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On Performance of Minimax Second-Order Slope-Estimating Designs Under Variations of the Model

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Summary

Minimization of the maximum variance of the estimated slope is taken as the optimality criterion. For regression in spherical regions optimal designs under the criterion are obtained for various second-order models. These designs are compared with one another under variation of the model. Performance of central composite designs under model variation is also investigated.

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

Introduction

In many practical situations, efficient estimation of the derivatives of the response function may be as important or possibly more important than estimation of the mean response. Since the designs that may enjoy desirable features in estimating the parameters or in estimating the mean response may not enjoy the same features in estimating the slopes, it is important to consider designs that are constructed with the objective of estimating slopes. Atkinson [1] appears to be the first in realizing this. For subsequent major works dealing with slopes the readers are requested to see the references in Mukerjee and Huda [5] and Myers, Khuri and Carter [6].

Mukerjee and Huda [5] developed optimal designs for minimization of the variance of the estimated slope maximized over all points in the factor space for the full second-order and third-order polynomial models over a spherical region. In the present paper we obtain the minimax designs for various second-order submodels of the full model. Further, we investigate the performance of the optimal designs under variation of the model.

2. *Minimax second-order designs.*

Consider a response surface design set-up with k quantitative factors $x_1,...,x_k$

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

$$E\{y(x)\} = f'(x)\,\beta$$

where f(x) is the vector of linearly independent polynomial terms in x and β is the corresponding vector of parameters. Let the observations be uncorrelated and homoscedastic, the common variance being, without loss of generality, taken to be unity.

A design ζ is a probability measure on X which allows estimation of β. If N experiments are performed according to ζ then N cov $(\hat{\beta}) = M^{-1}(\zeta)$ where $\hat{\beta}$ is the least squares estimator of β and $M(\zeta) = \int_X f(x) f'(x) \zeta(dx)$ is the information matrix of ζ. Further, $\hat{y}(x) = f'(x)\hat{\beta}$ is the estimated response and

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

is the vector of estimated slopes along the factor axes at point x. The variance of the estimated slope averaged over all directions is $tr\{cov(d\hat{y}(x)/dx)\}$. Let $V(x)=N\, tr\{cov(d\hat{y}(x)/dx)\}$ be the normalized variance. Then under the minimax criterion the objective is to

$$\underset{\zeta}{\text{Min}}\ \underset{x \in X}{\text{Max}}\ V(x)$$

Consider the following second-order models:

(F) $f'(x) = (1, x_1^2, \ldots, x_k^2;\ x_1x_2, \ldots, x_{k-1}x_k;\ x_1, \ldots, x_k)$,

(1) $f'(x) = (1, x_1^2, \ldots, x_k^2;\ x_1, \ldots, x_k)$,

(2) $f'(x) = (1, x_1x_2, \ldots, x_{k-1}x_k;\ x_1, \ldots, x_k)$,

(3) $f'(x) = (1, x_1^2, \ldots, x_k^2;\ x_1x_2, \ldots, x_{k-1}x_k)$,

(4) $f'(x) = (1, x_1^2, \ldots, x_k^2)$,

(5) $f'(x) = (1, x_1x_2, \ldots, x_{k-1}x_k)$.

Model (F) is the full second-order model and the remaining are various second-order submodels of it. Note that we are only considering models that are symmetric in the x_i's. It was shown in Mukerjee and Huda [5] that for model (F), the variance function V(x) attains its maximum when x is at the surface of X and that the optimal design is a rotatable one supported at the surface of X and the origin only. A second-order design ζ is rotatable (Box and Hunter, 1957) if

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

and all other moments upto order four are zero. When a second- order rotatable design ζ is used for model (F),

$$V(x) = \frac{2\left\{(k+1)\,\lambda_4 - (k-1)\,\lambda_2^2\right\}\rho_x^2}{\lambda_4\left\{(k+2)\,\lambda_4 - k\,\lambda_2^2\right\}} + \frac{(k-1)}{\lambda_4}\,\rho_x^2 + \frac{k}{\lambda_2}$$

where $\rho_x^2 = x'\,x = \Sigma\, x_i^2$.

Hence, for the model (F),

$$V = \operatorname*{Max}_{x \in X} V(x) = V_a + V_b + V_c,$$

where

$$V_a = \frac{2\left\{(k+1)\,\lambda_4 - (k-1)\,\lambda_2^2\right\}}{\lambda_4\left\{(k+2)\,\lambda_4 - k\,\lambda_2^2\right\}}\,,\quad V_b = \frac{(k-1)}{\lambda_4}\,,\quad V_c = \frac{k}{\lambda_2}$$

These three terms above arise from the components $(1,\ x_1^2, \ldots, x_k^2)$, $(x_1x_2, \ldots, x_{k-1}x_k)$ and $(x_1, \ldots, x_k)$, respectively in the model.

The minimum value of V is

$$V_{min} = \operatorname*{Min}_{\zeta} V = \{2 + k(k+4)^{1/2}\}^2$$

corresponding to the design ζ_F having $\lambda_4 = \lambda_2 / (k+2) = [(k+2)\,\{k+2/(k+4)^{1/2}\}]^{-1}$..

For the other models under consideration, V, the maximum value of V(x), is simply combinations of V_a, V_b and V_c. Further, it can be readily seen that the minimax designs will all have $\lambda_4 = \lambda_2 / (k+2)$ as in the case of model (F). Denoting the minimax designs for model (1), . . . , (5), by $\zeta_1, \ldots, \zeta_5$, respectively, it can also be shown that ζ_2 and ζ_5 are identical, have $\lambda_2 = 1/k$ and are singular in the context of other models. As an example consider the case of Model (1) for which

$$V = V_a + V_c = \frac{2\left\{(k+1)\,\lambda_4 - (k-1)\,\lambda_2^2\right\}}{\lambda_4\left\{(k+2)\,\lambda_4 - k\,\lambda_2^2\right\}} + \frac{k}{\lambda_2}$$

$$= \frac{2}{k}\left[\frac{(k-1)}{\lambda_4} + \frac{2}{\{(k+2)\,\lambda_4 - k\,\lambda_2^2\}}\right] + \frac{k}{\lambda_2}$$

which is strictly decreasing in λ_4. Since X is the unit sphere, $\lambda_4 \leq \lambda_2 / (k+2)$. Hence, for the minimax design ζ_1 we must have $\lambda_4 = \lambda_2/(k+2)$. On substituting this value of λ_4 in the expression we obtain

$$V = \frac{(3k+2)}{\lambda_2} + \frac{4}{1-k\,\lambda_2}$$ which is clearly minimized when

$\lambda_2 = 1 / [k+2\{k/(3k+2)\}^{1/2}]$ and the minimum value of V is

$$V_{min} = [\,2 + \{\,k\,(3k+2)\,\}^{1/2}\,]^2.$$

In Table 1 we present the formulae for V, V_{min} and λ_2 corresponding to the minimax designs for the various second-order models.

Table 1. Values of V, V_{min} and optimal λ_2

Model	V	V_{min}	λ_2
(F)	$V_a + V_b + V_c$	$\{\,2 + k\,(k+4)^{1/2}\,\}^2$	$\{\,k+2\,/\,(k+4)^{1/2}\,\}^{-1}$
(1)	$V_a + V_c$	$[2 + \{\,k\,(3k+2)\,\}^{1/2}\,]^2$	$[\,k+2\,\{\,k\,/\,(3k+2)\,\}^{1/2}\,]^{-1}$
(2)	$V_b + V_c$	$k\,(\,k^2 + 2k - 2)$	$1/k$
(3)	$V_a + V_b$	$\{\,2 + k\,(k+3)^{1/2}\,\}^2$	$[\,k + 2/\,(k+3)1/2)\,]^{-1}$
(4)	V_a	$2\,[2^{1/2} + \{\,k\,(k+1)\,\}^{1/2}\,]^2$	$[\,k + \{\,2k\,/\,(k+1)\,\}^{1/2}\,]^{-1}$
(5)	V_b	$(\,k-1\,)\,k\,(\,k+2\,)$	$1/k$

3. *Performance under model variation.*

The design ζ_2 ($\equiv \zeta_5$) is singular in the context of models other than (2) and (5). However, the designs ζ_F, ζ_1, ζ_3 and ζ_4 are non-singular for all the models and hence we can study the performance of these designs under various models. For any design ζ the minimax efficiency under a given model is defined as $V_{min}/V(\zeta)$ where $V(\zeta)$ is the value of V on using ζ and V_{min} is the minimum value of V on using minimax design for the corresponding model. Let $E_{F,1}, \ldots, E_{F,5}$ denote the efficiency of ζ_F under models (1), . . . , (5), respectively. Analogously, define $E_{i,j}$ as the efficiency of ζ_i under model (j) (i = 1, 3, 4 ; j = F, 1, 2, 3, 4, 5). Using the results stated in Section (2) we derive that

$$E_{F,1} = [\,2+\{k(3k+2)\}^{1/2}\,]^2 / [\{(3k+2)+2(k+4)^{1/2}\}\,\{k+2/(k+4)^{1/2}\}],$$

$$E_{F,2} = 1/[1+2/\{k(k+4)^{1/2}\}] = E_{F,5}\ ,$$

$$E_{F,3} = \{2+k(k+3)^{1/2}\}^2 / [\{k+2/(k+4)^{1/2}\}\,\{k(k+3)+2(k+4)^{1/2}\}],$$

$$E_{F,4} = [2+\{2k(k+1)\}^{1/2}]^2 / [\{2k+4/(k+4)^{1/2}\}\{(k+1)+(k+4)^{1/2}\}],$$

$$E_{1,F} = \{2+k(k+4)^{1/2}\}^2/[\{k+2k^{1/2}\}/(3k+2)^{1/2}\}\,\{k(k+4)+2(3k+2)^{1/2}/k^{1/2}\}],$$

$$E_{1,2} = 1/[1+2/\{k(3k+2)^{1/2}\}] = E_{1,5}\ ,$$

$$E_{1,3} = \{2+k(k+3)^{1/2}\}^2/[\{k+2k^{1/2}/(3k+2)^{1/2}\}\{k(k+3)+2(3k+2)^{1/2}/k^{1/2}\}],$$

$$E_{1,4} = 2[1+\{k(k+1)/2\}^{1/2}]^2/[\{k+2k^{1/2}/(3k+2)^{1/2}\}\{(k+1)+(3k+2)^{1/2}/k^{1/2}\}],$$

$$E_{3,F} = \{2+k(k+4)^{1/2}\}^2 / [\{k+2/(3k+2)^{1/2}\}\,\{k(k+4)+2(k+3)^{1/2}\}],$$

$$E_{3,1} = [2+\{k(3k+2)^{1/2}\}^2/[\{k+2/(k+3)^{1/2}\}\{(3k+2)+2(k+3)^{1/2}\}],$$

$$E_{3,2} = 1/[1+2/\{k(k+3)^{1/2}\}] = E_{3,5}\ ,$$

$$E_{3,4} = 2[1+\{k(k+1)/2\}^{1/2}]^2/[(k+2/(k+3)^{1/2}\}\,\{(k+1)+(k+3)^{1/2}\}],$$

$$E_{4,F} = \{2+k(k+4)^{1/2}\}^2 /[[k+\{2k/(k+1)\}^{1/2}][k(k+4)+\{8(k+1)/k\}^{1/2}]],$$

$$E_{4,1} = [2+\{k(3k+2)^{1/2}]^2 / [[k+\{2k/(k+1)\}^{1/2}][(3k+2)+\{8(k+1)/k\}^{1/2}]],$$

$$E_{4,2} = 1/[1+2^{1/2}/\{k(k+1)\}^{1/2}] = E_{4,5}\ ,$$

$$E_{4,3} = \{2+k(k+3)^{1/2}\}^2 / [[\,k+2^{1/2}\{k/(k+1)\}^{1/2}][k(k+3)+\{8(k+1)/k\}^{1/2}\,]].$$

From the results presented above it can be seen that all the efficiencies approach unity as k approaches infinity. However, for small values of k the efficiencies are quite different and can be far from unity. The actual numerical values of E_{ij}'s for k=2 to k=10 are provided in Table 2.

4. *Performance of Central Composite Designs*

The theoretically optimal designs considered in the earlier sections are all approximate designs. These designs are often unimplementable and can usually serve only as guidelines. In practice the experimenter is concerned with discrete (exact) designs for which it may be impossible to attain moments matching those of the theoretically optimal designs. None the less we may compare the available discrete designs with the optimal ones and implement those which perform well.

Table 2 : Numerical values of the efficiencies $E_{i,j}$'s (in %)

k	2	3	4	5	6	7	8	9	10
$E_{F,1}$	99.09	98.02	97.20	96.58	96.12	95.76	95.49	95.27	95.10
$E_{F,2}$	71.01	79.87	84.98	88.23	90.46	92.07	93.27	94.19	94.93
$E_{F,3}$	99.82	99.90	99.94	99.96	99.97	99.98	99.99	100.00	100.00
$E_{F,4}$	97.26	95.34	94.03	93.12	92.48	92.01	91.67	91.41	91.22
$E_{1,F}$	99.16	98.33	97.84	97.55	97.40	97.33	97.30	97.30	97.33
$E_{1,2}$	66.67	74.17	78.91	82.17	84.56	86.38	87.82	88.98	89.94
$E_{1,3}$	99.73	98.98	98.40	98.02	97.78	97.64	97.56	97.52	97.51
$E_{1,4}$	99.52	99.48	99.48	99.51	99.53	99.56	99.59	99.61	99.63
$E_{3,F}$	99.83	99.90	99.94	99.96	99.98	99.98	99.99	99.99	99.99
$E_{3,1}$	99.72	98.85	98.02	97.35	96.82	96.40	96.05	95.79	95.58
$E_{3,2}$	69.10	78.61	84.11	87.61	90.00	91.71	92.88	93.97	94.74
$E_{3,4}$	98.50	96.68	95.29	94.26	93.50	92.92	92.49	92.15	91.90
$E_{4,F}$	97.56	96.32	95.75	95.51	95.44	95.47	95.55	95.65	95.76
$E_{4,1}$	99.54	99.52	99.53	99.56	99.58	99.61	99.64	99.66	99.68
$E_{4,2}$	63.40	71.01	75.97	79.48	82.09	84.11	85.71	87.03	88.12
$E_{4,3}$	98.62	97.27	96.50	96.10	95.92	95.85	95.85	95.90	95.97

A class of discrete designs which are readily available and quite popular with the experimenters consists of the central composite second-order rotatable designs. A central composite design (CCD) is composed of the point-sets 2^{-p} s(a, . . . , a), s(b, 0, . . . , 0) and n_c replicates of the origin where s(x_1, . . . , x_k) denotes all distinct permutations of ($\pm x_1, \ldots, \pm x_k$) and 2^{-p} s(x_1, . . . , x_k) denotes any resolution V2^{-p}th fraction of it. We shall consider only the smallest of such fractions. For the design to be second-order rotatable it is necessary to have $b^2 = 2^{(k-p)/2} a^2$. Also since X is the unit ball the design has to be scaled so that the outermost points lie on the surface of X. This imposes the restriction that $a^2 = [\max \{k, 2^{(k-p)/2}\}]^{-1}$. Therefore, for a central composite design $N = 2^{k-p} + 2k + n_c$ and $\lambda_2 = \{2^{k-p} + 2^{(k-p+2)/2}\} a^2/N$, $\lambda_4 = 2^{k-p} a^4/N$.

In what follows we consider the efficiency of central composite designs. Let $E_{c,j}$ be the efficiency of central composite design when the model is Model (j) (j = F, 1, . . . , 5). For any k the values of $E_{c,j}$'s for various values of n_c may be readily computed. However, we present only the values of $E_{c,F}$, $E_{c,4}$, $E_{c,2}$ and $E_{c,5}$.

Since Model (F) is the 'largest' model and models (4) and (5) are the two 'smallest' models, $E_{c,j}$'s for other j's should lie between the values for these models. Tables 3,4 and 5 which follow provide the efficiencies for k=2 to k=10. The best values of n_c are the second largest ones among those for which efficiencies are tabulated.

Table 3 : Efficiency E_{cF} (in %) of CCD's

n_c \ k	2	3	4	5	6	7	8	9	10
0	00.00	01.95	00.00	42.68	06.74	26.55	00.00	49.22	36.58
1	75.55	74.33	75.97	79.04	78.65	64.29	80.14	59.96	67.67
2	95.19	90.83	92.46	86.16	91.46	74.28	92.81	64.33	75.40
3	99.85	95.19	98.47	87.66	95.64	78.42	97.29	66.55	78.65
4	99.15	95.33	99.96	87.24	96.99	80.38	99.15	67.78	80.28
5		93.71	99.66		97.11	81.29	99.87	68.49	81.14
6					96.59	81.65	99.99	68.89	81.57
7						81.65	99.77	69.08	81.76
8						81.44		69.13	81.78
9								69.09	81.69

5. *Discussion.*

Among the various second-order models considered, Model (5) is possibly the least useful one. It envisages a situation where the linear and quadratic main-effect terms are non-significant but the interaction terms are significant --- a highly unlikely set up. None the less the model was included in this study for the sake of completeness. For justification of considering optimal designs for other models, readers are requested to see Atkinson [2] who studied the performance of D-optimal designs under model variation.

From Table 2 it can be seen that ζ_3, the minimax design for Model (3), performs better on average than the other designs under model variation. This is to be somewhat expected. Model (3) includes all the second-order terms but not the linear terms. It is a model midway between the extremes Model (F) and Models (4) or (5). Thus Table 2 suggests that if the experimenter is not too sure of the correct second-order model, it will be better for him to use ζ_3.

Table 4 : Efficiency E_{c4} (in %) of CCD's

n_c \ k	2	3	4	5	6	7	8	9	10
0	00.00	00.91	00.00	07.49	01.99	08.46	00.00	20.77	18.18
1	60.32	53.35	48.92	56.29	46.38	34.45	41.71	33.77	33.61
2	85.30	76.55	72.69	72.37	67.75	49.48	62.90	42.38	47.39
3	95.80	87.67	85.55	80.35	79.66	59.08	75.36	48.44	56.33
4	99.52	92.91	92.81	84.43	86.81	65.51	83.33	52.88	62.51
5	99.85	94.98	96.87	86.37	91.24	70.04	88.69	56.23	66.98
6	98.43	95.27	99.00	87.07	94.00	73.30	92.39	58.81	70.32
7		94.50	99.88	86.99	95.66	75.67	95.00	60.84	72.86
8			99.95		96.58	77.41	96.83	62.45	74.82
9			99.47		96.98	78.67	98.12	63.74	76.36
10					97.01	79.58	98.99	64.77	77.56
11					96.76	80.21	99.55	65.60	78.52
12						80.63	99.86	66.27	79.26
13						80.88	99.99	66.80	79.85
14						80.99	99.97	67.23	80.30
15						80.99		67.56	80.64
16								67.81	80.89
17								68.00	81.07
18								68.13	81.18
19								68.21	81.23
20								68.26	81.24
21								68.26	81.20

Table 3, 4 and 5 illustrate the highly satisfactory performance of central composite designs. The maximum efficiencies achieved by the CCD's are generally extremely high. Only a small proportion of observations are needed at the centre points to achieve the maximum efficiencies. Further, near the maximum values the efficiencies are quite stable, i.e. there is little change when the number

Table 5 : Efficiency E_{c2} and E_{c5} (in %) of CCD's

	n_c \ k	2	3	4	5	6	7	8	9	10
$E_{c,2}$	0	100.00	95.96	100.00	87.03	97.16	81.51	100.00	68.92	81.76
	1	88.89	89.38	96.00	83.81	95.00	80.67	98.76	68.45	81.22
$E_{c,5}$	0	100.00	95.24	100.00	86.15	96.97	80.77	100.00	67.81	81.08
	1	88.89	88.89	96.00	82.96	94.81	79.75	98.76	67.35	80.54

of centre points is varied. The values of $E_{c,2}$ and $E_{c,5}$ are strictly decreasing as n_c is increased but for large k's the rate of decrease is very low.

It is to be noted that $E_{c,F}$'s were also considered in Huda [4] but the numerical values presented there were erroneous. The correct values presented in this paper were provided by Miss Manisha Gupta, a student of Dr. Aloke Dey, who pointed out the errors in a personal communication.

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