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NECESSARY AND SUFFICIENT CONDITIONS FOR $D-$ROTATABILITY OF SECOND-ORDER DESIGNS

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ABSTRACT

Designs for estimating slopes of a second-order response surface are considered and moment requirements of the design to be $D-$rotatable are investigated. It is shown that, within the class of balanced symmetric designs, a second-order design is $D-$rotatable if and only if it is rotatable in the ordinary (Box-Hunter (1957)) sense.

1. INTRODUCTION

Box and Hunter (1957) introduced the concept of rotatability of designs for exploration of response surfaces. A design is said to be rotatable if the variance of the estimated response at a point in the factor space is a function of the distance of the point from the center of the design, conventionally taken to be the origin of the factor space, after transformations if necessary. Rotatability is a highly desirable property of a response surface design when estimation of the absolute response is the main objective of the experimenter and little prior information is available about the nature of the response surface. Rotatable designs also form a very rich class in the sense that for polynomial regression models over hyperspherical regions, under many commonly used criteria, such as $D-$optimality, the optimal designs belong to this class (Kiefer (1960)). Consequently, a large volume of statistical literature on response surface designs involves rotatability.

In many response surface design set-ups the experimenter is often more interested in estimating the slopes of the response surface rather than the response itself, at various locations in the factor space. This is particularly true in situations where the objective is to optimize the response in some sense and the experimenter may be looking for maxima/minima or turning points in the surface. For such situations, Huda and Chowdhury (2004), Huda (2006) introduced the concept of $D-$(slope)-rotatability (or $D-$rotatability for short). A design is said to be $D-$rotatable if the determinant of the variance-covariance matrix of the estimated slopes at a point is a function of distance of the point from the origin. Analogously, a design is $A-$rotatable if instead the trace of the matrix is a function of the distance. While the concept of $D-$rotatability is new, the idea of $A-$rotatability has existed for some time and was introduced by Park (1987) who called it slope-rotatability over all directions

$(SROAD)$. Ying, Pukelsheim and Draper (1995a, b) provided some interesting results concerning $A-$rotatability of second-order designs. In what follows we consider $D-$rotatability of second-order response surface designs.

2. THE DESIGN SET-UP

Consider a response y depending on k quantitative factors $x_1, \cdots, x_k$ via a functional relationship $y = \phi(\underline{x})$, where $\underline{x} = (x_1, \cdots, x_k)'$. If y_i is an observation at the point $\underline{x}_i = (x_{1i}, \cdots, x_{ki})'$, it is assumed that $y_i = \phi(\underline{x}_i) + \varepsilon_i$, where ε_i's are uncorrelated zero mean errors with a common variance σ^2 taken to be unity without loss of generality. When the assumed model is a linear model, $\phi(\underline{x}) = f'(\underline{x})\theta$, where $f'(\underline{x})$ is a row 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 χ, which without loss of generality we take to be centered at the origin. If N trials are carried out according to ξ then $\operatorname{cov}(\hat{\theta}) = N^{-1}M^{-1}(\xi)$, where $\hat{\theta}$ is the least square estimate of θ and $M(\xi) = \int_\chi f(\underline{x})\, f'(\underline{x})\, \xi(d\underline{x})$ is the information matrix of ξ.

3. $D-$ROTATABILITY

The least squares estimate of the response $y(\underline{x})$ at a point $\underline{x}$ in the factor space is given by $\hat{y}(\underline{x}) = f'(\underline{x})\,\hat{\theta}$ whereby the column vector of estimated slopes along the factor axes is $d\hat{y}/d\underline{x} = (\partial\hat{y}/\partial x_1, \cdots, \partial\hat{y}/\partial x_k)'$. The variance-covariance matrix of $d\hat{y}/d\underline{x}$, normalized with respect to the number of observations, is given by

$$V(\xi, \underline{x}) = N \ \operatorname{cov}(d\hat{y}/d\underline{x}) = H(\underline{x})\, M^{-1}(\xi)\, H'(\underline{x}), \tag{3.1}$$

where $H(\underline{x})$ is the $k \times p$ matrix with $\partial f'(\underline{x})/\partial x_i$ as the $i-$th row. $V(\xi, \underline{x})$ depends on the design ξ through $M(\xi)$ and on the point $\underline{x}$ through $H(\underline{x})$ as (3.1) clearly illustrates. A design is said to be $A-$rotatable if $\operatorname{tr} V(\xi, \underline{x})$ depends on $\underline{x}$ only through $\underline{x}'\underline{x}$ and $D-$rotatable if $|V(\xi, \underline{x})|$ depends on $\underline{x}$ only through $\underline{x}'\underline{x}$.

Thus $A-$rotatability is concerned with invariance of the arithmetic average variance of the estimated slopes while $D-$roatability is concerned with the invariance of generalized variance of the estimated slopes. In terms of $e-$values of $V(\xi, \underline{x})$, $A-$ and $D-$rotatability are concerned with their arithmetic and geometric averages, respectively.

4. SECOND-ORDER DESIGNS

For a full second-order model, $f'(\underline{x})$ contains $p=(k+2)(k+1)/2$ terms of degree two or less in the x_i's that are involved in a polynomial of degree two. A design ξ is called a second-order design if it allows estimation of all the parameters in the second-order model. For the second-order model it is convenient to partition $f'(\underline{x})$ as $f'(\underline{x})=[f_1'(\underline{x}), f_2'(\underline{x}), f_3'(\underline{x})]$, where

$$f_1'(\underline{x})=(1, x_1^2, \cdots, x_k^2), \quad f_2'(\underline{x})=(x_1, \cdots, x_k)$$

and

$$f_3'(\underline{x})=(x_1x_2, \cdots, x_{k-1}x_k).$$

Accordingly, $M(\xi)$ is a partitioned matrix given by

$$M(\xi)=\begin{bmatrix} M_{11}(\xi) & M_{12}(\xi) & M_{13}(\xi) \\ M_{21}(\xi) & M_{22}(\xi) & M_{23}(\xi) \\ M_{31}(\xi) & M_{32}(\xi) & M_{33}(\xi) \end{bmatrix}, \tag{4.1}$$

where

$$M_{ij}(\xi)=\int_{\chi} f_i(\underline{x}) f_j'(\underline{x}) \xi(d\underline{x}), \quad (i, j=1,2,3).$$

Although $M(\xi)$ is symmetric, it is not algebraically feasible to obtain an inverse of $M(\xi)$ for an arbitrary design ξ and large k. However, for a symmetric design ξ, the odd moments of the design disappear, i.e.

$$\int_{\chi} x_i \, \xi(d\underline{x}) = \int_{\chi} x_i x_j \, \xi(d\underline{x}) = \int_{\chi} x_i^3 \, \xi(d\underline{x})$$

$$= \int_{\chi} x_i^2 x_j \, \xi(d\underline{x}) = \int_{\chi} x_i x_j x_l \, \xi(d\underline{x}) = 0, \quad (i \neq j \neq l = 1, \cdots, k)$$

and hence $M_{ij}(\xi)$ $(i \neq j)$ are null matrices, making $M(\xi)$ a block diagonal matrix, reducing (4.1) to

$$M(\xi)=Diag\{M_{11}(\xi), M_{22}(\xi), M_{33}(\xi)\} \tag{4.2}$$

and

$$M_{11}(\xi)=\begin{bmatrix} 1 & m' \\ m & M^* \end{bmatrix}$$

$$M_{22}(\xi)=Diag\{m_1, \cdots, m_k\}$$

$$M_{33}(\xi)=Diag\{m_{12}, m_{13}, \cdots, m_{k-1,k}\},$$

where

$$m = (m_1, \cdots, m_k)', \quad (M^*)_{ij} = m_{ij}, \quad m_i = \int_{\chi} x_i^2 \xi(d\,\underline{x}),$$

$$m_{ij} = \int_{\chi} x_i^2 x_j^2\, \xi(d\underline{x}), \quad (i, j = 1, \cdots, k).$$

If in addition the design ξ is balanced (permutation invariant) then $m_i = \alpha_2$, $m_{ii} = \alpha_4$ and $m_{ij} = \alpha_{22}$, $(i \neq j = 1, \cdots, k)$ and the non-null matrices in (4.2) are further simplified to

$$M_{11}(\xi) = \begin{bmatrix} 1 & \alpha_2 1_k' \\ \alpha_2 1_k & (\alpha_4 - \alpha_{22}) I_k + \alpha_{22} E_k \end{bmatrix}, \qquad M_{22}(\xi) = \alpha_2 I_k,$$

$$M_{33}(\xi) = \alpha_{22} I_{k^*}, \tag{4.3}$$

where 1_k is the $k-$component column vector of $1's$, I_k is the identity matrix of order k, $E_k = 1_k 1_k'$ and $k^* = k(k-1)/2$.

Under all the commonly used optimality criteria, the optimal designs belong to the class of symmetric balanced designs. Also, given the fact that $|V(\xi, \underline{x})|$ involves all elements of $V(\xi, \underline{x})$ it is most unlikely that there exist any $D-$rotatable design outside that class, although one can easily construct an $A-$rotatable design that is not symmetric or balanced [Ying *et al.* (1995a, b)]. In what follows we shall restrict our attention to the class of symmetric balanced designs. Note that the rotatable designs form a sub-class of the symmetric balanced designs and a second-order symmetric balanced design is rotatable if $\alpha_4 = 3\alpha_{22}$ [Box and Hunter (1957)].

5. NECESSARY AND SUFFICIENT CONDITIONS

In this section we present our main result in the form of a theorem which follows:

Theorem 5.1: A necessary and sufficient condition for a symmetric balanced second-order design ξ to be $D-$rotatable is that the design be rotatable.

Proof: Sufficiency

After some algebra, it can be seen from (4.3) that for a symmetric balanced second-order design ξ, (3.1) reduces to

$$V(\xi, \underline{x}) = (1/\alpha_2 + \rho^2/\alpha_{22}) I_K + \{4/(\alpha_4 - \alpha_{22}) - 2/\alpha_{22}\} Diag\{x_1^2, \cdots, x_k^2\}$$
$$+ [1/\alpha_{22} + 4\{1/\{\alpha_4 + (k-1)\alpha_{22} - k\alpha_2^2\} - 1/(\alpha_4 - \alpha_{22})\}/k]\, \underline{x}\underline{x}',$$

(5.1)

where $\rho^2 = \underline{x}'\underline{x}$.

For a rotatable design $\alpha_4 = 3\alpha_{22}$ and thus the second-term in the right hand side of (5.1) disappears making

$$V(\xi,\underline{x}) = (1/\alpha_2 + \rho^2/\alpha_{22})I_k + [1/\{(k+2)\alpha_{22} - k\alpha_2^2\} + (k-2)/(4\alpha_{22})](4/k)\underline{x}\underline{x}' \quad (5.2)$$

From (5.2) it is readily seen that the $e-$values of $V(\xi,\underline{x})$ are

$$(1/\alpha_2 + \rho^2/\alpha_{22}) + [1/\{(k+2)\alpha_{22} - k\alpha_2^2\} + (k-2)/(4\alpha_{22})](4\rho^2/k)$$

corresponding to the $e-$vector $\underline{x}$ and $(1/\alpha_2 + \rho^2/\alpha_{22})$ with multiplicity $k-1$ corresponding to e-vectors orthogonal to $\underline{x}$. Since the $e-$values depend on $\underline{x}$ through ρ^2 and $|V(\xi,\underline{x})|$ is the product of $e-$values, $|V(\xi,\underline{x})|$ is a function of ρ^2 only. Thus rotatability is a sufficient condition for $D-$rotatability.

Necessity

From (5.1) it is seen that $V(\xi,\underline{x})$ is of the form

$$V(\xi,\underline{x}) = aI_k + (b-c)\,Diag\,(x_1^2,\cdots,x_k^2) + c\,\underline{x}\underline{x}', \quad (5.3)$$

where

$$a = (1/\alpha_2 + \rho^2/\alpha_{22}),\ b-c = \{4/(\alpha_4 - \alpha_{22}) - 2/\alpha_{22}\}$$

and

$$c = \{1/\alpha_{22} + 4[1/\{\alpha_4 + (k-1)\alpha_{22} - k\alpha_2^2\} - 1/(\alpha_4 - \alpha_{22})]/k\}.$$

Now, the determinant of $V(\xi,\underline{x})$ from (5.3) is given by

$$|V(\xi,\underline{x})| = a^k + \sum_{m=1}^{k}\left[a^{k-m}(b-c)^{m-1}\{b+(m-1)c\}\left\{\sum_{1\le i_1<i_2<\cdots<i_m}^{k}\left(\prod_{j=i_1}^{i_m} x_j^2\right)\right\}\right]. \quad (5.4)$$

Therefore, for (5.4) to be a function of $\rho^2 = \underline{x}'\underline{x}$ only, it is necessary that all terms involving $m \ge 2$ on the right-hand side disappear which can happen only if $b-c=0$. But $b-c=0$ is equivalent to $\alpha_4 = 3\alpha_{22}$ which is the condition of rotatability. Thus rotatability is also a necessary condition for $D-$rotatability. This completes the proof of the theorem.

6. COMMENTS AND DISCUSSION

1. It is readily seen from (5.1) that for second-order designs rotatability is also a sufficient condition for $A-$rotatability which involves only the diagonal elements of $V(\xi, \underline{x})$.

2. Mukerjee and Huda (1985) observed that for a second-order design symmetry and balance are sufficient to make $tr\, V(\xi, \underline{x})$ become a function of ρ^2 only, but for third-order designs symmetry and balance were not sufficient. This result for

second-order designs was also presented Park (1987) as Corollary 1 of his theorem, while Corollary 2 presented sufficiency of rotatability.

3. Huda (2006) showed that for a symmetric balanced two-dimensional second-order design rotatability is a necessary and sufficient condition for $D-$rotatability. Thus the theorem in the present paper generalizes the earlier results.

4. It is possible to find $A-$rotatable second-order designs outside the class of symmetric balanced designs. Ying, *et al*. (1995a, b) presented several examples of asymmetric designs as well as unbalanced designs that were $A-$rotatable. Huda and Chowdhury (2004) also provided some unbalanced examples. However the requirements of $D-$rotatability, involving all elements of $V(\xi, \underline{x})$, are much more demanding and it is highly unlikely that there exist any $D-$rotatable design outside the symmetric balanced class and hence, in view of the theorem presented here, outside the rotatable class.

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