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MINIMAX SECOND-ORDER DESIGNS FOR DIFFERENCE BETWEEN ESTIMATED RESPONSES IN EXTRAPOLATION REGION

S. HUDA

Department of Statistics, King Saud University, Riyadh, Saudi Arabia

Rahul MUKERJEE

Stat-Math Division, Indian Statistical Institute, Calcutta, India

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Abstract: Minimization of the variance of the difference between estimated response at two points maximized over all pairs of points in the extrapolation region is taken as the criterion for selecting designs. Optimal designs under the criterion are derived for second-order models.

Keywords: extrapolation region, optimal designs, response surface designs, second order.

1. Introduction and preliminaries

In recent years it has been recognized that even in response surface designs the difference between estimated responses at two points is often of greater interest than the estimated response at an individual location in the factor space (see Herzberg, 1967; Atkinson, 1970; Hader and Park, 1978; Box and Draper, 1980; Mukerjee and Huda, 1985). In such situations, designs minimizing the variance of the difference between estimated responses at two points maximized over all pairs of points in the region of interest may be preferable to others. Huda and Mukerjee (1984) obtained the optimal second-order designs under this 'minimax' criterion when the region of interest and the region of experimentation are the same hypersphere. In the present paper, optimal second-order designs are derived taking the region of interest to be the extrapolation region consisting of a hyperspherical shell surrounding a hyperspherical region of experimentation.

Let $x_1, \ldots, x_k$ be k quantitative factors under investigation and let $\mathscr{X} = \{x = (x_1, \ldots, x_k); \sum_{i=1}^{k} x_i^2 \leqslant 1\}$ be the region of experimentation. The region of interest $\bar{\mathscr{X}}$ is the extrapolation region given by $\bar{\mathscr{X}} = \{x;\ 1 \leqslant \sum_{i=1}^{k} x_i^2 \leqslant R^2\}$. Let the expected value of the response $y(x)$ at point x be given by a second degree polynomial regression model. Observations are assumed to be uncorrelated and to have a common variance which, without loss of generality, is taken to be unity.

A design ξ is a probability measure on $\mathscr{X}$. In what follows we shall only be concerned with rotatable designs since it is well-known (Kiefer, 1960) that for polynomial regression in hyperspherical regions, the optimal designs under the type of criterion considered are also rotatable. Herzberg (1967) derived that for a second-order rotatable design

$$\begin{aligned} N \operatorname{Var}\{\hat{y}(x) - \hat{y}(z)\} &= c^{-1}\left(\rho_x^2 + \rho_z^2 - 2\rho_x\rho_z \cos\theta\right) \\ &\quad + f^{-1}\rho_x^2\rho_z^2(1 - \cos^2\theta) \\ &\quad + \left\{2f\left((k+2)f - kc^2\right)\right\}^{-1} \\ &\qquad \times \left\{(k+1)f - (k-1)c^2\right\}\left(\rho_x^2 - \rho_z^2\right)^2, \quad (1) \end{aligned}$$

where $\hat{y}(x)$, $\hat{y}(z)$ are the estimated responses at points x, z, $\rho_x^2 = \sum_{i=1}^k x_i^2$, $\rho_z^2 = \sum_{i=1}^k z_i^2$, $\theta = \cos^{-1}(\sum_{i=1}^k x_i z_i / \rho_x \rho_z)$. N is the number of experiments performed according to ξ, $c = \int_{\mathscr{X}} x_i^2 \xi(dx)$, $f = \frac{1}{3}\int_{\mathscr{X}} x_i^4 \xi(dx)$ $(i = 1, 2, \ldots, k)$. Since the region $\mathscr{X}$ is a hypersphere of unit radius, we have (cf. Box and Hunter (1957))

$$0 < c < 1/k, \quad kc^2/(k+2) < f \leqslant c/(k+2). \tag{2}$$

The rest of the paper considers the problem of selecting c and f, subject to (2), such that the maximum of $N \operatorname{Var}\{\hat{y}(x) - \hat{y}(z)\}$, over $x, z \in \bar{\mathscr{X}}$, is minimized.

2. The minimax design

As in Huda and Mukerjee (1984), it can be readily seen from (1) that the only admissible designs for the problem under consideration are those for which $f = c/(k+2)$. Further, one of the points maximizing $N \operatorname{Var}\{\hat{y}(x) - \hat{y}(z)\}$ is always on the outer surface of $\bar{\mathscr{X}}$, i.e., at a distance R from the origin. Hence the problem may be rewritten as

$$\underset{0<c<1/k}{\text{Minimize}} \quad \underset{1/R \leqslant t \leqslant 1, 0 \leqslant \theta \leqslant \pi}{\text{Maximum}} \; V(c, t, \theta)$$

where $t = \rho_z / R$ and

$$\begin{aligned} V(c, t, \theta) = {} & c^{-1}R^2(1 + t^2 - 2t\cos\theta) \\ & + c^{-1}R^4 t^2 (1 - \cos^2\theta)(k+2) \\ & + \{2c(1-kc)\}^{-1} R^4 (1-t^2)^2 \\ & \quad \times \{(k+1) - (k-1)(k+2)c\}. \end{aligned}$$

Partial differentiation with respect to θ shows that for fixed c, $t (0 < c < 1/k,\ 1/R \leqslant t \leqslant 1)$, $V(c, t, \theta)$ has a unique maximum over θ $(0 \leqslant \theta \leqslant \pi)$ at $\theta_0 = \cos^{-1}\{-(R^2 t(k+2))^{-1}\}$. Writing $V(c, t)$ for $V(c, t, \theta_0)$, it may be seen that

$$V(c, t) = h_1(c) + h_2(c)t^2 + h_3(c)t^4,$$

where $h_1(c)$, $h_2(c)$, $h_3(c)$ are functions exclusively of c and $h_3(c) > 0$, for every c $(0 < c < 1/k)$. Hence for each fixed c, the maximum of $V(c, t)$, over t, is attained either at $t = 1$ or at $t = 1/R$. Thus the problem reduces to finding c $(0 < c < 1/k)$ such that $\max\{V(c, 1), V(c, 1/R)\} = V(c)$, say, is minimized.

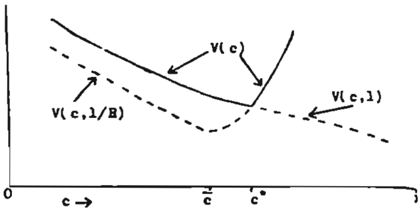

Fig. 1.

It is easily seen that $V(c, 1/R) \leqslant V(c, 1)$ for all c such that $0 < c \leqslant c^*$, where

$$\begin{aligned} c^* = {} & (R^2+1)(k+3) \\ & /\{(R^2+1)(k+2)(k+1) - 4\} \\ & < 1/k. \end{aligned}$$

Also $V(c, 1/R) = V(c, 1)$ if and only if $c = c^*$. Now $V(c, 1) = \{(k+2)R^2 + 1\}^2/(k+2)c$ is strictly decreasing in c. Further, differentiation with respect to c shows that $V(c, 1/R)$ has a unique minimum at $c = \bar{c}$, where

$$\bar{c} = \left[k + k^{1/2}(R^2 - 1) \Big/ \left\{ (k+3)\left(R^2 + \frac{1}{k+2}\right) + \tfrac{1}{2}(R^2-1)^2(k+1) \right\}^{1/2} \right]^{-1}$$

It may be seen that $\bar{c} < c^*$ for all $k \geqslant 1$. Therefore, for the optimal design we must have $c = c^*$. A rough sketch of $V(c, 1)$, $V(c, 1/R)$ and $V(c)$ is provided in Figure 1 in order to illustrate our derivation of the optimal design.

3. Comments

From the value of c^* it can be seen that the optimal design puts mass

$$a(k, R) = \{2(R^2+1) - 4\} \Big/ \{(R^2+1)(k+2)(k+1) - 4\}$$

at the origin and mass $1 - a(k, R)$ uniformly distributed over the surface of the hypersphere $\mathscr{X}$. Thus our optimal design always puts greater mass on the surface than that put by second-order D-optimal design, which puts mass

$$k(k+3)/\{(k+1)(k+2)\}$$

on the surface. However, in the limit $R \to \infty$, our optimal design converges to the D-optimal design. On the other hand, $\lim_{R \to 1}$, $a(k, R) = 0$, and as expected the optimal design converges to a singular design putting all the mass on the surface of the hypersphere $\mathscr{X}$. Construction of discrete (exact) designs with $c = c^*$ is not considered here. However, many of the available second-order rotatable designs can be seen to have c close to the optimal value c^*.

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