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PERFORMANCE OF SECOND-ORDER A-MINIMAX OPTIMAL DESIGNS FOR ESTIMATING SLOPES UNDER MODEL VARIATION

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ABSTRACT. A-minimax optimality is considered as a criterion for selecting designs to estimate the slopes of a response surface. Optimal designs under the criterion are obtainded for several second-order models over spherical regions. The relative perfomance of optimal designs is investigated.

1. INTRODUCTION

Huda and Al-Shiha (2000) generalized the concepts of A-, D- and E-optimality criteria to the A-, D- and E-minimax optimality criteria, respectively in order to consider the situation where primary interest of the experimenter is in estimation of axial slopes of the response surface. Under the A-minimax criterion the objective is to choose the design which minimizes the trace of the variance-covariance matrix of the estimated axial slopes at a point maximized over all points in the region of interest within the factor space. This criterion is in fact what had been simply called the "minimax criterion" in Mukerjee and Huda (1985) who provided the optimal designs for the full second- and third-order models over spherical regions.

In the present paper, assuming the regions of interest and experiment to be identical, A-minimax optimal designs are derived for several second-order models over spherical regions. In addition the performance of optimal designs for a given model when used as a design for other models is also investigated.

AMS Subject classification: 62K99, 62K05.
Key Words and Phrases: A-minimax designs, estimation of slopes, response surface, second-order designs.

Consider the standard response surface design set-up in which the response y depends on k quantitative factors $x_1, \ldots, x_k$ through a smooth relationship $y = \emptyset(\underline{x})$ where $\underline{x} = (x_1, \ldots, x_k)'$. The observation y_i on the response at point $\underline{x}_i = (x_{1i}, \ldots, x_{ki})'$ is given by $y_i = \emptyset(\underline{x}_i) + e_i$ where the e_i's are zero-mean uncorrelated random errors with a constant variance σ^2. Suppose further that $\emptyset(\underline{x}) = f'(\underline{x})\theta$ where $f'(\underline{x})$ is a row vector of p linearly independent functions of $\underline{x}$, and θ is the corresponding column vector of unknown parameters. A design ξ is a probability measure on the experimental region $\mathcal{X}$. If N trials are peformed according to ξ then $(N/\sigma^2)cov(\hat{\theta}) = M^{-1}(\xi)$ where $\hat{\theta}$ is the least squares estimator of θ and $M(\xi) = \int_{\mathcal{X}} f(\underline{x})f'(\underline{x})\xi(d\underline{x})$ is the information matrix of ξ. The least squares estimator of the response at the point $\underline{x}$ is $\hat{y}(\underline{x}) = f'(\underline{x})\hat{\theta}$. The column vector of estimated slopes along the axial directions at the point $\underline{x}$ is given by $d\hat{y}/d\underline{x} = (\partial\hat{y}(\underline{x})/\partial x_1, \ldots, \partial\hat{y}(\underline{x})/\partial x_k)' = H(\underline{x})\hat{\theta}$ where $H(\underline{x})$ is a $k \times p$ matrix whose i-th row is $\partial f'(\underline{x})/\partial x_i (i = 1, \ldots, k)$. Then denoting $(N/\sigma^2)Cov(d\hat{y}(\underline{x})/d\underline{x})$ by $V(\xi, \underline{x})$ we obtain that $V(\xi, \underline{x}) = H(\underline{x})M^{-1}(\xi)H'(\underline{x})$. Under the A-minimax optimality criterion the objective is to $min_\xi \max_{\underline{x}\epsilon\Re} trV(\xi, \underline{x})$ where $\Re$ is the region of interest.

In what follows we consider $\Re = \mathcal{X}$ where $\mathcal{X}$ is a spherical region of radius R. Without loss of generality, $\mathcal{X}$ is taken to be centered at the origin with radius $R = 1$. Further, $\emptyset(\underline{x})$ is taken to be corresponding to a second-order model. In view of the results in Mukerjee and Huda (1985) it is sufficient to restrict to the class of rotatable designs, a sub-class of the permutation-invariant symmetric designs. Rotatable designs were introduced by Box and Hunter (1957) and have $var\{\hat{y}(\underline{x})\}$ constant at points equidistant from the centre of the design.

2. MODELS AND THE OBJECTIVE FUNCTIONS

The six second-order models under consideration are the following

$$\begin{aligned}
M1 &: f'(\underline{x}) = f_1'(\underline{x}), \\
M2 &: f'(\underline{x}) = (f_1'(\underline{x}), f_2'(\underline{x})), \\
M3 &: f'(\underline{x}) = (f_1'(\underline{x}), f_3'(\underline{x})), \\
M4 &: f'(\underline{x}) = (f_1'(\underline{x}), f_2'(\underline{x}), f_3'(\underline{x})), \\
M5 &: f'(\underline{x}) = (1, f_3'(\underline{x})), \\
M6 &: f'(\underline{x}) = (1, f_2'(\underline{x}), f_3'(\underline{x})),
\end{aligned}$$

where

$$f_1'(\underline{x}) = (1, x_1^2, \ldots, x_k^2), f_2'(\underline{x}) = (x_1, \ldots, x_k) and f_3'(\underline{x}) = (x_1x_2, \ldots, x_{k-1}x_k).$$

Clearly, model $M1$ is a submodel of $M2$ and $M3$ while $M4$ is the full second-order model, containing all other models as submodels.

A second-order rotatable design ξ is characteized by only two non-zero moments, namely $\lambda_2 = \int_{\mathcal{X}} x_i^2 \xi(d\underline{x})$ and $\lambda_4 = \int_{\mathcal{X}} x_i^2 x_j^2 \xi(d\underline{x}) = \frac{1}{3} \int_{\mathcal{X}} x_i^4 \xi(d\underline{x})$ $(i \neq j = 1, \ldots, k)$. Since $\mathcal{X}$ is the unit ball, the restrictions on these moments are $0 < k\lambda_2^2 \leq (k+2)\lambda_4 \leq \lambda_2 \leq 1/k$ and for non-singularity of the design all inequalities except the second-last must be strict ones. Here non-singularity refers to estimability of all the parameters of a full second-order model.

Let $V_i(\xi, \underline{x})$ denote $V(\xi, \underline{x})$ for the i-th model. Then it is readily seen that $V_i(\xi, \underline{x})$ are given by

$$\begin{aligned}
V_1(\xi, \underline{x}) &= U_1(\xi, \underline{x}), \\
V_2(\xi, \underline{x}) &= U_1(\xi, \underline{x}) + U_2(\xi, \underline{x}), \\
V_3(\xi, \underline{x}) &= U_1(\xi, \underline{x}) + U_3(\xi, \underline{x}), \\
V_4(\xi, \underline{x}) &= U_1(\xi, \underline{x}) + U_2(\xi, \underline{x}) + U_3(\xi, \underline{x}), \\
V_5(\xi, \underline{x}) &= U_3(\xi, \underline{x}), \\
V_6(\xi, \underline{x}) &= U_2(\xi, \underline{x}) + U_3(\xi, \underline{x}),
\end{aligned}$$

where

$$\begin{aligned}
U_1(\xi, \underline{x}) &= \frac{2}{\lambda_4} Diag\{x_1^2, \ldots, x_k^2\} + \frac{4}{k}[\frac{1}{\{(k+2)\lambda_4 - k\lambda_2^2\}} - \frac{1}{2\lambda_4}]\underline{x}\underline{x}', \\
U_2(\xi, \underline{x}) &= \frac{1}{\lambda_2} I_k \text{ and } U_3(\xi, \underline{x}) = \frac{1}{\lambda_4}[\rho^2 I_k - 2\ Diag\{x_1^2, \ldots, x_k^2\} + \underline{x}\underline{x}'],
\end{aligned}$$

$\rho^2 = \underline{x}'\underline{x}$ and I_k is the identity matrix of order k. It follows that

$$\begin{aligned}
trV_1(\xi,\underline{x}) &= [\tfrac{2(k-1)}{k\lambda_4} + \tfrac{4}{k\{(k+2)\lambda_4 - k\lambda_2^2\}}]\rho^2, \\
trV_2(\xi,\underline{x}) &= \tfrac{k}{\lambda_2} + [\tfrac{2(k-1)}{k\lambda_4} + \tfrac{4}{k\{(k+2)\lambda_4 - k\lambda_2^2\}}]\rho^2, \\
trV_3(\xi,\underline{x}) &= [\tfrac{(k-1)(k+2)}{k\lambda_4} + \tfrac{4}{k\{(k+2)\lambda_4 - k\lambda_2^2\}}]\rho^2, \\
trV_4(\xi,\underline{x}) &= \tfrac{k}{\lambda_2} + [\tfrac{(k-1)(k+2)}{k\lambda_4} + \tfrac{4}{k\{(k+2)\lambda_4 - k\lambda_2^2\}}]\rho^2, \\
trV_5(\xi,\underline{x}) &= \tfrac{(k-1)\rho^2}{\lambda_4}, \quad trV_6(\xi,\underline{x}) = \tfrac{k}{\lambda_2} + \tfrac{(k-1)}{\lambda_4}\rho^2,
\end{aligned}$$

all of which are strictly increasing in ρ^2 and hence

$$\begin{aligned}
V_1(\lambda_2,\lambda_4) &= \tfrac{2(k-1)}{k\lambda_4} + \tfrac{4}{k\{(k+2)\lambda_4 - k\lambda_2^2\}}, \\
V_2(\lambda_2,\lambda_4) &= \tfrac{k}{\lambda_2} + \tfrac{2(k-1)}{k\lambda_4} + \tfrac{4}{k\{(k+2)\lambda_4 - k\lambda_2^2\}}, \\
V_3(\lambda_2,\lambda_4) &= \tfrac{(k-1)(k+2)}{k\lambda_4} + \tfrac{4}{k\{(k+2)\lambda_4 - k\lambda_2^2\}}, \\
V_4(\lambda_2,\lambda_4) &= \tfrac{k}{\lambda_2} + \tfrac{(k-1)(k+2)}{k\lambda_4} + \tfrac{4}{k\{(k+2)\lambda_4 - k\lambda_2^2\}}], \\
V_5(\lambda_2,\lambda_4) &= \tfrac{(k-1)}{\lambda_4} \text{ and } V_6(\lambda_2,\lambda_4) = \tfrac{k}{\lambda_2} + \tfrac{(k-1)}{\lambda_4},
\end{aligned}$$

where $V_i(\lambda_2,\lambda_4) = Max_{\underline{x}\epsilon\mathcal{X}}\ trV_i(\xi,\underline{x})$.

3. A-MINIMAX OPTIMAL DESIGNS

Let ξ_i dentoe the A-minimax optimal design for the i-th model $(i = 1,\ldots,6)$. Since each $V_i(\lambda_2,\lambda_4)$ is strictly decreasing in λ_4, the ξ_i must have $\lambda_4 = \lambda_2/(k+2)$, the highest possible value, reducing the objective function $V_i(\lambda_2,\lambda_4)$ to $V_i(\lambda_2)$, respectively where

$$\begin{aligned}
V_1(\lambda_2) &= \frac{2(k+1)}{\lambda_2} + \frac{4}{(1-k\lambda_2)}, \quad V_2(\lambda_2) = \frac{3k+2}{\lambda_2} + \frac{4}{(1-k\lambda_2)}, \\
V_3(\lambda_2) &= \frac{k(k+3)}{\lambda_2} + \frac{4}{(1-k\lambda_2)}, \quad V_4(\lambda_2) = \frac{k(k+4)}{\lambda_2} + \frac{4}{(1-k\lambda_2)}, \\
V_5(\lambda_2) &= \frac{(k-1)(k+2)}{\lambda_2} \text{ and } V_6(\lambda_2) = \frac{k^2+2k-2}{\lambda_2}.
\end{aligned}$$

It is obvious that $V_5(\lambda_2)$ and $V_6(\lambda_2)$ are minimized when λ_2 has the maximum allowed value, i.e. $\lambda_2 = 1/k$. Thus ξ_5 and ξ_6 are indentical, have $\lambda_2 = \lambda_{2(5)} = \lambda_{2(6)} = 1/k$, and therefore are singular for the models $M1 - M4$.

Now each of the $V_i(\lambda_2)$ is of the form $\frac{A_i}{\lambda_2} + \frac{B}{1-k\lambda_2}$ which, by differentiation with respect to λ_2, can be seen to be minimized when $\lambda_2 = \lambda_{2(i)} = 1/[k + \sqrt{kB/A_i}]$ $(i = 1,2,3,4)$ where $B = 4$ and $A_1 = 2(k+1), A_2 = (3k+2), A_3 = k(k+3), A_4 = k(k+4)$. Thus ξ_i, the optimal design for the i-th model has $\lambda_2 = \lambda_{2(i)}$ $(i = 1,2,3,4)$ where

$$\lambda_{2(1)} = 1/[k + \sqrt{2k/(k+1)}], \qquad \lambda_{2(2)} = 1/[k + 2\sqrt{k/(3k+2)}],$$
$$\lambda_{2(3)} = 1/[k + 2/\sqrt{(k+3)}], \qquad \lambda_{2(4)} = 1/[k + 2\sqrt{(k+4)}].$$

The values of $\lambda_{2(i)}$ for some selected values of k are provided in Table 1 which follows.

Table 1. Values of λ_2 for the A-minimax optimal designs

k	$\lambda_{2(1)}$	$\lambda_{2(2)}$	$\lambda_{2(3)}$	$\lambda_{2(4)}$	$\lambda_{2(5)} = \lambda_{2(6)}$
2	0.3170	0.3333	0.3455	0.3551	0.5000
3	0.2367	0.2473	0.2620	0.2662	0.3333
4	0.1899	0.1973	0.2103	0.2124	0.2500
5	0.1590	0.1643	0.1752	0.1765	0.2000
6	0.1368	0.1409	0.1500	0.1508	0.1667
7	0.1202	0.1234	0.1310	0.1315	0.1429
8	0.1071	0.1098	0.1162	0.1167	0.1250
9	0.0967	0.0989	0.1044	0.1047	0.1111
10	0.0881	0.0899	0.0947	0.0949	0.1000
50	0.0195	0.0196	0.0199	0.0199	0.0200
100	0.0099	0.0099	0.0100	0.0100	0.0100

4. RELATIVE PERFORMANCE

The A-minimax efficiency of a design ξ is defined as

$$\{Max_{\underline{x}\epsilon\mathcal{X}}\ trV(\xi^*, \underline{x})\}/\{Max_{\underline{x}\epsilon\mathcal{X}}\ trV(\xi, \underline{x})\}$$

where ξ^* is the A-minimax optimal design.

We are particularly interested in finding out how well the design ξ_i performs for the j-th model $(j \neq i)$. Let A_{ij} denote the A-minimax efficiency of ξ_i when ξ_i is used as a design for the j-th model $(j \neq i)$. Then it is readily seen that

$$A_{ij} = V_j(\lambda_{2(j)})/V_j(\lambda_{2(i)}) \qquad (i \neq j = 1,2,3,4).$$

Also, $A_{56} = A_{65} = 1$, $A_{5j} = A_{6j} = 0$ $(j = 1,2,3,4)$, $A_{i5} = A_{i6} = k\lambda_{2(i)}$ $(i = 1,2,3,4)$. The numerical values of the A_{ij} corresponding to some selected values of k are presented in Table 2 which follows.

Table 2. Relative efficiencies A_{ij} (in %)

k	2	3	4	5	6	7	8	9	10	20	50	100	1000
A_{12}	99.54	99.52	99.53	99.56	99.58	99.61	99.64	99.66	99.68	99.81	99.91	99.95	99.99
A_{13}	98.62	97.27	96.51	96.10	95.92	95.85	95.86	95.90	95.98	96.88	98.24	98.97	99.87
A_{14}	97.56	96.32	95.75	95.51	95.44	95.47	95.55	95.65	95.76	96.82	98.23	98.97	99.87
A_{15}	63.40	71.01	75.98	79.48	82.09	84.11	85.71	87.03	88.12	93.54	97.28	98.61	99.86
A_{21}	99.52	99.48	99.51	99.53	99.56	99.59	99.59	99.61	99.63	99.63	99.89	99.94	99.99
A_{23}	99.73	98.99	98.40	98.03	97.78	97.64	97.56	97.52	97.51	97.86	98.71	99.22	99.90
A_{24}	99.16	98.33	97.84	97.55	97.40	97.33	97.30	97.31	97.33	97.81	98.70	99.22	99.90
A_{25}	66.67	74.17	98.91	82.17	84.56	86.38	87.82	88.98	89.94	94.63	97.76	98.86	99.88
A_{31}	98.50	96.68	95.29	94.26	93.49	90.92	92.49	92.15	91.90	91.13	91.97	93.26	97.20
A_{32}	99.72	99.85	98.02	97.35	96.82	96.40	96.06	95.79	95.58	94.74	94.97	99.68	98.15
A_{34}	99.83	99.90	99.94	99.96	99.98	99.98	99.99	99.99	99.99	100	100	100	100
A_{35}	69.10	78.61	84.11	87.61	90.00	91.71	92.99	93.97	94.74	97.96	99.45	99.80	99.99
A_{41}	97.26	95.34	94.03	93.12	92.48	92.01	91.67	91.41	91.22	90.81	91.87	93.22	97.20
A_{42}	99.09	98.02	97.20	96.58	96.12	95.76	95.49	95.27	95.10	94.51	94.90	95.66	98.15
A_{43}	99.82	99.90	99.94	99.96	99.97	99.98	99.99	99.99	99.99	100	100	100	100
A_{45}	71.01	79.87	84.98	88.24	90.46	92.07	93.27	94.19	94.93	98.00	99.46	99.80	99.99

5. CONCLUSIONS

The values of A_{ij} in Table 2 show that there isn't much difference in the relative performances of ξ_1, ξ_2, ξ_3 and ξ_4 although on average ξ_4 is slightly better. Among the four, ξ_4 has best performance for models $M5$ and $M6$. Hence, the recommendation would be that the experimenter, when unsure about the true model, might stick to ξ_4, the optimal design for the full second-order model.

Also, it is obvious from the expressions for $V_i(\lambda_2)$ and $\lambda_{2(i)}$ that in the limit k going to infinity, all non-zero A_{ij}'s converge to unity. Table 2 clearly illustrates this. The table also shows that as k increases from 2 there is initially a decline in the A_{ij}'s except for $j = 5$ (and 6) for which the increase starts immediately.

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