Slope rotatability over all directions designs

LISA H. YING[1], FRIEDRICH PUKELSHEIM[2] & NORMAN R. DRAPER[3],
[1] *Exxon Chemical Co., Linden, NJ,* [2] *Institut für Mathematik, Universität Augsburg and*
[3] *Department of Statistics, University of Wisconsin*

SUMMARY *Slope rotatability over all directions (SROAD) is a useful concept when the slope of a second-order response is to be studied. SROAD designs ensure that knowledge of the slope is acquired symmetrically, whatever direction later becomes of more interest as the data are analyzed. Some standard second-order designs are SROAD, but here we explore designs for two and three dimensions, which do not have the full symmetries of such standard designs but which still possess the SROAD property.*

1 Introduction

In some response surface applications, attention focuses on the estimation of differences in response, or slopes rather than the absolute value of the response variable. It is then natural to consider the variance measure for the slope of the fitted surface at any given point. On the assumption that equal information in all directions about the design origin was important, Hader and Park (1978) introduced the idea of slope rotatability and discussed it in the context of central composite designs. Later, Park (1987) introduced the concept of second-order slope rotatability over all directions (SROAD), and gave necessary and sufficient conditions for a design to have this property based on the precision matrix. However, only a few simple types of SROAD design have been discussed in the literature. The purpose of this paper is to investigate the moment structures of SROAD designs in detail for the two- and three-factor cases, and so to find alternative SROAD designs. We begin with some general k-dimensional groundwork.

2 SROAD

Let us suppose that the response variable y satisfies a functional relationship in k predictor variables, $x_1, x_2, \ldots, x_k$ of the general form

$$y_i = \eta(\mathbf{x}_i) + \varepsilon_i$$

where y_i is the observed response taken at a selected combination, $\mathbf{x}_i = (x_{1i}, x_{2i}, \ldots, x_{ki})'$ of the predictor variables $\mathbf{x} = (x_1, x_2, \ldots, x_k)'$ and $i = 1, 2, \ldots, N$. The ε_i terms are assumed to be uncorrelated random errors with zero means and constant variance σ^2. We assume that η can be represented adequately in a restricted region of interest by a second-order polynomial, i.e.

$$\eta(\mathbf{x}) = \beta_0 + \sum_{i=1}^{k} \beta_i x_i + \sum_{i=1}^{k} \sum_{j \geq i}^{k} \beta_{ij} x_i x_j = \mathbf{z}_\mathbf{x}' \boldsymbol{\beta} \tag{1}$$

where $\mathbf{z}_\mathbf{x}' = (1, x_1, x_2, \ldots, x_k, x_1^2, x_2^2, \ldots, x_k^2, x_1 x_2, \ldots, x_{k-1} x_k)$ and $\boldsymbol{\beta}$ is the vector of correspondingly subscripted coefficients. The least-squares estimator of $\boldsymbol{\beta}$ is $\mathbf{b} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{y}$, where $\mathbf{X}$ is the matrix of values of $\mathbf{z}_\mathbf{x}'$ taken at the N design points and $\mathbf{y}$ is the $N \times 1$ vector of y observations. The variance–covariance matrix of $\mathbf{b}$ is $\operatorname{var}(\mathbf{b}) = \sigma^2(\mathbf{X}'\mathbf{X})^{-1}$. It is traditional to call $N^{-1}\mathbf{X}'\mathbf{X}$ the 'moment matrix' and its inverse $N(\mathbf{X}'\mathbf{X})^{-1}$ the 'precision matrix'.

The first derivatives (slopes) of $\eta(\mathbf{x})$ at a general point $\mathbf{u} = (u_1, \ldots, u_k)'$ in the x-space are

$$\left.\frac{\partial \hat{y}}{\partial x_i}\right|_{\mathbf{u}} = b_i + 2 b_{ii} u_i + \sum_{j \neq i} b_{ij} u_j \tag{2}$$

Let us denote the estimated slope vector by

$$\mathbf{g}(\mathbf{u}) = \left(\frac{\partial \hat{y}}{\partial x_1}, \frac{\partial \hat{y}}{\partial x_2}, \ldots, \frac{\partial \hat{y}}{\partial x_k}\right)_{\mathbf{u}}' = \mathbf{A}\mathbf{b} \tag{3}$$

say. Thus, the estimated derivative at any point $\mathbf{u}$ in the direction specified by a $k \times 1$ vector of direction cosines, i.e. $\mathbf{c}' = (c_1, c_2, \ldots, c_k)$, is $\mathbf{c}'\mathbf{g}(\mathbf{u})$, where $\mathbf{c}'\mathbf{c} = 1$. The variance of this is

$$V_c(\mathbf{u}) = \operatorname{var}[\mathbf{c}'\mathbf{g}(\mathbf{u})] = \sigma^2 \mathbf{c}'\mathbf{A}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{A}'\mathbf{c} \tag{4}$$

The (integrated) averaged value of $V_c(\mathbf{u})$ over all possible directions, i.e. the averaged slope variance, is

$$\bar{V}(\mathbf{u}) = \frac{\sigma^2}{k} \operatorname{tr}[\mathbf{A}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{A}'] \tag{5}$$

(see Park, 1987, pp. 450–451). $\bar{V}(\mathbf{u})$ is a function of the point $\mathbf{u}$, through $\mathbf{A}$, and also is a function of the design, through $\mathbf{X}$. A k-dimensional design is said to be SROAD if $\bar{V}(\mathbf{u})$ at the point $\mathbf{u}$ depends only on the distance of the point $\mathbf{u}$ from the design origin (Park, 1987). The necessary and sufficient conditions for a second-order design to be SROAD are as follows (Park, 1987):

(1) $2\operatorname{cov}(b_i, b_{ii}) + \sum_{j=1, j \neq i}^{k} \operatorname{cov}(b_j, b_{ij}) = 0$, for all i
(2) $2[\operatorname{cov}(b_{ii}, b_{ij}) + \operatorname{cov}(b_{jj}, b_{ij})] + \sum_{l=1, l \neq i,j}^{k} \operatorname{cov}(b_{il}, b_{jl}) = 0$, for any (i, j), when $i \neq j$
(3) $4\operatorname{var}(b_{ii}) + \sum_{j=1, j \neq i}^{k} \operatorname{var}(b_{ij})$, equal for all i

Some designs given by Park (1987, p. 452) followed from his corollary.

Corollary 1. If the following moment conditions are satisfied, then the design is slope rotatable over all directions:

(1) all odd-order moments are 0 (i.e. $[i]=[ij]=[iij]=[iii]=[iiij]= \ldots =0$);
(2) $[ii]$ are equal for all i;
(3) $[iiii]$ are equal for all i;
(4) $[iijj]$ are equal for all $i \neq j$.

The quantities in square brackets denote the moments of the design. For example, we have $N^{-1}\sum_{u=1}^{N} x_{iu}=[i]$, $N^{-1}\sum_{u=1}^{N} x_{iu}^2 x_{ju}=[iij]$, and so on. If any subscript i, j, ..., appears an odd number of times, then the moment is odd; otherwise, it is even.

This corollary is framed using moment conditions for specific types of design that are known to be rotatable (i.e. $\mathrm{var}(\hat{y}(\mathbf{u}))$ is a function only of $\mathbf{u}'\mathbf{u}$; see Box & Hunter, 1957, p. 205) or slope rotatable over axial directions (i.e. $\mathrm{var}(\partial\hat{y}/\partial x_i|\mathbf{u})$ is a function only of $\mathbf{u}'\mathbf{u}$ and $\mathrm{var}(\partial\hat{y}/\partial x_i|\mathbf{u})$ are the same for all $i=1, \ldots, k$; see Hader & Park, 1978, p. 414). The corollary thus implies that we have the following relationship among designs:

$$\text{rotatable} \subset \text{slope rotatable over all directions}$$

This means that the class of SROAD designs contains the class of rotatable designs. Thus, there must be a much wider choice of SROAD designs. In particular, we have found some with unbalanced moment structures and some with unbalanced point arrangements. Odd-order moments of an SROAD design could be non-zero. The types of SROAD designs vary from dimension to dimension. We discuss $k=2$ and $k=3$ dimensions here, giving examples of designs that are SROAD but which do not belong to the classes of rotatable designs and designs that are slope rotatable over axial directions. None of these designs has been given by previous authors.

3 Two-dimensional SROAD designs

Park's necessary and sufficient conditions for SROAD designs are based on the precision matrix, i.e. $N(\mathbf{X}'\mathbf{X})^{-1}$. It would be much more convenient if we could find necessary and sufficient conditions for SROAD designs based on the moment matrix rather than the precision matrix. It appears, however, that it may not be possible to have general necessary and sufficient conditions for any dimension, without added assumptions. For two dimensions, for example, we have the following.

Lemma 1. For the two-dimensional case, suppose all odd moments of order 4 or less are 0, except [12], [1112] and [1222], (i.e. $[i]=[iij]=[iii]=0$). Then, the design is SROAD if and only if the following hold:

(1) $[1112]+[1222]=([11]+[22])[12]$
(2) $[1111]+[22]^2=[2222]+[11]^2$

This can be proved by inverting the general 6×6 moment matrix symbolically, using the MAPLE matrix program and imposing the SROAD conditions on the result. We now look at some specific examples.

Example 1. Let us consider the design points $(-a, -b)$, (a, b), $(-\alpha, 0)$, $(\alpha, 0)$, $(0, -\alpha)$, $(0, \alpha)$; and $(0, 0)$, n_0 times. This is a 2^{2-1} design $(x_1 x_2 = ab)$ plus two pairs of axial points at distances $\pm\alpha$, plus n_0 center points, in conventional notation. When $\alpha^2 = (n_0 + 4)(a^2 + b^2)/4$, the design is SROAD. For example, if $n_0 = 4$, $a = 1$ and $b = 2$, then $\alpha = 10^{1/2} = 3.162$, as shown in Fig. 1.

The corresponding moment matrix is

$$\frac{1}{N}\mathbf{X}'\mathbf{X} = \begin{pmatrix} 1 & . & . & 2.2 & 2.8 & 0.4 \\ . & 2.2 & 0.4 & . & . & . \\ . & 0.4 & 2.8 & . & . & . \\ 2.2 & . & . & 20.2 & 0.8 & 0.4 \\ 2.8 & . & . & 0.8 & 23.2 & 1.6 \\ 0.4 & . & . & 0.4 & 1.6 & 0.8 \end{pmatrix}$$

where . denotes 0 here as well as in examples following. This SROAD design has an unbalanced moment structure, i.e. $[11] \neq [12]$ and $[1111] \neq [2222]$, and three non-zero odd moments.

Example 2. Let us suppose that we add two more points $(-b, -a)$ and (b, a) to the design in example 1. Then, when $\alpha^2 = (n_0 + 4)(a^2 + b^2)/4$, the design is SROAD. For example, if $n_0 = 4$, $a = 1$ and $b = 2$, then $\alpha = 10^{1/2} = 3.162$, as in Fig. 2.

This design has a balanced moment structure. The corresponding moment matrix is

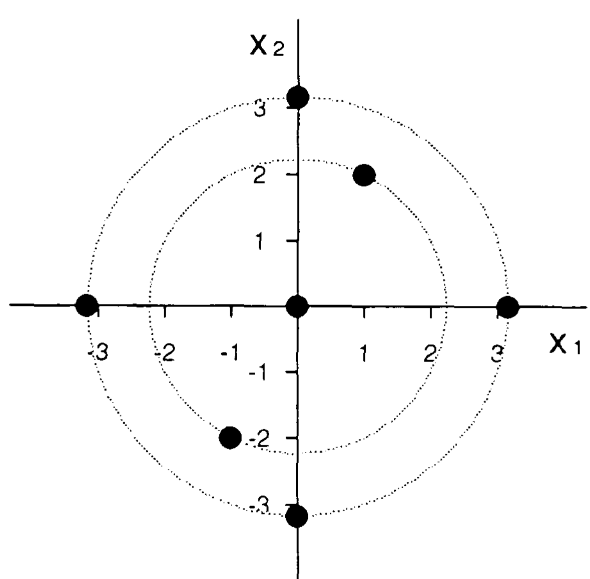

FIG. 1. Design points of example 1 ($n_0 = 4$, $a = 1$, $b = 2$, $\alpha = 3.162$).

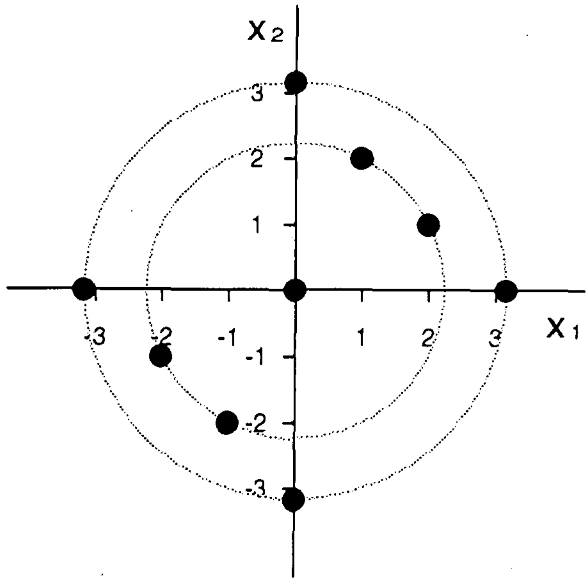

FIG. 2. Design points of example 2 ($n_0=4$, $a=1$, $b=2$, $\alpha=3.162$).

$$\frac{1}{N}\mathbf{X}'\mathbf{X}=\begin{pmatrix} 1 & . & . & 2.5 & 2.5 & .67 \\ . & 2.5 & .67 & . & . & . \\ . & .67 & 2.5 & . & . & . \\ 2.5 & . & . & 19.5 & 1.33 & 1.67 \\ 2.5 & . & . & 1.33 & 19.5 & 1.67 \\ .67 & . & . & 1.67 & 1.67 & 1.33 \end{pmatrix}$$

Example 3. Let us consider the design of Box and Draper (1987, Exercise 15.2, due originally to A. M. Herzberg). The design points are $(0, -a)$, $(0, a)$, $(-b, -c)$, $(b, -c)$, $(-b, c)$, (b, c); and $(0, 0)$, n_0 times. Let us suppose that a, b and c are all positive. Then, when

$$(a^4-2b^4+2c^4)\,n_0+4(a^4-b^4+c^4-2a^2c^2)=0 \tag{6}$$

the design is SROAD. For example, if $a=1$, $b=2$ and $n_0=3$, then $c=2.0813$, as in Fig. 3.

The moment matrix of this design is

$$\frac{1}{N}\mathbf{X}'\mathbf{X}=\begin{pmatrix} 1 & . & . & 1.78 & 2.15 & . \\ . & 1.78 & . & . & . & . \\ . & . & 2.15 & . & . & . \\ 1.78 & . & . & 7.11 & 7.70 & . \\ 2.15 & . & . & 7.70 & 8.56 & . \\ . & . & . & . & . & 7.70 \end{pmatrix}$$

It should be noted that $[11]\neq[22]$ and $[1111]\neq[2222]$.

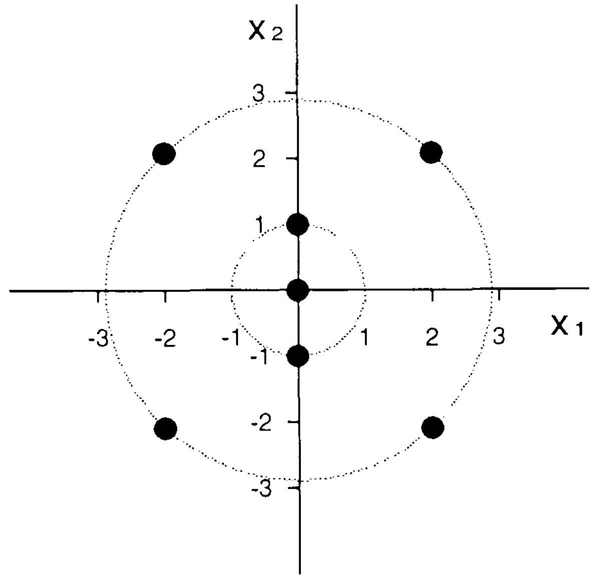

FIG. 3. Design points of example 3 ($n_0=3$, $a=1$, $b=2$, $c=2.0813$).

Example 3 consists of a rectangle ($\pm b$, $\pm c$), two axial points (0, $\pm a$) and n_0 center points, and there are various other possibilities that involve different comparative magnifications of the rectangle and the axial points. Another set of solutions, for example, is $a=1$, $c=1$ and $b=3n_0/(4+2n_0)$; for $n_0=1$, $b=0.8409$, the axial points are at the midpoints of the top and bottom of the rectangle, and [11] = [1122] and [22] = [2222]. When equation (6) holds for all n_0, we have

$$a^4-2b^4+2c^4=0$$

$$a^4-b^4+c^4-2a^2c^2=0$$

simultaneously, providing the solution $a=2c$, $b=c(3^{1/2})$. This design is fully rotatable and, hence, necessarily is SROAD. It is, in fact, a regular hexagon on a circle of radius $2c$.

4 Three-dimensional SROAD designs

In three dimensions, the moment structures of SROAD designs are much more complicated than those in two dimensions, as will be seen. With some added conditions, we find, in general, two kinds of moment structure, shown in Lemmas 2 and 3 below.

Lemma 2. For the three-dimensional case, if all odd moments of order 4 or less are 0, except [123], then the design is SROAD if and only if the following hold:

$$\begin{aligned}&\lambda_{11}/(\lambda_{11}\lambda_{2233}-\lambda_{123}^2)-\lambda_{22}/(\lambda_{22}\lambda_{1133}-\lambda_{123}^2)\\&\quad-4[2\lambda_{33}(\lambda_{22}\lambda_{2233}-\lambda_{11}\lambda_{1133})+(\lambda_{33}^2-\lambda_{3333})(\lambda_{1111}-\lambda_{2222})\\&\quad+\lambda_{3333}(\lambda_{11}^2-\lambda_{22}^2)+(\lambda_{1133}^2-\lambda_{2233}^2)]/\varphi=0\end{aligned}\tag{7}$$

and

$$
\begin{aligned}
&\lambda_{11}/(\lambda_{11}\lambda_{2233}-\lambda_{123}^2)-\lambda_{33}/(\lambda_{33}\lambda_{1122}-\lambda_{123}^2)\\
&\quad -4[2\lambda_{22}(\lambda_{33}\lambda_{2233}-\lambda_{11}\lambda_{1122})+(\lambda_{22}^2-\lambda_{2222})(\lambda_{1111}-\lambda_{3333})\\
&\quad +\lambda_{2222}(\lambda_{11}^2-\lambda_{33}^2)+(\lambda_{1122}^2-\lambda_{2233}^2)]/\varphi=0
\end{aligned}
\tag{8}
$$

Here, we have

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

and $\lambda_{ii}=[ii]$, $\lambda_{ijk}=[ijk]$, $\lambda_{iiii}=[iiii]$ and $\lambda_{iijj}=[iijj]$ for $i\neq j\neq k=1, 2, 3$.

The moment matrix of such a design has the form

$$
\frac{1}{N}\mathbf{X}'\mathbf{X}=\begin{pmatrix}
1 & \cdot & \cdot & \cdot & \lambda_{11} & \lambda_{22} & \lambda_{33} & \cdot & \cdot & \cdot\\
- & \lambda_{11} & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \lambda_{123}\\
\cdot & \cdot & \lambda_{22} & \cdot & \cdot & \cdot & \cdot & \cdot & \lambda_{123} & \cdot\\
\cdot & \cdot & \cdot & \lambda_{33} & \cdot & \cdot & \cdot & \lambda_{123} & \cdot & \cdot\\
\lambda_{11} & \cdot & \cdot & \cdot & \lambda_{1111} & \lambda_{1122} & \lambda_{1133} & \cdot & \cdot & \cdot\\
\lambda_{22} & \cdot & \cdot & \cdot & \lambda_{1122} & \lambda_{2222} & \lambda_{2233} & \cdot & \cdot & \cdot\\
\lambda_{33} & \cdot & \cdot & \cdot & \lambda_{1133} & \lambda_{2233} & \lambda_{3333} & \cdot & \cdot & \cdot\\
\cdot & \cdot & \cdot & \lambda_{123} & \cdot & \cdot & \cdot & \lambda_{1122} & \cdot & \cdot\\
\cdot & \cdot & \lambda_{123} & \cdot & \cdot & \cdot & \cdot & \cdot & \lambda_{1133} & \cdot\\
\cdot & \lambda_{123} & : & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \lambda_{2233}
\end{pmatrix}
$$

Three special cases of Lemma 2 are as follows.

Case 1. SROAD designs exist which have a non-zero [123] moment. For example, a design is SROAD if it meets the following requirements:

(1) all odd-order moments up to and including order four, except [123], are 0;
(2) $[ii]$ are equal for all i, $[iiii]$ are equal for all i and $[iijj]$ are equal for all $i\neq j$.

Example 4. Let us consider the three-dimensional SROAD Hartley-type designs with $(10+n_0)$ points (Hartley, 1959): (i) 2^{3-1} fractional factorial with $\mathbf{I}=123$; (ii) three pairs of axial points at distance α; (iii) n_0 center points. For this design, $[ii]N=4+2\alpha^2$, $[123]N=[iijj]N=4$ and $[iiii]N=4+2\alpha^4$. The design is SROAD for any α and n_0. The Hartley design can be orthogonally blocked for the second-order model fit. For example, if we divide the original design into two blocks—one consisting of four runs from a 2^{3-1} design plus n_{01} center points, and the other consisting of the six runs from the axial points plus n_{02} center points—blocking is orthogonal. The first condition for orthogonal blocks (see Box & Draper, 1987, p. 509) is obviously satisfied. The second condition is satisfied if $\alpha^2=2(6+n_{02})/[(4+n_{01})]$.

It should be noted that, when we rotate the x axes, some or all third-order moments other than [123] will become non-zero. This means that there are moment structures of SROAD designs even more complicated than those which satisfy Lemma 2, because rotation does not change the SROAD property of a design, by definition.

Example 5. Bose and Draper (1959) gave an infinite class of second-order rotatable designs which combined point sets with non-zero third moments which cancelled out. We can use part of such a design, retaining a non-zero third moment for this particular point set and adding a set of axial points. Our selected design consists of these point sets: (i) $(\pm a, \pm b, \pm c)$, $(\pm c, \pm a, \pm b)$, $(\pm b, \pm c, \pm a)$ subject to $x_1x_2x_3 = abc$, 12 points; (ii) $(\pm \alpha, 0, 0)$, $(0, \pm \alpha, 0)$, $(0, 0, \pm \alpha)$, six points; and (iii) n_0 center points.

In this case, $[ii]N = 4(a^2 + b^2 + c^2) + 2\alpha^2$, $[123]N = 12abc$, $[iiii]N = 4(a^4 + b^4 + c^4) + 2\alpha^4$, $[iijj]N = 4(a^2b^2 + a^2c^2 + b^2c^2)$, for $i \neq j$, and the design is SROAD for any values of a, b, c and α, and any number of center points. Similarly to the Hartley design blocking, we can divide this design into two blocks, one consisting of the first 12 runs plus n_{01} center points and the other consisting of the six axial points plus n_{02} center points. The design is orthogonally blocked when $\alpha^2 = 2(a^2 + b^2 + c^2)(6 + n_{02})/(12 + n_{01})$.

Example 6. In the notation of Draper and Herzberg (1968), $\frac{1}{2}S(a, a, a)$ with $\mathbf{I} = 123$ denotes the half-fraction of a 2^3 design, such that $\sum x_1x_2x_3 = 4a^3$; $S(a, a, \ldots, a)$ denotes the full 2^k factorial design or 'cube' $(\pm a, \pm a, \ldots, \pm a)$; and $S(\alpha, 0, \ldots, 0)$ denotes the $2k$ axial points $(\pm \alpha, 0, \ldots, 0), \ldots, (0, \ldots, 0, \pm \alpha)$. Then, the design which contains the following points is SROAD for any values of a, b, α and n_0:

(1) $\frac{1}{2}S(a, a, a)$ with $\mathbf{I} = 123$ (four points);
(2) $\frac{1}{2}S(b, b, b)$ with $\mathbf{I} = -123$ (four points);
(3) $S(\alpha, 0, 0)$ (six points);
(4) n_0 center points.

For this case, $[ii]N = 4(a^2 + b^2) + 2\alpha^2$, $[123]N = 4(a^3 - b^3)$, $[iiii]N = 4(a^4 + b^4) + 2\alpha^4$ and $[iijj]N = 4(a^4 + b^4)$, for $i \neq j$. (It is also possible to have an SROAD design with multiple point sets of this type.) When $\alpha^2 = 2(a^2 + b^2)(6 + n_{02})/(8 + n_{01})$, the design is also orthogonally blocked if the design is divided into two blocks, one consisting of runs from $\frac{1}{2}S(a, a, a)$ and $\frac{1}{2}S(b, b, b)$ plus n_{01} center points and another one consisting of runs from $S(\alpha, 0, 0)$ plus n_{02} center points.

Case 2. If the following moment conditions are satisfied, then the design is SROAD:

(1) all odd-order moments up to and including four are 0;
(2) $\lambda_{11} = \lambda_{22}$, $\lambda_{1111} = \lambda_{2222}$ and $\lambda_{1133} = \lambda_{2233}$;
(3) $\lambda_{3333} = \varphi_1/\varphi_2$, where

$$\varphi_1 = (\lambda_{1111}^2 - \lambda_{1122}^2)[4\lambda_{1122}\lambda_{1133} - \lambda_{33}^2(\lambda_{1122} - \lambda_{1133})]$$
$$+ 2\lambda_{1133}^2(\lambda_{1111} + \lambda_{1122})(\lambda_{1133} - 2\lambda_{11}\lambda_{33}) + 4\lambda_{33}^2\lambda_{1111}\lambda_{1122}\lambda_{1133}$$
$$- 2\lambda_{1122}\lambda_{1133}(\lambda_{1111} - \lambda_{1122})(\lambda_{1133} - 2\lambda_{11}\lambda_{33} + 4\lambda_{11}^2)$$
$$\varphi_2 = (\lambda_{1122} - \lambda_{1133})(\lambda_{1122}^2 - \lambda_{1111}^2) + 4\lambda_{1111}\lambda_{1122}\lambda_{1133}$$
$$+ 2\lambda_{11}^2[\lambda_{1122}(\lambda_{1111} - \lambda_{1122}) - \lambda_{1133}(\lambda_{1111} + \lambda_{1122})]$$

This type of design is not balanced for all coordinates. For example, λ_{11} is not necessarily equal to λ_{33}, etc.

Example 7. Here, we consider hybrid-type designs. Roquemore (1976) proposed his hybrid designs:

> to achieve the same degree of orthogonality as central composite or regular polyhedral designs, to be near-minimum-point in size, to be near-rotatable, and to possess some ease in coding. Hybrid designs for k variables may be viewed as composite designs (with center point) for $(k-1)$ variables which have been augmented with a column for variable k and, possibly, another row or two.

Roquemore (1976, p. 420) gave three three-dimensional hybrid designs, which he called 310, 311A and 311B. These are not SROAD as they stand. If we use a similar idea, however, i.e. choose a design such that the first $(k-1)$ variables form an SROAD design in $(k-1)$ dimensions, and add a further variable, we can obtain an SROAD design in k variables (here, $k=3$). Let us suppose that we choose a design that has a structure similar to Roquemore's 311A, with points $(-b, -b, c)$, $(b, -b, c)$, $(-b, b, c)$, (b, b, c), $(-a, 0, -c)$, $(a, 0, -c)$, $(0, -a, -c)$, $(0, a, -c)$, $(0, 0, -d)$, $(0, 0, d)$; and $(0, 0, 0)$ n_0 times. Such a design will satisfy condition 1 if $a = b(2^{1/2})$ and automatically satisfies condition (2). Condition (3) reduces to

$$4c^2(n_0+2)(4b^4 - c^4) + 8c^2d^2(2c^2 - d^2) + n_0 d^4(b^2 - 5c^2) = 0 \tag{9}$$

There are infinite solutions. For example, for any n_0, c and d values which satisfy

$$\phi \equiv n_0^2 + 64y(n_0+2)[4y^3(n_0+2) - 16y^2 + (8+5n_0)y] > n_0^2 \tag{10}$$

the design is SROAD if

$$x = [\phi^{1/2} - n_0][32y(n_0+2)]^{-1} \tag{11}$$

where $x = b^2/d^2$ and $y = c^2/d^2$. In particular, when $c = d[(73^{1/2}-3)/32]^{1/2}$ and $b = [(d^2-c^2)/2]^{1/2} = d[(35-73^{1/2})/64]^{1/2}$, the design is SROAD for any d and any n_0.

Case 3. Here, we extend example 3 from two dimensions to three dimensions. We need all odd moments as zero, $[ii]$ unequal, $[iiii]$ unequal and $[iijj]$ unequal (where $i \neq j$). Let us consider the design with the following points: (i) $(\pm b, \pm c, \pm d)$, eight points; (ii) $(0, \pm a, \pm g)$, four points; (iii) $(0, 0, \pm f)$, two points; (iv) $(0, 0, 0)$, n_0 times. When a, b, c, d, f, g and n_0 satisfy

$$[8f^4(a^2-c^2)^2 + 16f^2(a^2-c^2)(c^2g^2 - a^2d^2) + f^4 n_0(a^4 + 2c^4)$$
$$+ 4(n_0+2)(c^2g^2 - a^2d^2)^2]a^{-4}b^{-4}f^{-4}/(2n_0) - (a^2g^2 + 2c^2d^2)^{-1}/4$$
$$+ (8b^2d^2)^{-1} - [(f^4+2g^4)n_0 + 4(f^2-g^2)^2]a^{-4}f^{-4}/n_0 = 0$$

and

$$[(f^4+2g^4)n_0+4(f^2-g^2)^2]a^{-4}f^{-4}+(c^{-2}-d^{-2})n_0 b^{-2}/8-2(n_0+2)f^{-4}=0$$

the design is SROAD. For example, if $a=0.5$, $c=f=1$, $g=0.25$ and $n_0=2$, we obtain $b=1.180$ and $d=0.047$ by solving the above equations. The corresponding moment matrix has its same-order even moments all different.

In the next lemma, we present SROAD designs with several non-zero odd moments.

Lemma 3. Suppose a design satisfies

$$\begin{aligned}
[12]=[13]=[23]&=\tau_{22}\\
[1123]=[1223]=[1233]&=\tau_{43}\\
[1112]=[2223]=[1333]&=\tau_{44}\\
[1113]=[1222]=[2333]&=\tau_{45}
\end{aligned}$$

all other odd-order moments are 0, and

$$\begin{aligned}
[11]=[22]=[33]&=\tau_{21}\\
[1111]=[2222]=[3333]&=\tau_{41}\\
[1122]=[1133]=[2233]&=\tau_{42}
\end{aligned}$$

Then, the design is SROAD if and only if the following holds:

$$\begin{aligned}
&(\tau_{44}+\tau_{45})[\tau_{21}^2(2\tau_{42}+3\tau_{43})+2\tau_{22}^2(\tau_{41}+2\tau_{42})\\
&\quad+2\tau_{21}\tau_{22}(\tau_{42}-\tau_{41}+4\tau_{43})-2(\tau_{41}\tau_{42}-\tau_{44}\tau_{45})\\
&\quad+\tau_{43}(\tau_{41}-4\tau_{42}-2\tau_{43})]+(\tau_{44}^2+\tau_{45}^2)[\tau_{21}(\tau_{21}-8\tau_{22})-\tau_{42}]\\
&\quad+\tau_{41}(\tau_{41}+\tau_{42})(\tau_{22}^2-\tau_{43})+\tau_{21}^2\{\tau_{43}[3\tau_{41}-7(\tau_{42}+\tau_{43})]\\
&\quad-\tau_{44}\tau_{45})\}-\tau_{22}^2[4\tau_{43}(\tau_{41}+2\tau_{42})+2\tau_{42}^2]+2\tau_{21}\tau_{22}\\
&\quad\times[(\tau_{41}-\tau_{42})(2\tau_{42}-3\tau_{43})+2(\tau_{43}^2-\tau_{44}\tau_{45})]+2(\tau_{44}^3+\tau_{45}^3)\\
&\quad+\tau_{44}\tau_{45}(\tau_{41}-4\tau_{43})+6\tau_{42}^2\tau_{43}+\tau_{43}^2(4\tau_{41}+3\tau_{42})=0
\end{aligned}\tag{12}$$

The moment matrix of this kind of design has the form

$$\frac{1}{N}\mathbf{X}'\mathbf{X}=\begin{pmatrix}
1 & \cdot & \cdot & \cdot & \tau_{21} & \tau_{21} & \tau_{21} & \tau_{22} & \tau_{22} & \tau_{22}\\
\cdot & \tau_{21} & \tau_{22} & \tau_{22} & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot\\
\cdot & \tau_{22} & \tau_{21} & \tau_{22} & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot\\
\cdot & \tau_{22} & \tau_{22} & \tau_{21} & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot\\
\tau_{21} & \cdot & \cdot & \cdot & \tau_{41} & \tau_{42} & \tau_{42} & \tau_{44} & \tau_{45} & \tau_{43}\\
\tau_{21} & \cdot & \cdot & \cdot & \tau_{42} & \tau_{41} & \tau_{42} & \tau_{45} & \tau_{43} & \tau_{44}\\
\tau_{21} & \cdot & \cdot & \cdot & \tau_{42} & \tau_{42} & \tau_{41} & \tau_{43} & \tau_{44} & \tau_{45}\\
\tau_{22} & \cdot & \cdot & \cdot & \tau_{44} & \tau_{45} & \tau_{43} & \tau_{42} & \tau_{43} & \tau_{43}\\
\tau_{22} & \cdot & \cdot & \cdot & \tau_{45} & \tau_{43} & \tau_{44} & \tau_{43} & \tau_{42} & \tau_{43}\\
\tau_{22} & \cdot & \cdot & \cdot & \tau_{43} & \tau_{44} & \tau_{45} & \tau_{43} & \tau_{43} & \tau_{42}
\end{pmatrix}$$

Example 8. The design points $(-a,\ -b,\ -c)$, $(a,\ b,\ c)$, $(-b,\ -c,\ -a)$, $(b,\ c,\ a)$, $(-c,\ -a,\ -b)$, $(c,\ a,\ b)$, $(\pm\alpha, 0, 0)$, $(0, \pm\alpha, 0)$, $(0, 0, \pm\alpha)$; and $(0, 0, 0)$ n_0 times, satisfy the conditions of Lemma 3 with

$$\tau_{21}=2(a^2+b^2+c^2+\alpha^2)/N$$

$$\tau_{22}=2(ab+ac+bc)/N$$

$$\tau_{41}=2(a^4+b^4+c^4+\alpha^4)/N$$

$$\tau_{42}=2(a^2b^2+a^2c^2+b^2c^2)/N$$

$$\tau_{43}=2(a^2bc+ab^2c+abc^2)/N$$

$$\tau_{44}=2(a^3b+ac^3+b^3c)/N$$

$$\tau_{45}=2(a^3c+ab^3+bc^3)/N$$

For example, if we choose $n_0=1$, $a=0.1$, $b=0.2$ and $c=0.5$, we obtain an SROAD design with $\alpha=0.9683$ from equation (12).

Acknowledgements

N. R. Draper gratefully acknowledges partial support from the Wisconsin Alumni Research Foundation via the Graduate School of the University of Wisconsin; from the National Security Agency via Grant MDA904-92-H-3096; and from the German Alexander von Humboldt Stiftung. We are grateful to the referee for a careful reading and many suggested improvements.

Correspondence: N. Draper, Department of Statistics, University of Wisconsin, Madison, WI 53706, USA.

REFERENCES

BOSE, R. C. & DRAPER, N. (1959) Second order rotatable designs in three dimensions, *Annals of Mathematical Statistics*, 30, pp. 1097–1112.

BOX, G. E. P. & HUNTER, J. S. (1957) Multifactor experimental designs for exploring response surfaces, *Annals of Mathematical Statistics*, 28, pp. 195–241.

BOX, G. E. P. & DRAPER N. R. (1987) *Empirical Model Building and Response Surfaces* (New York, Wiley).

DRAPER, N. R. & HERZBERG, A. M. (1968) Further second order rotatable designs, *Annals of Mathematical Statistics*, 39, pp. 1995–2000.

HADER, R. J. & PARK, S. H. (1978) Slope-rotatable central composite designs, *Technometrics*, 20, pp. 413–417.

HARTLEY, H. O. (1959) Smallest composite designs for quadratic response surfaces, *Biometrics*, 15, pp. 611–624.

PARK, S. H. (1987) A class of multifactor designs for estimating the slope of response surfaces, *Technometrics*, 29, pp. 449–453.

ROQUEMORE, K. G. (1976) Hybrid designs for quadratic response surfaces, *Technometrics*, 18, pp. 419–423.