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MINIMAX CENTRAL COMPOSITE DESIGNS TO ESTIMATE THE SLOPE OF A SECOND-ORDER RESPONSE SURFACE

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SUMMARY

Minimization of the variance of the slope maximized over all points in the design region is taken as the optimality criterion. For spherical regions and second-order models the performance of central composite rotatable designs under this criterion is investigated. The number of centre points needed to maximize the efficiency is derived.

Keywords : Optimal design, Response surface, Second-order designs, Central composite designs.

Introduction

Even in response surface designs the difference between responses at two points may be more important than the response at individual locations (Huda and Mukerjee, [3]). If differences at adjacent points are involved, estimation of the local slope of the response surface acquires importance. Many researchers have taken up the problem of estimating slope since the pioneering work by Atkinson [1]. Recently, Mukerjee and Huda [4] introduced minimization of the variance of the estimated slope maximized over all points in the design region as a criterion and derived the optimal second- and third-order designs for spherical regions. The optimal designs under this minimax criterion were found to belong to the class of rotatable designs introdueed by Box and Hunter [2].

Unfortunately, the theoretically optimal designs are often not implementable. The mass distribution may have irrational weights which do not correspond to any discrete design. It is therefore important to study the performance of discrete designs which the experimenter can actually use. Central composite second-order rotatable designs are readily available and often used in experimental work. In this paper we examine the performance of these designs and determine the number of centre points required to maximize the efficiency.

2. Variance of the Slope

Consider k quantitative factors $x_1, \ldots, x_k$ taking values in a k-ball X assumed, without loss of generally, to be of unit radius, i.e., $X = \{x = (x_1, \ldots x_k) : \Sigma\, x_i^2 \leqslant 1\}$ and suppose that the response $y(x)$ at point x is given by the second-order polynomial

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

Let the observations be uncorrelated, with a common variance which, without loss of generality, is taken to be unity.

A second-order design ξ is a probability measure on X which allows estimation of all the parameters in (1). If N experiments are performed in accordance with ξ then $N \operatorname{cov}(\hat{\beta}) = M^{-1}(\xi)$, where $\hat{\beta}$ is the least squares estimator of β and $M(\xi) = \int_X f(x) f'(x)\, \xi(dx)$ is the information matrix of ξ. The vector of estimated slopes along the factor axes at point x is given by

$$d\hat{y}(x)/dx = (\partial\hat{y}(x)/\partial x_1, \ldots, \partial\hat{y}(x)/\partial x_k)' \text{ where } \hat{y}(x) = f'(x)\,\hat{\beta}.$$

The variance of the estimated slope averaged over all directions is $\operatorname{tr}\{\operatorname{cov}(d\hat{y}(x)/dx)\}$. Let $v(x) = N \operatorname{tr}\{\operatorname{cov}(d\hat{y}(x)/dx)\}$. Then under the minimax criterion the objective is to

$$\operatorname*{Min}_{\xi} \operatorname*{Max}_{x \epsilon X} v(x)$$

In Mukerjee and Huda [4] it was shown that $v(x)$ attains its maximum when x is at the surface of X and that the optimal design is a rotatable one. A second-order design ξ is rotatable if

$$\int_X x_i^2\, \xi(dx) = \lambda_2, \int_X x_i^4\, \xi(dx) = 3 \int_X x_i^2 x_j^2\, \xi(dx) = 3\lambda_4 \; (i \neq j = 1, \ldots, k),$$

and all other design moments up to order four are zero. For a rotatable design, it can be shown that the maximum value of $v(x)$ is

$$\begin{aligned} v = k\lambda_2^{-1} + \{k(k+3)\,\lambda_4 - (k-1)\,(k+2)\,\lambda_2^2\}\,[\lambda_4\,\{(k \\ + 2)\,\lambda_4 - k\lambda_2^2\}]^{-1}, \end{aligned} \tag{2}$$

which is minimized, as shown in Mukerjee and Huda [4], when

$$\lambda_4 = (k+2)^{-1}\,\lambda_2 = (k+2)^{-1}\,\{k + 2\,(k+4)^{-1/2}\}^{-1} \qquad (3)$$

In practice, we are always concerned with discrete designs for which the weights are integer multiples of N^{-1}. Thus, the optimal design moments specified in (3) may not be achieved by implementable designs. Therefore, it is of interest to know how well an implementable design performs in comparison with the optimal design. As a measure of efficiency we take the ratio of the value of (2) for the optimal design to that for the design under consideration.

3. Central Composite Rotatable Designs

A central composite design consists of the point-sets $2^{-p}S\,(a, \ldots, a)$, $S(b, 0, \ldots, 0)$ and n_c replicates of the origin where $S(x_1, \ldots, x_k)$ denotes all distinct permutations of $(\pm\, x_1, \ldots, \pm\, x_k)$ and $2^{-p}\,S(x_1, \ldots, x_k)$ denotes any 'Resolution V' 2^{-p}th fraction of it. We shall consider only the smallest such fractions. In order that a design be second-order rotatable, It is necessary to have $b^2 = 2^{(k-p)/2}a^2$. Further, to ensure that the outermost points of the design lie on the surface of the design region, we need $a^2 = [\max\,\{2^{(k-p)/2}, k\}]^{-1}$. These give

$$\begin{aligned} \lambda_2 &= \{2^{k-p} + 2^{(k-p+2)/2}\}\,a^2/(2^{k-p} + 2k + n_c), \\ \lambda_4 &= 2^{k-p}\,a^4/(2^{k-p}) + 2k + n_c). \end{aligned} \qquad (4)$$

Substituting (4) in (2), we obtain ν as a function n_c. Treating n_c as a continuous variable and differentiating ν with respect to n_c we obtain the value of n_c minimizing ν given as a root of a simple quadratic equation in n_c. Since n_c needs to be an integer, the best value of n_c is given by one of the pair closest to the root. As an example consider the case $k = 4$ where for the minimax design, using (2) and (3), we obtain $\nu = 146.834$. For the central composite second-order rotatable design, $f = 0$, $a^2 = 0.25$, $b^2 = 1$, $\lambda_2 = 6/(24 + n_c)$, $\nu = 4(24 + n_c)\,(3 + 2n_c)/3n_c$. Clearly, treating n_c as continuous, ν is minimized when $n_c = 3\sqrt{2}$. Therefore, the optimal integer value of n_c is one of 4 or 5. Substituting these values of n_c in ν it is found that the optimal n_c is 4 when $\nu = 177.333$ and hence the design has 82.8% efficiency.

The best values of n_c, corresponding to efficiencies indicated by $*$ are given in Table 1 for $k = 2(1)10$.

4. Discussion

Theoretically optimal designs are often unimplementable and usually

TABLE 1—EFFICIENCY E OF CENTRAL COMPOSITE DESIGNS

k	f	a^2	N	n_c	E	(*percentage*)
2	0	2^{-1}	$8 + n_c$	0	0	
				1	47.42	
				2	59.75	
				3	62.68	*
				4	62.24	
3	0	3^{-1}	$14 + n_c$	0	1.48	
				1	56.50	
				2	69.04	
				3	72.35	
				4	72.46	*
				5	71.23	
4	0	4^{-1}	$24 + n_c$	0	0	
				1	62.93	
				2	77.01	
				3	81.57	
				4	82.80	*
				5	82.55	
5	1	5^{-1}	$26 + n_c$	0	37.10	
				1	68.71	
				2	74.89	
				3	76.20	*
				4	75.84	
6	1	6^{-1}	$44 + n_c$	0	6.04	
				1	70.48	
				2	81.96	
				3	85.71	
				4	86.92	
				5	87.02	*
				6	86.56	

Table 1 (*contd. on page* 158)

Table 1 (*contd. from page* 157)

k	f	a^2	N	n_c	E	(*percentage*)
7	1	8^{-1}	$78 + n_c$	0	24.99	
				1	58.81	
				2	67.95	
				3	71.73	
				4	73.52	
				5	74.36	
				6	74.68	
				7	74.69	*
				8	74.50	
8	2	8^{-1}	$80 + n_c$	0	0	
				1	74.40	
				2	86.17	
				3	90.32	
				4	92.05	
				5	92.72	
				6	92.83	*
				7	92.62	
9	2	$2^{-7/2}$	$146 + n_c$	0	46.20	
				1	56.29	
				2	60.39	
				3	62.47	
				4	63.63	
				5	64.29	
				6	64.66	
				7	65.54	*
				8	64.90	

Table 1 (*contd. on page* 159)

Table 1 (*contd. from page* 158)

k	f	a^2	N	n_c	E (*percentage*)
10	3	$2^{-7/2}$	$148 + n_c$	0	34.63
				1	64.07
				2	71.39
				3	74.47
				4	76.01
				5	76.82
				6	77.24
				7	77.41
				8	77.43 *
				9	77.34

serve as guidelines. In order to have some idea about the performance of discrete designs which can be implemented, these designs should be compared with optimal designs. A given design, even if not optimal, may be preferred to others if it has higher efficiency than the others.

In this paper we have studied the performance of central composite second-order rotatable designs under the minimax criterion introduced in Mukerjee and Huda [4]. For $k = 2$ to $k = 10$ these designs seem to perform reasonably well under our criterion and are known to perform much better under the more usual criteria such as D-optimality. Very few centre points are needed to reach the maximum efficiency. Near the optimal value, there is little change in efficiency on variation of the number of centre points. In practice, the experimentor may use larger number of centre points than that recommended by our findings, especially if he is also concerned with other considerations like estimation of error variance with high precision.

Another class of second-order rotatable designs worth investigation using the minimax criterion is that consisting of designs derived through balanced incomplete block designs. Work in that direction is currently in progress.

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