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A Note on Slope-Rotatability of Designs

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Abstract

Various notions of slope-rotatability of response surface designs are considered. Existing results are reviewed and some current problems are discussed. Two new examples of unbalanced symmetric A-rotatable second-order designs in two dimensions are provided.

Keywords and Phrases: A-, D- and E- (slope)- rotatability, Balanced designs, Response surface designs, Symmetric designs.

AMS Classification: 62K99.

1 Introduction

Since its introduction by Box and Hunter (1957), rotatabilty has been considered to be a desirable property of response surface designs, particularly when very little prior information is available about the nature of the response surface being investigated. Unlike in classical designs, in response surface designs usually the interest is in estimating the response at various points in the factor space and rotatability of the design ensures that the variance of the estimated response at a point is a function of the distance of the point from the centre of the design, conveniently taken to be the origin. However, since the factors in response surface experiments are usually all quantitative, smooth functional relationship is assumed to exist between the response and the factors, and sometimes the investigator has greater interest in estimating the slopes of the response surface. 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. When estimation of slopes is of greater interest, it is preferable to have notions of rotatability in terms of the estimated slopes rather than the estimated response.

Several concepts of slope-rotability (or rotatability in terms of slopes) have been introduced in recent years for dealing with second-order designs. In particular, Hader and Park (1978) introduced slope-rotatability over axial directions and Park (1987) introduced slope-rotatability over all directions (SROAD). In what follows we consider more general notions of slope-rotatability

2 Background

Consider the usual response surface design set-up involving an univariate response y depending on k quantitative factors $x_1, \cdots, x_k$ through a smooth functional relationship $y = \emptyset(x, \theta)$ where $x = (x_1, \cdots, x_k)^t$ and $\theta = (\theta_1, \cdots, \theta_p)^t$ is a p-component column vector of unknown parameters. A design ξ is a probability measure on the experimental region χ which is that part of the factor space in which experimentation is permissible. Let y_i be the observation at the point $x_i = (x_{i1}, \cdots, x_{ik})^t$ $(i = 1, \cdots, N)$ chosen according to the design ξ. It is assumed that $y_i = \emptyset(x_i, \theta) + e_i$ 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. Typically, it will be the least squares estimate. Then $\hat{y}(z) = \emptyset(z, \hat{\theta})$ is the estimated response at a point z. Further, $d\hat{y}/dz = (\partial\hat{y}(z)/\partial z_1, \cdots, \partial\hat{y}(z)/\partial z_k)^t$ is the column vector of estimated slopes along the factor axes at a point z. Let $V(\xi, z)$ denote (N/σ^2) cov $(d\hat{y}/dz)$, the standardized variance-covariance matrix of the estimated slopes where N is the total number of trials. Note that $V(\xi, z)$ depends both on the design ξ used and on the point z at which the slopes are estimated.

It is also worth noting that 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 estimated directional derivative at point z in the direction specified by the vector of direction cosines $c = (c_1, \cdots, c_k)^t$ is $c^t d\hat{y}/dz$. Further, $\{(d\hat{y}/dz)^t(d\hat{y}/dz)\}^{-1/2} d\hat{y}/dz$ is the direction in which the derivative is largest.

3 Notions of slope-rotatability

Since we are dealing with the $k \times k$ matrix $V(\xi, z)$ when we are concerned with slopes, there are several possibilities for defining slope-rotatability, each corresponding to a different scalar function of the matrix. We may consider the following concepts of slope rotatablity.

(a) A design ξ is to be called A-(slope)-rotatable if and only if $trV(\xi, z)$ depends on z through $\rho^2 = z^t z$.

(b) A design ξ is to be called D-(slope)-rotatable if and only if the determinant of $V(\xi, z)$ depends on z through $\rho^2 = z^t z$.

(c) A design ξ is to be called E-(slope)-rotatable if and only if the largest eigen-value of $V(\xi, z)$ depends on z through $\rho^2 = z^t z$.

(d) A design ξ is to be called Axially-(slope)-rotatable if and only if $V(\xi, z)_{ii}$ $(i = 1, \cdots, k)$ depend on z through $\rho^2 = z^t z$ where $V(\xi, z)_{ii}$ is the i-th diagonal element of $V(\xi, z)$.

4 Linear model set-up

In the linear model set-up, $\emptyset(x, \theta) = f^t(x)\theta$ with $f^t(x) = (f_1(x), \cdots, f_p(x))$ containing p linearly independent functions of x. In this case the least squares estimate $\hat{\theta}$ has the variance-covariance matrix 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. Further $(N/\sigma^2)var\{\hat{y}(x)\} = f'(x)M^{-1}(\xi)f(x)$, and the standardized variance-covariance matrix of $d\hat{y}/dx$ is given by $V(\xi, z) = (N/\sigma^2)cov(d\hat{y}/dz) = H(z)M^{-1}(\xi)H'(z)$ where $H(z)$ is a $k \times p$ matrix whose i-th row is $\partial f^t(z)/\partial z_i = (\partial f_1(z)/\partial z_i, \cdots, \partial f_p(z)/\partial z_i)$.

The linear models most widely used in response surface designs are the polynomial models for which $f(x)$ contains the terms of a polynomial of order (degree) d in x. When $d = 1$ the model is called a first-order model, when $d = 2$ the model is a second-order model and so on. If all the terms of a polynomial of degree d are included in the model then $f(x)$ (and θ) contains ${}_{k+d}C_d$ components. For example, in the first-order model one may write $f^t(x) = (1, x_1 \cdots, x_k)$. For the second-order model it is often convenient to write $f^t(x) = (1, x_1^2, \cdots, x_k^2,\ x_1, \cdots, x_k,\ x_1x_2, \cdots, x_{k-1}x_k)$. For the third-order model the most convenient expression for $f^t(x)$ seems to be $f^t(x) = (1, x_1^2, \cdots, x_k^2,\ x_1x_2, \cdots, x_{k-1}x_k,\ x_1x_2x_3, \cdots, x_{k-2}x_{k-1}x_k,\ g_1^t(x), \cdots, g_k^t(x))$ where $g_i^t(x) = (x_i, x_i^3, x_ix_1^2, \cdots, x_ix_{i-1}^2, x_ix_{i+1}^2, \cdots, x_ix_k^2)$ $(i = 1, \cdots, k)$. In what follows only the polynomial models are to be considered. A design ξ is called a d-th order design if it permits estimation of all the parameters of a d-th order model. Most of the literature on response surface designs deal with $d \leq 3$ except when $k = 1$.

It would be interesting to find the necessary and sufficient conditions for a d-th order design to be slope-rotatable. Past literature has been concerned with $d = 2$ only. In what follows we also consider the second-order designs only.

5 Slope-rotatable designs

A d-th order design ξ is called symmetric if all the "odd moments" up to order $2d$ are zero, that is, if $\int\limits_{\chi} x_1^{d_1} \cdots x_k^{d_k}\ \xi(dx) = 0$ whenever one or more of the d_i's are odd integers and $\sum\limits_{i=1}^{k} d_i \leq 2d$. A design ξ is called balanced (permutation invariant) if the moments are invariant with respect to permutations of the factors $x_1, \cdots, x_k$.

Hader and Park (1975) studied Axial-slope-rotatability of a special class of second-order designs, namely the central composite designs and derived the necessary and sufficient conditions for such rotatability in terms of the elements of $M^{-1}(\xi)$. They called this kind of slope-rotatability "rotatability over axial directions". Park (1987) studied A-rotatability of second-order designs, derived the necessary and sufficient conditions for it and termed it "slope-rotatability over all directions (SROAD)". Ying et al (19995a, b) considered A-rotatability of second-order designs and found some examples from outside the class of symmetric balanced designs and also obtained for some special classes of designs the necessary and sufficient conditions in terms of the elements of $M(\xi)$, thus providing deeper insight into the structure of such designs.

The elements of the information matrix $M(\xi)$, i.e. the moments of a design ξ may be denoted by [i] = $\int\limits_{\chi} x_i \xi(dx)$, [ij] = $\int\limits_{\chi} x_i x_j \xi(dx)$, [iij] = $\int\limits_{\chi} x_i^2 x_j \xi(dx)$, and so on.

For a second-order design only the moments of order 4 and less are involved and consequently, if the design is symmetric and balanced, the only non-zero moments are [ii] = α_2, [iiii] = α_4 and [iijj] = α_{22}, say, $(i \neq j = 1, \cdots, k)$. Then one may write $M(\xi) = diag\{M_1(\xi), \alpha_2 I_k, \alpha_{22} I_{k'}\}$ where $k' = k(k-1)/2$, I_k is the identity matrix of order k, $M_1(\xi) = \begin{bmatrix} 1 & \alpha_2 1^t{}_k \\ \alpha_2 1_k & (\alpha_4 - \alpha_{22}) I_k + \alpha_{22} E_k \end{bmatrix}$, $E_k = 1_k 1_k^t$ and 1_k is the k-component column vector of 1's. Further,

$$\begin{aligned} V(\xi, z) &= (1/\alpha_2 + \rho^2/\alpha_{22}) + \{4/(\alpha_4 - \alpha_{22}) - 2/\alpha_{22}\}\ diag\{z_1^2, \cdots, z_k^2\} \\ &\quad + (1/\alpha_{22} + 4[1/\{\alpha_4 + (k-1)\alpha_{22} - k\alpha_2^2\} - 1/(\alpha_4 - \alpha_{22})]/k) z z^t \quad (1) \end{aligned}$$

where $\rho^2 = z^t z$. (cf. Huda and Al-Shiha (2000)).

From (1) it follows that for a second-order symmetric balanced design to be D-rotatable a sufficient condition is that the design be rotatable (in the Box and Hunter (1957) sense). It is yet to be determined if rotatability is also a necessary condition for D-rotatability. The matter is currently under investigation.

Note that A-rotatability is concerned with the trace of $V(\xi, z)$ which involves only the diagonal elements of $V(\xi, z)$. Equation (1) shows that for second-order designs symmetry and balance are sufficient conditions for A-rotatability. Rotatability (i.e. $\alpha_4 = 3\alpha_{22}$) is not necessary. In fact it is possible to construct A-rotatable designs that are not symmetric and balanced. For example when $k = 2$, the information matrix for a second-order symmetric design ξ is given by

$$M(\xi) = \text{diag}\,\{ \begin{bmatrix} 1 & [11] & [22] \\ [11] & [1111] & [1122] \\ [22] & [1122] & [2222] \end{bmatrix}, \text{diag}\,\{[11],\ [22],\ [1122]\}\ \}, \text{ and}$$

$$H(z) = \begin{bmatrix} 0 & 2z_1 & 0 & 1 & 0 & z_2 \\ 0 & 0 & 2z_2 & 0 & 1 & z_1 \end{bmatrix}. \text{ Consequently, } V(\xi, z) \text{ is given by}$$

$$V(\xi, z) = \begin{bmatrix} 4D([2222]-[22]^2)z_1^2 + 1/[11] + z_2^2/[1122], & -4D([1122]-[11][22])z_1z_2 + z_1z_2/[1122] \\ -4D([1122]-[11][22])z_1z_2 + z_1z_2/[1122], & 4D([1111]-[11]^2)z_2^2 + 1/[22] + z_1^2/[1122] \end{bmatrix}$$

where D = 1/{[1111][2222]-[1122]^2- [11]^2[2222] + 2[11][22][1122] - [22]^2[1111]}.

Thus for a 2-dimensional symmetric second-order design to be A-rotatable, the necessary and sufficient condition is that

$$[2222] + [11]^2 = [1111] + [22]^2. \qquad (2)$$

It is very easy to construct symmetric designs satisfying condition (2) and two simple examples are as follows.

Example 1. Consider, a two dimensional design with one trial at each of ($\pm a$, $\pm b$), ($\pm c$, 0), (0, $\pm c$) and n_0 trials at the origin (0, 0). Clearly the design satisfies (2) and hence is A -rotatable if $c^2 = (a^2 + b^2)(n_0 + 4)/4$. This design is not balanced for arbitrary values of a and b. Figure 1 shows the design for specific values $a = 2$, $b = 1$ and $n_0 = 4$ (giving $c = \sqrt{10}$, [11] = 3, [22] = 2, [1111] = 22 and [2222] = 17).

Example 2. Consider a design given by one trial at each of ($\pm a$, $\pm a$), ($\pm b$, 0), (0, $\pm c$) and n_0 centre points. This design satisfies (2) if $a^2 = (b^2 + c^2)\ (n_0 + 6)/8$ and is A-rotatable. It is also not balanced for arbitrary values of b and c. Figure 2 shows the design for the specific values $b = 1$, $c = 3$ and $n_0 = 2$ (giving $a = \sqrt{10}$, [11] = 4.2, [22] = 5.8, [1111] = 40.2, [2222] = 56.2).

Ying et al (1995a, b) studied in depth the problem of A-rotatability of second-order designs and the interested readers should see the asymmetric examples therein.

Equation (1) also shows that rotatability is a sufficient condition for E-rotatability of second-order designs. But it is not yet known if it is also a necessary condition. The matter is under investigation.

6 Comments

More work needs to be done regarding D- and E-rotatability. In particular, it would be very useful to obtain in terms of the elements of $M(\xi)$ the necessary and sufficient conditions for a design to be D- or E-rotatable. The investigation might be quite difficult to carry out for a general d-th order design. However, it may be possible to do the investigation in depth for second-order designs in low dimensions, say for k = 2 or 3, in order to provide some idea about the complexity of the problem in higher dimensions.

Figure 1. Plot of Trial Points for Example 1

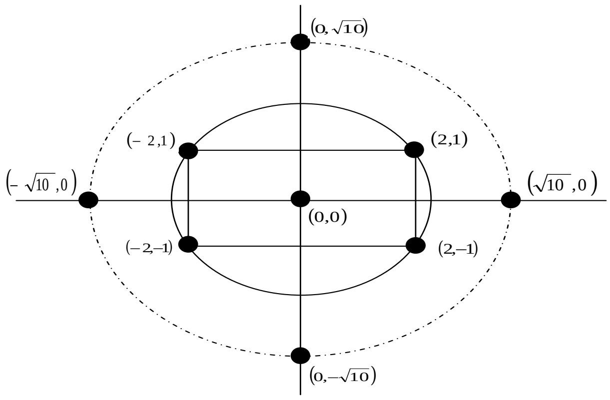

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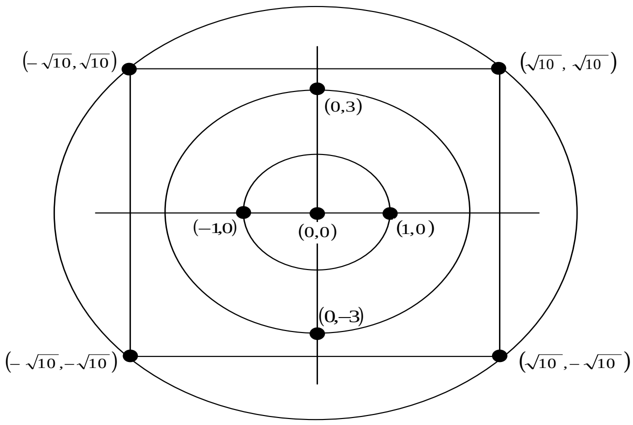
Figure 2. Plot of Trial Points for Example 2



From the definitions given in Section 3 it is clear that an Axially- (slope)-rotatable design is automatically A-(slope)-rotatable. For second-order designs this has been pointed out in Anjaneyulu et al (1997).

A large volume of work has been done in the past regarding construction of second-order slope-rotatable designs. The interested readers are requested to see Victorbabu and Narasimham (1996) and references therein.

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