of the k-ball. Using the standard notation for rotatable designs, one may write $\alpha_2 = \lambda_2$ and $\alpha_4 = 3\alpha_{22} = 3\lambda_4$. The values of λ_2 leading to the minimax designs and certain other interesting comparisons between our minimax designs and the standard D-optimal designs are tabulated for $2 \leqslant k \leqslant 8$ in §4.

3. Minimax third-order designs

Here the factor space $\mathscr{X}$ and the linear model are as in the preceding section with the only change that

$$E\{y(x)\} = \beta_0 + \sum_{i=1}^{k} \beta_i x_i + \sum_{j=1}^{k} \sum_{i=1}^{j} \beta_{ij} x_i x_j + \sum_{u=1}^{k} \sum_{j=1}^{u} \sum_{i=1}^{j} \beta_{iju} x_i x_j x_u,$$

a third-degree polynomial.

In the third-order case symmetry alone does not ensure that the trace of the dispersion matrix of $d\hat{y}/dx$ will be a function of ρ_x^2; in fact, this can be readily verified by considering the simplest situation with $k = 2$. In view of the findings in the second-order case, only rotatable designs will be considered. This is also justified following Kiefer (1960) since it can be shown analogously that the optimal design under our criterion will also be rotatable. For a third-order design the conditions for rotatability are

$$\int x_i^2 \,\xi(dx) = \lambda_2, \quad \int x_i^4 \,\xi(dx) = 3 \int x_i^2 x_j^2 \,\xi(dx) = 3\lambda_4 \quad (i \neq j),$$

$$\int x_i^6 \,\xi(dx) = 5 \int x_i^4 x_j^2 \,\xi(dx) = 15 \int x_i^2 x_j^2 x_u^2 \,\xi(dx) = 15\lambda_6 \quad (i \neq j \neq u),$$

$$\lambda_2 > 0, \quad (k+2)\lambda_4 > k\lambda_2^2, \quad (k+4)\lambda_2\lambda_6 > (k+2)\lambda_4^2,$$

and all other moments up to order six are zero.

Then if one makes use of the expressions for $M(\xi)$ and $M^{-1}(\xi)$ for such designs as by

Gardiner, Grandage & Hader (1959) and Box & Draper (1980) and proceeds exactly as for second-order designs, one obtains the trace of the covariance matrix of $d\hat{y}/dx$ as $a(\lambda)+b(\lambda)\rho_x^2+c(\lambda)\rho_x^4$, where

$$a(\lambda) = D_1 k(k+4)\lambda_6,$$
$$b(\lambda) = D_2\{k(k+3)\lambda_4-(k-1)(k+2)\lambda_2^2\}-2D_1(k+2)\lambda_4,$$
$$c(\lambda) = \tfrac{1}{2}D_1\lambda_6^{-1}\{k(k+5)\lambda_2\lambda_6-(k^2+3k-4)\lambda_4^2\},$$
$$D_1 = \{(k+4)\lambda_2\lambda_6-(k+2)\lambda_4^2\}^{-1}, \quad D_2 = [\lambda_4\{(k+2)\lambda_4-k\lambda_2^2\}]^{-1}, \quad \rho_x^2 = \sum_{i=1}^{k} x_i^2.$$

Since $(k+4)\lambda_2\lambda_6 > (k+2)\lambda_4^2$, it can be seen that $c(\lambda) > 0$; but $b(\lambda)$ may be positive or negative. Hence, if we assume as before that $R = 1$ without loss of generality, it is evident that the quantity $a(\lambda)+b(\lambda)\rho_x^2+c(\lambda)\rho_x^4$ is maximum at either $\rho_x = 1$ or at $\rho_x = 0$ according as $b(\lambda)+c(\lambda)$ is positive or not. As such, our objective function, namely the trace of the covariance matrix of $d\hat{y}/dx$ maximized over the factor space, becomes, say,

$$\phi(\lambda) = a(\lambda)+\max\{b(\lambda)+c(\lambda), 0\}, \tag{6}$$

which we have to minimize by suitably choosing $\lambda_2, \lambda_4, \lambda_6$.

If $R = 1$, then $\lambda_4 < (k+2)^{-1}\lambda_2$ and if we apply this condition, partial differentiation with respect to λ_6 shows $a(\lambda)+b(\lambda)+c(\lambda)$ to be decreasing in λ_6 for fixed λ_2 and λ_4. The same holds trivially for $a(\lambda)$. Therefore, $\phi(\lambda)$ is decreasing in λ_6 for fixed λ_2 and λ_4, and in order to minimize $\phi(\lambda)$ one should take λ_6 at its maximum possible value for given λ_2 and λ_4.

Now if μ be a probability measure over $[0,1]$, then subject to the constraints $\int z^i\mu(dz) = h_i$ $(i = 1, 2)$, the maximum of $\int z^3\mu(dz)$ is attained if μ has a support over exactly two points namely $(1-h_1)^{-1}(h_1-h_2) = z_0$, say, and 1. This can be proved (Karlin & Studden, 1966, Ch. 2) by observing that the function

$$l(z) = (1+z+z^2)\{(1-h_2)^{-1}(1+z)+(1-h_1)^{-1}h\}^{-1},$$

where

$$h = -(h_1-h_2)(2-h_1-h_2)\{(1-h_2)(1+h_1-2h_2)\}^{-1},$$

is a minimum for $0 \leqslant z \leqslant 1$ at z_0, and hence the inequality

$$(1+z+z^2)(1-z) \geqslant l(z_0)\{(1-h_2)^{-1}(1-z^2)+(1-h_1)^{-1}h(1-z)\}$$

holds for $0 \leqslant z \leqslant 1$, providing an upper bound for z^3 in this range which is attainable if and only if $z = z_0$ or 1.

In view of the above, for given λ_2, λ_4, in order to maximize λ_6, the design measure ξ should put all the mass at the surface of the ball and an inner spherical shell: incidentally, the same phenomenon happens with the D-optimal designs (Galil & Kiefer, 1979). Denoting by ρ the radius of the inner shell, and w the mass distributed uniformly over it, one gets

$$\lambda_2 = k^{-1}(1-w+w\rho^2), \quad \lambda_4 = \{k(k+2)\}^{-1}(1-w+w\rho^4),$$
$$\lambda_6 = \{k(k+2)(k+4)\}^{-1}(1-w+w\rho^6), \tag{7}$$

and, accordingly, the objective function (6) becomes, say,

$$\phi_1(w,\rho) = a_1(w,\rho)+\max\{b_1(w,\rho)+c_1(w,\rho), 0\},$$

where, for $0 < w, \rho < 1$,

$$a_1(w,\rho) = B(1-w+w\rho^6)\,k^2,$$

$$b_1(w,\rho) = (1-w+w\rho^4)^{-1}(k-1)(k+2)^2 - 4\{w(1-w)(1-\rho^2)^2\}^{-1} - 2B(1-w+w\rho^4)\,k(k+2),$$

$$c_1(w,\rho) = \tfrac{1}{2}(1-w+w\rho^6)^{-1}(k^2+3k-4)\,k(k+4) + B(1-w+w\rho^2)\,k(k+8),$$

$$B = \{w(1-w)\rho^2(1-\rho^2)^2\}^{-1}.$$

The form of the function ϕ_1 is too cumbersome to allow analytical solution. Following Galil & Kiefer (1979), we therefore proceed numerically. We start with the function $a_1(w,\rho)+b_1(w,\rho)+c_1(w,\rho)$ and obtain numerically the combination of w and ρ that minimizes this over $0 < w, \rho < 1$. If for this combination of w and ρ, $b_1(w,\rho)+c_1(w,\rho) > 0$, then clearly this gives the optimal solution in terms of minimization of $\phi_1(w,\rho)$. This procedure operates successfully for $2 \leqslant k \leqslant 8$ and the optimal combinations of w and ρ are given in §4. Then it is routine to compute $\lambda_2, \lambda_4, \lambda_6$ from (7). Results for $k \geqslant 9$ have not been derived since the available rotatable exact designs for such cases require too many trials to be of practical use. However, it is felt from our computational experience that the method will be successful even for $k = 9$ and 10 and possibly for still higher values of k.

4. Computational results

The optimal choices of design parameters for second- and third-order designs are given in Table 1, which shows also some comparisons between our designs and the D-optimal

Table 1. *Values of optimal design parameters for minimax design; D-efficiency E_k of minimax design; efficiency e_k of D-optimal design*

		$k=2$	$k=3$	$k=4$	$k=5$	$k=6$	$k=7$	$k=8$
Second-order design	λ_2	0·355	0·266	0·212	0·176	0·151	0·131	0·116
	E_k	0·960	0·963	0·967	0·971	0·974	0·977	0·979
	e_k	0·909	0·898	0·899	0·902	0·906	0·911	0·914
Third-order design	ρ	0·504	0·529	0·545	0·556	0·564	0·570	0·574
	w	0·465	0·381	0·319	0·271	0·234	0·205	0·181
	E_k	0·951	0·935	0·930	0·931	0·935	0·937	0·939
	e_k	0·899	0·851	0·823	0·806	0·796	0·789	0·786

ones. The D-efficiencies of the minimax designs appear to be fairly satisfactory. The D-efficiency of a design is defined in the usual way by taking pth root of the ratio of determinants, where p is the number of parameters. To judge the D-optimal designs under the minimaxity criterion, we take as a measure of efficiency the ratios of the maximum trace of the dispersion matrix of the estimated slope vector for the D-optimal designs to that of the minimax designs. The D-optimal designs perform well but not so well as our optimal designs do under the criterion of D-optimality. In making these comparisons, the findings of Galil & Kiefer (1979) have been used.

The efficiency of some exact designs under the minimax criterion has been investigated. For example in the second-order case with $k = 3$ the 'cube + cross − polytope' design with some centre points has a maximum efficiency of approximately 0·95 attained when only three centre points are added.

ACKNOWLEDGEMENT

The authors are grateful to the referee for his constructive suggestions.

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[*Received May* 1984. *Revised August* 1984]