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On Invariance Properties of A- and D- Minimax Designs for Estimating Slopes of a Reduced Second-order Model

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Abstract

The A- and D-minimax criteria are concerned with minimization with respect to the design the trace and determinant, respectively, of the covariance matrix of the estimated axial slopes at a point, maximized over all points in the region $I\!R$ of interest in the factor space. It is shown that for the reduced multifactor second-order model containing an intercept term and the pure quadratic terms only the D-minimax design is invariant with respect to the choice of the region $I\!R$. It is further shown that the A-minimax design among the balanced designs is also invariant with respect to $I\!R$. The necessary and sufficient conditions for invariance of A-minimax designs in two and three dimensions are also provided.

Keywords and Phrases: A-minimax designs; Balanced designs; D-minimax designs; Response surface designs; Second-order model.

AMS Classification: Primary 62k99; Secondary 62k05.

1 Introduction

Consider the standard response surface experimental design set up in which it is assumed that an univariate response y depends on k quantitative factors $x_1, \ldots, x_k$ through a smooth functional relationship $y = \phi(x, \theta)$ where $x = (x_1, \ldots, x_k)^t$ and $\theta = (\theta_1, \ldots, \theta_p)^t$ is a column vector of unknown parameters. Let χ be the experimental region, i.e. the region of the factor space in which experimentation is permitted. A design ξ is a probability measure on χ. If y_i is the observation at the point $x_i = (x_{i1}, \ldots, x_{ik})^t$ $(i = 1, \ldots, N)$ chosen according to the design ξ, it is assumed that $y_i = \phi(x_i, \theta) + e_i$ where the e_i's are uncorrelated, zero-mean random errors with a constant variance σ^2. Let $\hat{\theta}$ be the estimate of θ. Then $\hat{y}(z) = \phi(z, \hat{\theta})$ is the corresponding estimate of the response at a point $z = (z_1, \ldots, z_k)^t$. Further, $d\hat{y}/dz = (\partial\hat{y}(z)/\partial z_1, \ldots, \partial\hat{y}(z)/\partial z_k)^t$ is the column vector of estimated slopes along the factor axes at the point. Typically, the method of least squares may be used for the estimation. Let $V(\xi, z)$ denote (N/σ^2) cov$(d\hat{y}/dz)$, the standardized variance-covariance matrix of the estimated slopes. Obviously $V(\xi, z)$ depends both on the design ξ used and on the point z at which the axial slopes are estimated.

In many situations estimation of slopes of a response surface is of greater interest than estimation of the response surface itself (see for example, Atkinson (1970), Mukerjee and Huda (1985)). This is particularly true in situations where the experimenter is interested in optimizing the response and needs to determine points where the maximum (or minimum) occurs. The vector dy/dz not only displays the rates of change along the axial directions but also provides information about the rates of change in other directions. The directional derivative at point z in the direction specified by the vector of direction cosines $c = (c_1, \ldots, c_k)^t$ is $c^t dy/dz$. Further $\{(dy/dz)^t(dy/dz)\}^{-1/2} dy/dz$ is the direction in which the directional derivative is largest. This well-known result from multivariate calculus provides added justification for concentrating on estimation of slopes along the axial directions.

Under the traditional A-, D- and E-optimality criteria the objective is to minimize with respect to the design

$$tr\ cov(\hat{\theta}) = \sum_{i=1}^{p} \lambda_i,$$

$$|cov(\hat{\theta})| = \prod_{i=1}^{p} \lambda_i,$$

$$\max\{\lambda_1, \ldots, \lambda_p\},$$

respectively, where λ_i $(i = 1, \ldots .p)$ are the e-values of $cov(\hat{\theta})$. Huda and Al-Shiha (1999, 2000) generalized these concepts to consider situations where estimation of slopes is the primary interest of the experimenter and defined the A-, D- and E-minimax criteria as follows:

$$\min_{\xi} \max_{z \in I\!R} tr\ V(\xi, z) (= \sum_{i=1}^{k} \beta_i(\xi, z)),$$

$$\min_{\xi} \max_{z \in I\!R} |V(\xi, z)| (= \prod_{i=1}^{k} \beta_i(\xi, z)),$$

$$\min_{\xi} \max_{z \in I\!R} \max\{\beta_1(\xi, z), \ldots, \beta_k(\xi, z)\},$$

respectively, where $\beta_i(\xi, z)$ $(i = 1, \ldots, k)$ are the e-values of $V(\xi, z)$ and $I\!R$ is the region of interest in the factor space. Often $I\!R = \chi$ but that need not be the case always. We shall assume that $I\!R$ is bounded.

2 Second-order model

A substantial part of statistical literature on experimental design is concerned with linear models. In the linear model set-up, $\phi(x, \theta) = f^t(x)\theta$ with $f^t(x) = (f_1(x), \ldots, f_p(x))$ containing p linearly independent functions of x. Then the least squares estimate $\hat{\theta}$ has the variance-covariance matrix $cov(\hat{\theta})$ given by $(N/\sigma^2)cov(\hat{\theta}) = M^{-1}(\xi)$ where $M(\xi) = \int_\chi f(x)f^t(x)\xi(dx)$ is the information matrix of ξ. Also, $(N/\sigma^2)var(\hat{y}(z)) = f^t(z)M^{-1}(\xi)f(z)$ and

$$V(\xi, z) = H(z)M^{-1}(\xi)H^t(z), \tag{1}$$

where $H(z)$ is a $k \times p$ matrix whose i-th row is $\partial f^t(z)/\partial z_i = (\partial f_1(z)/\partial z_i, \ldots, \partial f_p(z)/\partial z_i)$ $(i = 1, \ldots, k)$.

The linear models most commonly used in response surface designs are the polynomial models. A polynomial model of order d is one for which $f(x)$ contains the terms of a polynomial of degree d and less in x. For example when $d = 2$ the model is called a second-order model. A full second-order model in k variables contains $(k+2)(k+1)/2$ terms in $f(x)$ (and in θ). In what follows we consider a reduced second-order model containing the intercept and the pure quadratic terms only, given by

$$f^t(x) = (1, x_1^2, \ldots, x_k^2). \tag{2}$$

Note that the second-order models are widely used in industry and even reduced second-order models such as (2) may have practical usefulness (cf. Schwabe and Wong (2003)).

3 Invariance property of A- and D- minimax designs

When the model is specified by (2), the information matrix $M(\xi)$ is given by

$$M(\xi) = \begin{bmatrix} 1 & m' \\ m & M \end{bmatrix}, \tag{3}$$

where $m' = (m_1, \ldots, m_k)$ with $m_i = \int_\chi x_i^2 \xi(dx)$ and M is a $k \times k$ matrix with diagonal elements $m_{ii} = \int_\chi x_i^4 \xi(dx)$ and off-diagonal elements $m_{ij} = \int_\chi x_i^2 x_j^2 \xi(dx)$ $(i \neq j = 1, \ldots, k)$. Further,

$$H(z) = [0, 2\ \text{Diag}\{z^t\}], \tag{4}$$

where 0 is the k-component column vector of 0's. Then assuming M to be non-singular and using the standard results on inverse of partitioned matrices, from (3) we have

$$M^{-1}(\xi) = \begin{bmatrix} a & -am'M^{-1} \\ -aM^{-1}m & M^{-1} + aM^{-1}mm'M^{-1} \end{bmatrix}, \tag{5}$$

where $a = 1/(1 - m'M^{-1}m)$.

3.1 D-minimax design

Under the D-minimax optimality criterion the objective is to $\min_{\xi} \max_{z \in I\!R} |V(\xi, z)|$. But substituting for $H(z)$ from (4) and $M^{-1}(\xi)$ from (5) into (1), we obtain that for the reduced second-order model,

$$V(\xi, z) = 4 \text{ Diag}\{z^t\}[M^{-1} + aM^{-1}mm'M^{-1}] \text{ Diag}\{z^t\}. \tag{6}$$

From (6) it follows that

$$|V(\xi, z)| = 4^k |M^{-1} + aM^{-1}mm'M^{-1}| (\prod_{i=1}^{k} z_i^2). \tag{7}$$

Clearly, the objective function (7) is separable in the arguments ξ and z. The only term depending on z is $(\prod_{i=1}^{k} z_i^2)$ and the term $|M^{-1} + aM^{-1}mm'M^{-1}|$ depends only on the design ξ and does not involve z at all. Hence, the D-minimax design ξ_D^* has to minimize $|M^{-1} + aM^{-1}mm'M^{-1}|$ and the same ξ_D^* will be optimum whatever $I\!R$ is. This may be stated as the following theorem.

Theorem 1. *For the reduced second-order model containing the intercept and pure quantitative terms only, the D-minimax design is invariant with respect to the region $I\!R$ over which estimation of slopes is of interest.*

3.2 A-minimax design

Under A-minimax optimality criterion, the objective is to $\min_{\xi} \max_{z \in I\!R} trV(\xi, z)$. Now from (6) we obtain that

$$trV(\xi, z) = \sum_{i=1}^{k} (V(\xi, z))_{ii} = 4 \sum_{i=1}^{k} v_{ii} z_i^2, \tag{8}$$

where $v_{ii} = (M^{-1} + aM^{-1}mm'M^{-1})_{ii}$ $(i = 1, \ldots, k)$.

If the design ξ is balanced, then $v_{ii} = v(i = 1, \ldots, k)$ (say) and it follows from (8) that $trV(\xi, z) = 4v\rho_z^2$ where $\rho_z^2 = \sum_{i=1}^{k} z_i^2$. Then the objective function is again separable in the arguments and the A-minimax design ξ_A^* has to minimize v, the same ξ_A^* being optimum whatever $I\!R$ is. This may be stated as the following.

Theorem 2. *For the reduced second-order model containing the intercept and pure quadratic terms only, the A-minimax design within the class of balanced deigns is invariant with respect to the region $I\!R$ over which estimation of slopes is of interest.*

The question that arises naturally is "Is the condition of balance also necessary for invariance of the A-minimax design?" This can be easily answered by looking at the special case of $k = 2$. Then letting $[ii] = \int_\chi x_i^2 \xi(dx)$, $[iiii] = \int_\chi x_i^4 \xi(dx)$ $(i = 1, 2)$ and $[1122] = \int_\chi x_1^2 x_2^2 \xi(dx)$, it is readily seen that $v_{11} = v_{22}$ if and only if $[1111]+[22]^2 = [2222]+[11]^2$. It is easy to construct designs satisfying this requirement and the two-dimensional designs presented in Huda and Chowdhury (2004) are such. For $k = 3$, the necessary and sufficient condition is $v_{11} = v_{22} = v_{33}$ which is true if and only if

$$\begin{aligned}
&[1111][22]^2 + [2222][11]^2 + [1122]^2 - [1111][2222] - 2[1122][11][22] \\
&= [1111][33]^2 + [3333][11]^2 + [1133]^2 - [1111][3333] - 2[1133][11][33] \\
&= [2222][33]^2 + [3333][22]^2 + [2233]^2 - [2222][3333] - 2[2233][22][33]
\end{aligned}$$

where $[ii] = \int_\chi x_i^2 \xi(dx)$, $[iiii] = \int_\chi x_i^4 \xi(dx)$ and $[iijj] = \int_\chi x_i^2 x_j^2 \xi(dx)$ $(i \neq j = 1, 2, 3)$. The problem of finding necessary and sufficient condition in the general case of $k \geq 4$ is currently under investigation.

4 Remarks

Remark 1. For the reduced second-order model the D-minimax design is the same for all regions over which estimation of the slopes is of interest. Thus the region $I\!R$ can be completely arbitrary. In particular, it may be irregular in shape, disjoint from the experimental region χ or may even consist of a finite number of points. The condition that $I\!R$ be bounded is needed so that the minimax optimality criterion is well defined.

Remark 2. Experimenters usually prefer the use of balanced designs because of their simplicity of analysis (and also construction at times). Thus the invariance result concerning A-minimax optimality criterion also should be of interest to experimenters.

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